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Ansys Chemkin Input Manual



ANSYS, Inc.
Southpointe
2600 Ansys Drive
Canonsburg, PA 15317
ansysinfo@ansys.com
<http://www.ansys.com>
(T) 724-746-3304
(F) 724-514-9494

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Chapter 1: Introduction

The [Chemkin Input Manual \(p. 1\)](#) is designed to serve as a reference to Ansys Chemkin users who require more information about the input parameters needed in defining a chemically reacting flow simulation. In particular, information about syntax and format of chemical reaction mechanism input files, thermodynamic data, and transport-property data are described in detail. In addition, detailed information about all of the input parameters associated with reactor models, including default values and usage guidelines, are included in the Keywords section.

The Ansys Chemkin Interface guides users through problem setup and execution, as well as quick analysis with the Chemkin Visualizer. The operation of the Chemkin Interface and Post-Processing are described in detail in [Chemkin Getting Started Guide](#). In some cases, however, users may wish to work from the command line instead of the User Interface and manually assemble Reactor Model input files. For this purpose, the [Chemkin Input Manual \(p. 1\)](#) describes the necessary syntax and usage of the reactor-input Keywords, as well as a quick reference of what keywords are available for each Reactor Model.

For background information on the equations and theory behind the input parameters, the [Chemkin Theory Manual](#) provides further reading. In many cases, equations in the [Chemkin Theory Manual](#) are references in the discussions of reactor parameter input Keywords.

In [Thermodynamic Data \(p. 3\)](#) through [Transport Database \(p. 97\)](#), the syntax and format required for thermodynamic, gas-phase kinetics, surface kinetics, and transport-property input data are described. [Description and Properties of Particles \(p. 105\)](#) has the description of fundamental particle properties for Particle Tracking. [CHEMKIN Project Input: Keyword Syntax and Rules \(p. 123\)](#) provides an overview of the syntax and rules for Keyword input, which make up the Reactor Model input files. Reactor Model input files are ordinarily created by the User Interface but can also be manually assembled for command-line usage. [Reference Guide to Project Input Keywords \(p. 125\)](#) provides a Quick Reference of the Keywords, organized by Reactor Model and other concepts, while [Alphabetical Listing of Project Input Keywords \(p. 139\)](#) contains alphabetical listings of keywords.

Chapter 2: Thermodynamic Data

Any chemical species that appears in a problem must have thermodynamic data associated with it. The format required for these data is described in this chapter. Also [Standard State Enthalpies and Entropies at 298 K \(p. 11\)](#) includes a discussion and listing of the standard-state enthalpies and entropies for the data contained in the therm.dat database file, which is included with every Ansys Chemkin installation.

Thermodynamic data may be extracted from a database file (for example, therm.dat) and/or read from the *Gas-phase Kinetics* or *Surface Kinetics* input file. If all of the thermodynamic data are to be extracted from a database file, then no thermodynamic data input in the *Gas-phase Kinetics* or *Surface Kinetics* input file is required. However, if you want to override information in the database or to provide data on species not in the database, then thermodynamic data are needed in the *Gas-phase Kinetics* or *Surface Kinetics* input file. In any case, the format for the information is the same.

2.1. Thermodynamic Data Format

Ansys Chemkin expects the thermodynamic data to be provided in a specific format. In addition to the fourteen polynomial fitting coefficients (described in [Standard-state Thermodynamic Properties in the Chemkin Theory Manual](#)), the database also contains the species' name, its elemental composition, its electronic charge, and an indication of its phase (gas, liquid or solid). The data for each species requires four formatted lines of length 80 characters. [Figure 2.1: Excerpts from the therm.dat Thermodynamic Database File \(p. 4\)](#) is a sample of the lines required for a species and [Table 2.1: Summary of the Rules for Thermodynamic Data \(p. 4\)](#) provides a detailed specification of the format required for entry of thermodynamics data. The first two lines in [Figure 2.1: Excerpts from the therm.dat Thermodynamic Database File \(p. 4\)](#) are required at the top of a thermodynamic database file; the first line specifies that the following is a set of thermodynamic data, while the second line provides the three temperatures used in the fitting process (a low temperature, break temperature, and high temperature). You must also adhere to these specifications when placing thermodynamic data within the *Gas-phase Kinetics* or *Surface Kinetics* input file.

Ansys Chemkin allows two salient formats based on the number of coefficients used in fitting the data: 7-coefficient and 9-coefficient. In the Ansys Chemkin documentation, the latter is referred to as the NASA9 format, acknowledging its origin. In this chapter, details of the 7-coefficient format are presented first, while the specifics of NASA9 usage in Ansys Chemkin are described in [Input in 9-Coefficient Format \(NASA9\) \(p. 33\)](#).

2.2. Default Data Format

The default format for thermodynamic data (see [Table 2.1: Summary of the Rules for Thermodynamic Data \(p. 4\)](#) and [Table 2.2: Fortran Format Descriptions \(p. 6\)](#)) is a minor modification of that used by Gordon and McBride [1] (p. 375) for the Thermodynamic Database in the NASA Chemical Equilibrium code. However, Ansys Chemkin allows a different midpoint temperature for the fits to the properties of each chemical species. Chemkin also allows a species to be composed of a maximum of nine elements, not four, on Line 3. Additional extensions allowed by Chemkin for multiple temperature ranges and for

very large molecular clusters are described in [Using More than Two Temperature Ranges \(p. 8\)](#) and [Creating Very Large Molecules with Unlimited Number of Elements \(p. 8\)](#), respectively. Despite these extensions, however, Chemkin can use the NASA database directly without any modification. The format conventions are summarized in [Table 2.2: Fortran Format Descriptions \(p. 6\)](#).

As indicated in [Table 2.1: Summary of the Rules for Thermodynamic Data \(p. 4\)](#), the pertinent information includes the species name, the elemental composition of the species, and the temperature ranges over which the polynomial fits to thermodynamic data are valid. The fits to C_p^o/R , H^o/RT , and S^o/R consist of seven coefficients for each of two temperature ranges, see [Equation 2.18](#), [Equation 2.22](#) and [Equation 2.28](#) of the [Chemkin Theory Manual](#). Further information about the fitting procedure can be found in the [Chemkin Theory Manual](#) as well as [Using Utilities \(p. 109\)](#).

Note:

Some users enhance the Thermodynamic Data block with additional data, such as tags for liquid fuel properties, SMILES, etc. These property tags are described in [Format for Property Tagging in the Chemkin Reaction Workbench User's Manual](#). The supplemental data are used by several Ansys Chemkin features, including the Reaction Path Analyzer (see the [Chemkin Visualization Manual](#)) and the Surrogate Blend Optimizer (see the [Chemkin Reaction Workbench User's Manual](#)).

Figure 2.1: Excerpts from the *therm.dat* Thermodynamic Database File

```

THERMO
  300.000  1000.000  5000.000
(CH2O)3      70590C  3H   60   3   G  0300.00  4000.00  1500.00    1
  0.01913678E+03  0.08578044E-01-0.08882060E-05-0.03574819E-08  0.06605142E-12    2
-0.06560876E+06-0.08432507E+03-0.04662286E+02  0.06091547E+00-0.04710536E-03    3
  0.01968843E-06-0.03563271E-10-0.05665403E+06  0.04525264E+03    4
AL          62987AL  1   G  0300.00  5000.00  0600.00    1
  0.02559589E+02-0.10632239E-03  0.07202828E-06-0.02121105E-09  0.02289429E-13    2
  0.03890214E+06  0.05234522E+02  0.02736825E+02-0.05912374E-02-0.04033937E-05    3
  0.02322343E-07-0.01705599E-10  0.03886794E+06  0.04363879E+02    4
END

```

Table 2.1: Summary of the Rules for Thermodynamic Data

Line #	Contents	Format ^[a]	Note in following table ^[b]	Column
1	THERMO (or THERMO ALL) ^[c]	Free	c	Any
2	Temperature ranges for 2 sets of coefficients: lowest T, common T, and highest T ^[d]	3F10.0	d	1 to 30
3	Species name (must start in Column 1)	16A1	e	1 to 16
	Date (not used)	6A1	f	19 to 24

Line #	Contents	Format ^[a]	Note in following table [b]	Column
	Atomic symbols and formula	4(2A1, I3)	g	25 to 44
	Phase of species (S, L, or G for solid, liquid, or gas)	A1	h	45
	Low temperature	E10.0	i	46 to 55
	High temperature	E10.0	i	56 to 65
	Common temperature (if needed, else blank)	E8.0	j	66 to 73
	Atomic symbols and formula (if needed, else blank)	2A1, I3	k	74 to 78
	The integer 1. This is a mandatory element and must appear in column 80.	I1	l	80
	Atomic symbols and formula (if needed, else blank), or & to indicate continuation to next line (See Creating Very Large Molecules with Unlimited Number of Elements (p. 8) for further information)	4(2A1, I3)	g	81 to 100
4	Coefficients a_1 through a_5 in Equation 2.18 , Equation 2.22 and Equation 2.28 of the Chemkin Theory Manual , for upper temperature interval	5(E15.8)	m	1 to 75
	The integer 2	I1	l	80
5	Coefficients a_6 , a_7 for upper temperature interval, and a_1 , a_2 , and a_3 for lower temperature interval	5(E15.8)	m	1 to 75
	The integer 3	I	l	80
6	Coefficients a_4 , a_5 , a_6 , a_7 for lower temperature interval	4(E15.8)	n	1 to 60
	The integer 4	I1	l	80
..	Repeat lines 3 - 6 for each species			
last	End (Optional, end of thermodynamic data.)	Free	c	Any

[a] The format string in this column follows the convention of FORTRAN documentation, as detailed in the notes provided in [Table 2.2: Fortran Format Descriptions](#) (p. 6).

[b] See [Table 2.2: Fortran Format Descriptions](#) (p. 6)

[c] Use only when all thermodynamic data are to be taken from Pre-processor input.

[d] When inserting thermodynamic data directly in the *Gas-phase Kinetics* and *Surface Kinetics* input files, Line 2 should only be included with THERMO ALL option (See *Gas-phase Kinetics* and *Surface Kinetics* for more information).

Table 2.2: Fortran Format Descriptions

Note	Format	Format Description ^[a]
c	FREE	The particular input described can be in any column of the input line.
d	3F10.0	3 Floating-point (real) values are allowed; each is allocated 10 columns.
e	16A1	16 Alpha-numeric characters are allowed in these columns (some may be blank).
f	6A1	6 Alpha-numeric characters are allowed in these columns (some may be blank).
g	4(2A1,I3)	There can be 4 sets of data; each set is allowed 2 Alpha-numeric columns (an element symbol) followed by 3 columns containing an Integer value (element count).
h	A1	1 Alpha-numeric character is allowed.
i	E10.0	10 columns are allocated for a real value, and scientific notation (E format) is allowed.
j	E8.0	8 columns are allocated for a real value, and scientific notation (E format) is allowed.
k	2A1,I3	2 Alpha-numeric columns (an element symbol) followed by 3 columns for an integer value (element count).
l	I1	One column is allowed for an integer value.
m	5(E15.8)	5 real values are allowed, with 15 columns allocated for each value, and scientific notation is allowed to have up to 8 values after the decimal point.
n	4(E15.8)	4 real values are allowed, with 15 columns allocated for each value, and scientific notation is allowed to have up to 8 values after the decimal point.

[a] From [Table 2.1: Summary of the Rules for Thermodynamic Data \(p. 4\)](#)

The first thermodynamic data line must start with the word THERMO (or THER). If the data appears inside of a *Gas-phase Kinetics* or *Surface Kinetics* input file, then the addition entry ALL (that is, the first line reads THERMO ALL) tells the pre-processor that all thermodynamic data for the species associated with that chemistry input are included in the chemistry input file. This will cause the pre-processor not to try to open or read a Thermodynamic database file.

If the data are in a thermodynamics database file, or if THERMO ALL precedes within a *Gas-phase Kinetics* or *Surface Kinetics* input file, then the next line must be Line 2 of [Table 2.1: Summary of the Rules for Thermodynamic Data \(p. 4\)](#). Otherwise Line 2 is skipped. In any case, the subsequent thermodynamic data lines must be in the format of Lines 3 - 6 of [Table 2.1: Summary of the Rules for Thermodynamic Data \(p. 4\)](#). (For the THERMO option within a kinetics input file, the midpoint temperature

is taken from Line 2 information already in the Thermodynamic Database associated with the chemistry set.)

Figure 2.2: Examples of Thermodynamic Data (p. 7) shows some examples of thermodynamic property input, as they might occur within a *Gas-phase Kinetics* input file. In these examples for OH, OH⁺, and OH⁻, it is seen from columns 25 - 34 that the elemental composition of each molecule is one O atom and one H atom. In addition, columns 35 - 39 indicate that two of the species, OH⁺, and OH⁻, are ionic since they contain -1 and +1 electrons (E), respectively. The G in column 45 indicates that all three species are gaseous. (This phase information is ignored by *Gas-phase Kinetics*.) The 1000.00 in columns 66 - 73 for OH indicates that the common temperature between the high- and low-temperature fits is 1000.00 K. If columns 66 - 73 are left blank, as they are for OH⁺ and OH⁻, then the common temperature is that given in columns 11 - 20 in Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4), which in this example is in the Thermodynamic Database. An alternative format is shown for OH if more than two temperature ranges are required. In this case the molecule has a different name, "MyOH", but the elemental composition is the same as for OH. The line after the elemental composition contains the TEMP description of minimum, common, and maximum temperatures, and a set of coefficients for each temperature range, ordered from highest to lowest.

Figure 2.2: Examples of Thermodynamic Data

```

THERMO
OH          1212860  1H  1      G  0300.00  5000.00  1000.00      1
0.02882730E+02 0.10139743E-02-0.02276877E-05 0.02174683E-09-0.05126305E-14      2
0.03886888E+05 0.05595712E+02 0.03637266E+02 0.01850910E-02-0.16761646E-05      3
0.02387202E-07-0.08431442E-11 0.03606781E+05 0.13588605E+01      4
OH+         1212860  1H  1E -1  G  0300.00  5000.00      1
0.02719058E+02 0.15085714E-02-0.05029369E-05 0.08261951E-09-0.04947452E-13      2
0.15763414E+06 0.06234536E+02 0.03326978E+02 0.13457859E-02-0.03777167E-04      3
0.04687749E-07-0.01780982E-10 0.15740294E+06 0.02744042E+02      4
OH-         1212860  1H  1E  1  G  0300.00  5000.00      1
0.02846204E+02 0.10418347E-02-0.02416850E-05 0.02483215E-09-0.07775605E-14      2
-0.01807280E+06 0.04422712E+02 0.03390037E+02 0.07922381E-02-0.01943429E-04      3
0.02001769E-07-0.05702087E-11-0.01830493E+06 0.12498923E+01      4
MyOH        00  1H  1  0  0G  300.000  5000.000      0 1
TEMP  300.000  1000.000  2500.000  5000.000
0.30563941E+01 0.89059362E-03-0.20849917E-06 0.24115927E-10-0.10516720E-14
0.37260112E+04 0.44780081E+01
0.34298433E+01-0.25250392E-03 0.80470663E-06-0.33336490E-09 0.43425671E-13
0.37097800E+04 0.26751302E+01
0.37695923E+01-0.59256858E-03-0.21359336E-06 0.13644331E-08-0.63575666E-12
0.35908836E+04 0.78130486E+00
END

```

The following is a summary of the possibilities for specifying thermodynamic data:

- **Case 1:** All thermodynamic data from database file
 1. A database file is opened during pre-processing (for example, *therm.dat*).
 2. No THERMO data required in the *Gas-phase* or *Surface Kinetics* input file.
- **Case 2:** Thermodynamic data from database and input files
 1. A database file is opened during pre-processing (for example, *therm.dat*).
 2. Include the following lines in the *Gas-phase* or *Surface Kinetics* input file, after the species data:

THERMO

Data in [Table 2.1: Summary of the Rules for Thermodynamic Data \(p. 4\)](#) format (lines 3 - 6 repeated) for each
END

- **Case 3:** All thermodynamic data from input file

1. No Thermodynamic database file is required.
2. Include the following lines in the *Gas-phase* or *Surface Kinetics* input file, after the species data:

THERMO ALL

Data in [Table 2.1: Summary of the Rules for Thermodynamic Data \(p. 4\)](#)

format (lines 3 - 6 repeated) for at least all species named in the species data

END

2.2.1. Using More than Two Temperature Ranges

An alternative input data format allows specification of more than two temperature ranges. Use of this format provides more flexibility in describing the thermodynamic data for complex functions of temperature. This alternative approach is summarized in [Table 2.3: Alternative Format for Specifying More than Two Temperature Ranges \(p. 8\)](#). The alternative lines used in place of lines 4 - 6 of [Table 2.1: Summary of the Rules for Thermodynamic Data \(p. 4\)](#). Line 1 specifies all of the temperature values that define the temperature intervals. Lines 2 and Line 3 are then repeated for each specified temperature interval, in descending order of temperature ranges.

Table 2.3: Alternative Format for Specifying More than Two Temperature Ranges

Alternative lines for more than 2 temperature intervals (in place of Lines 4 - 6 in Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4)):			
Line #	Contents	Format	Column
1	TEMP followed by space-delimited minimum fit temperature, common temperatures in increasing order, and maximum fit temperature.	A4, Free	1 to 80
2	Coefficients $a_1 - a_5$ for a temperature interval	5(E15.8)	1 to 75
3	Coefficients a_6, a_7 for a temperature interval	2(E15.8)	1 to 30

2.2.2. Creating Very Large Molecules with Unlimited Number of Elements

There are some cases where you may want to define very large molecules that contain many elements or that may be composed of a very large number of atoms for a particular element. For this purpose, Chemkin extends the thermodynamic data format to allow you to provide an unlimited number of elements and unconstrained composition. [Figure 2.3: Examples of Very Large Molecules \(p. 9\)](#) shows an example (for illustration purposes only) of using this extended format to describe a molecule called CLUSTER1 that consists of 2326 carbon atoms, 895 hydrogen atoms, 18 nitrogen atoms, 53 oxygen atoms, and 32 sulfur atoms. The extended format is enabled by putting a & character at the end of Line 3 ([Table 2.1: Summary of the Rules for Thermodynamic Data \(p. 4\)](#)), in column 81. Any number of continuation lines may subsequently be included by adding an ampersand (&) at the end of a preceding line. The composition information used on these continuation lines is in free format, which

consists of an element symbol, followed by the number of those atoms in the molecule, followed by another element symbol, and so forth.

Figure 2.3: Examples of Very Large Molecules

```

CLUSTER1      121086                G   300.000  5000.000 1000.00      1&
C 2326  H 895 N 18  O 53  S 32

  2.60208700e+00-1.78708100e-04 9.08704100e-08-1.14993300e-11 3.31084400e-16      2
  8.54215400e+04 4.19517700e+00 2.49858500e+00 8.08577700e-05-2.69769700e-07      3
  3.04072900e-10-1.10665200e-13 8.54587800e+04 4.75345900e+00                      4

```

2.2.3. Surface-Coverage Dependent Enthalpy of Surface Species

The enthalpy of surface species can be specified to be dependent on surface coverage by entering a block of data starting with HFCOV within a block of thermodynamics data that is being specified for surface species. Coverage-dependent coefficients are a subset of the thermodynamic data, and are specified at the end of the surface thermodynamic data input. The linear coverage-dependent coefficients are explicitly specified under the HFCOV block, as shown below. The required input for each line consists of the species (*species_name*) whose enthalpy is dependent on the second mentioned species coverage (*species_name*), and the coverage-dependent coefficient. The coverage-dependent coefficients must be specified in units of Kelvin.

*Species_name*_j *Species_name*_m *c*_{j,m}

Figure 2.4: HFCOV Thermodynamic Auxiliary Keyword Example

```

THERMO
O(S)          C   OH   OO   1AG 1S  0300.00  5000.00 1000.00      1
  0.02542059E+02-0.02755061E-03-0.03102803E-07 0.04551067E-10-0.04368051E-14      2
  0.02923080E+06 0.04920308E+02 0.02946428E+02-0.16381665E+02 0.02421031E-04      3
  -0.16028431E-08 0.03890696E-11 0.02914764E+06 0.02963995E+02                      4
C2H4(S)       C   2H   4O   OAG 1S  0298.00  5998.00 1298.00      1
  0.68302018E+01 0.10144574E-01-0.34419787E-05 0.52897660E-09-0.30353490E-13      2
  -0.98191467E+04-0.14816284E+02-0.40212793E+00 0.23298220E-01-0.80872187E-05      3
  -0.25065598E-08 0.15984527E-11-0.71721868E+04 0.24925868E+02                      4
Cl(S)         C   OH   OCl 1AG 1S  0298.00  5998.00 1298.00      1
  0.68302018E+01 0.10144574E-01-0.34419787E-05 0.52897660E-09-0.30353490E-13      2
  -0.98191467E+04-0.14816284E+02-0.40212793E+00 0.23298220E-01-0.80872187E-05      3
  -0.25065598E-08 0.15984527E-11-0.71721868E+04 0.24925868E+02                      4

HFCOV ! UNITS ARE KELVIN (ENTHALPY UNITS/GAS CONSTANT)

O(S) O(S)      17966.784

O(S) C2H4(S)   -1811.777

O(S) Cl(S)     1409.160

C2H4(S) Cl(S)  -4932.058

END

END

```

2.2.4. Gas Species Radiation Absorption Coefficients

For a gas species to absorb or emit infrared energy, its molecular structure must allow rotational and vibrational transitions and change in dipole moment. Accordingly, all monatomic species, such as O and H, and homonuclear diatomic species, such as O₂, H₂, and N₂, are "transparent" with respect to thermal radiation transfer. Most species that are actively absorbing and emitting infrared energy in flames can be neglected in the radiation calculation because they either have very low concentrations (for example, NO and NO₂) or exist in cooler regions of the flow domain (for example, hydrocarbon fuel species and CH₃ OH). The most important radiating species in hydrocarbon flames are CO₂ and H₂ O. The next important gas species are CO and CH₄, which emit about 1/10 as much infrared energy as the two dominant species.

The Planck mean absorption coefficients a for CO₂, H₂ O, CO, and CH₄ can be calculated by a narrow-band absorption coefficient model such as RADCAL [3] (p. 375). Since narrow-band calculations require integrating absorption-line intensities over all wavelengths, direct integration of a narrow-band model into the radiation model would greatly decrease the computational performance. To incorporate good absorption coefficient data without sacrificing performance, polynomials are fitted to temperature to represent the absorption coefficient data for individual gas species [4] (p. 375).

Two types of temperature polynomials are accepted by the radiation model for gas species:

- **Polynomial 1:**

$$a_i(T) = \sum_j c_j T^j \quad \text{with } j=0, \dots, 6. \quad (\text{m}^{-1}\text{atm}^{-1}) \quad (2.1)$$

- **Polynomial 2:**

$$a_i(T) = \sum_j c_j / T^j \quad \text{with } j=0, \dots, 6. \quad (\text{m}^{-1}\text{atm}^{-1}) \quad (2.2)$$

The curve-fitting parameters c_j are entered as optional-data lines in the thermodynamic data file or in the thermodynamic data section of the mechanism input file. The absorption coefficient data line is formatted as

```
![_ AbsorptionCoefficient=" polynomial_form Tmin Tmax c0 c1 c2 c3 c4 c5 c6 " _]
```

AbsorptionCoefficient is the tag indicating the data are for species absorption coefficient calculation. polynomial_form indicates the form of polynomial used to fit the absorption coefficient. This must have a value of 1.0 or 2.0, corresponding to Equation 2.1 (p. 10) or Equation 2.2 (p. 10), respectively. Tmin is the lower temperature bound in [K] for the fitted curve to be valid. Tmax is the upper temperature bound in [K] for the fitted curve to be valid. c_j are the seven parameters of the polynomial.

This data line must appear before the thermodynamic data of the associated gas species. Different gas species can use a different form of polynomial. Each gas species can have as many as two absorption-coefficient data lines, which allows two sets of parameters of different temperature ranges. If there are two tag lines for a given gas species, they must be of the same type of polynomial and the low-temperature line should appear before the high-temperature line. The gas radiation model will not be activated if no absorption-coefficient data are included in the thermodynamic data file.

For example, the absorption coefficient data of CO are fitted to two type-1 polynomials over temperature ranges of 300–750 K and 750–2500 K, with the coefficients included in the optional-data lines as follows:

```
! [_ AbsorptionCoefficients=" 1 300 750 4.8E0 -6.95E-2 2.96E-4 -4.26E-7 2.03E-10 0 0 " _]
! [_ AbsorptionCoefficients=" 1 750 2500 10. -1.2E-2 4.78E-6 -5.87E-10 -2.53E-14 0 0 " _]
CO TPIS79C 10 1 00 00G 200.000 3500.000 1000.000 1
2.71518561E+00 2.06252743E-03-9.98825771E-07 2.30053008E-10-2.03647716E-14 2
-1.41518724E+04 7.81868772E+00 3.57953347E+00-6.10353680E-04 1.01681433E-06 3
9.07005884E-10-9.04424499E-13-1.43440860E+04 3.50840928E+00 8.67100000E+03 4
```

2.3. Standard State Enthalpies and Entropies at 298 K

Table 2.4: Standard State Enthalpies and Entropies at 298 K (p. 11) contains the standard state enthalpies and entropies for 778 species that are in the thermodynamic database file, *therm.dat* (see Figure 2.1: Excerpts from the *therm.dat* Thermodynamic Database File (p. 4) and Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4) for the data and formats), which is included with all Ansys Chemkin installs. The values in the table were determined by evaluating the polynomial expressions (Equation 2.3 (p. 11) and Equation 2.4 (p. 11) of the Chemkin Theory Manual) at the standard temperature of 298 K. Note the measured or derived data for $H^o(298)$ and $S^o(298)$ that were used in generating the coefficients in *therm.dat* are also included in Table 2.4: Standard State Enthalpies and Entropies at 298 K (p. 11) for comparison.

$$H^o(298) = RT \left[a_1 + \frac{a_2}{2} T + \frac{a_3}{3} T^2 + \frac{a_4}{4} T^3 + \frac{a_5}{5} T^4 + \frac{a_6}{T} \right] \quad (2.3)$$

$$S^o(298) = R \left[a_1 \ln T + a_2 T + \frac{a_3}{2} T^2 + \frac{a_4}{3} T^3 + \frac{a_5}{4} T^4 + a_7 \right] \quad (2.4)$$

The units for enthalpies are (kcal)/mole and for entropies cal/(mole · K). The entries in Table 2.4: Standard State Enthalpies and Entropies at 298 K (p. 11) correspond to the *therm.dat* distributed with Ansys Chemkin.

Table 2.4: Standard State Enthalpies and Entropies at 298 K

Species	$H^o(298)$ kcal/mole		$S^o(298)$ cal/(mole·K)	
	Data	Fit	Data	Fit
(CH ₂ O) ₃	–110.70	–110.71	69.42	69.38
(CH ₃) ₂ SiCH ₂	12.30	12.37	80.37	82.41
AL	78.80	78.80	39.30	39.30
AL ₂ H ₆	21.35	21.35	62.75	62.75
AL ₂ ME ₆	–61.20	–61.20	131.05	131.06
ALAS	107.33	107.32	60.65	60.65
ALH	62.00	62.00	44.88	44.87
ALH ₂	41.95	41.95	54.40	54.40
ALH ₃	18.83	18.83	52.30	52.30
ALME	19.75	19.75	60.68	60.68
ALME ₂	12.75	12.75	77.40	77.40
ALME ₃	–20.30	–20.30	83.68	83.68

Species	$H^o(298)$ kcal/mole		$S^o(298)$ cal/(mole·K)	
	Data	Fit	Data	Fit
AR	0.00	0.00	36.98	36.98
AR+	364.91	364.91	39.75	39.74
AS	75.48	75.48	43.53	43.52
AS2	47.08	47.08	59.83	59.83
AS3	65.35	65.35	77.53	77.53
AS4	37.13	37.13	78.45	78.45
ASALME	70.00	70.00	81.60	81.60
ASALME2	63.25	63.25	91.00	91.00
ASGAET	82.75	82.75	95.20	95.20
ASGAET2	69.55	69.55	109.83	109.83
ASGAME	83.50	83.50	85.75	85.75
ASGAME2	81.25	81.25	91.00	91.00
ASGAMEH	93.75	93.75	84.73	84.73
ASH	61.75	61.75	50.20	50.20
ASH2	42.25	42.25	46.45	46.45
ASH3	16.63	16.63	55.65	55.65
ASME	59.20	59.20	63.80	63.80
ASME2	34.20	34.20	79.50	79.50
ASME3	2.93	2.93	85.78	85.78
B	133.80	133.80	36.65	36.64
B(S)	0.00	0.00	1.41	1.41
BCL	33.80	33.80	50.94	50.94
BCL2	-19.00	-19.00	65.14	65.15
BCL3	-96.31	-96.31	69.33	69.33
BE	78.25	78.25	32.54	32.54
BE(S)	0.00	0.00	2.28	2.28
BE2SIO4(S)	-506.03	-506.03	15.34	15.33
BE3B2O6(S)	-741.96	-741.96	24.00	23.97
BE3N2(A)	-140.60	-140.60	8.16	8.15
BE3N2(L)	-116.40	-116.41	9.43	9.41
BEAL2O4(S)	-549.90	-549.90	15.84	15.84
BEB2O4	-323.00	-323.00	78.08	78.08
BEBO2	-115.20	-115.20	63.40	63.41
BEBR	28.71	28.71	54.59	54.59
BEBR2	-54.80	-54.80	65.44	65.44
BEBR2(S)	-85.00	-85.00	24.00	23.99

Species	$H^{\circ}(298)\text{kcal/mole}$		$S^{\circ}(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
BECL	14.50	14.50	51.98	51.98
BECL2	-86.10	-86.10	60.26	60.26
BECL2(A)	-117.34	-117.34	19.76	19.75
BECL2(B)	-118.60	-118.60	18.12	18.11
BECLF	-137.00	-137.00	58.89	58.89
BEF	-40.60	-40.60	49.15	49.14
BEF2	-190.25	-190.25	54.36	54.36
BEF2(L)	-244.27	-244.28	14.32	14.32
BEH	76.77	76.77	42.24	42.23
BEH+	276.40	276.40	40.76	40.75
BEH2	30.00	30.00	41.35	41.33
BEH2O2	-161.70	-161.70	55.89	55.91
BEH2O2(A)	-215.80	-215.81	12.80	12.78
BEH2O2(B)	-216.50	-216.51	12.00	11.98
BEI	40.63	40.63	56.69	56.69
BEI2	-15.30	-15.30	69.65	69.65
BEI2(S)	-45.10	-45.11	28.80	28.78
BEN	101.98	101.98	49.87	49.87
BEO(A)	-145.40	-145.39	3.29	3.31
BEO(B)	-143.80	-143.79	3.97	3.99
BEOH	-27.40	-27.40	50.07	50.07
BES(S)	-56.00	-56.00	8.85	8.84
BESO4(A)	-287.00	-287.01	18.64	18.60
BESO4(B)	-286.73	-286.75	18.94	18.91
BESO4(GAM)	-282.06	-282.07	24.09	24.06
BN	-59.97	-59.97	3.54	3.53
C	171.29	171.29	37.76	37.76
C(S)	0.00	0.00	1.37	1.37
C+	432.47	432.02	36.94	36.93
C-	140.61	140.61	36.16	36.16
C2	200.22	200.23	47.63	47.63
C2-	106.00	106.00	46.96	46.96
C2CL3	54.37	54.36	79.93	79.89
C2CL5	7.38	7.39	94.52	94.75
C2CL6	-32.43	-32.44	93.15	93.04
C2F6	-321.20	-321.20	79.37	79.38

Species	$H^o(298)\text{kcal/mole}$		$S^o(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
C2H	135.00	135.00	51.10	49.55
C2H2	54.19	54.19	48.00	48.01
C2H3	0.00	68.41	0.00	55.32
C2H4	12.54	12.54	52.40	52.37
C2H5	0.00	28.01	0.00	60.13
C2H6	0.00	-20.04	0.00	54.72
C2HCL	51.10	51.10	57.81	57.82
C2HCL5	-35.19	-35.19	91.61	91.51
C2N	133.00	133.00	55.16	55.16
C2N2	73.87	73.87	57.71	57.72
C2O	68.50	68.50	55.68	55.67
C3	196.00	196.00	56.68	56.66
C3H2	129.39	129.60	62.01	64.81
C3H2(S)	141.43	141.43	59.74	59.75
C3H4	47.67	47.63	57.99	57.94
C3H4C	67.99	68.00	57.94	57.95
C3H4P	45.77	45.77	58.89	58.89
C3H6	0.00	4.89	0.00	61.51
C3H8	0.00	-24.82	0.00	64.56
C3O2	-22.38	-22.38	65.96	65.96
C4	232.00	232.00	54.54	54.55
C4H	0.00	155.08	0.00	60.89
C4H10	-32.02	-31.84	70.94	71.79
C4H2	0.00	111.70	0.00	59.77
C4H6	0.00	34.96	0.00	68.16
C4H8	0.00	-0.13	0.00	73.55
C5	234.00	234.01	57.81	57.82
C5H	0.00	185.99	0.00	62.20
C5H12	0.00	-34.98	0.00	83.48
C5H2	0.00	165.23	0.00	63.69
C5H5	63.83	63.84	68.10	68.13
C5H6	0.00	31.99	0.00	64.45
C6H	0.00	213.15	0.00	74.10
C6H10	0.00	-1.00	0.00	74.75
C6H14	0.00	-39.91	0.00	92.87
C6H2	0.00	169.66	0.00	70.92

Species	$H^{\circ}(298)\text{kcal/mole}$		$S^{\circ}(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
C6H3	0.00	158.45	0.00	76.30
C6H4	99.66	99.67	68.25	68.26
C6H5	79.42	79.43	69.81	69.82
C6H5(L)	140.58	140.58	83.39	84.26
C6H5O	10.34	10.35	74.86	74.87
C6H5OH	-25.13	-25.01	76.96	76.93
C6H6	0.00	19.81	0.00	64.35
C6H7	47.94	47.96	73.07	73.07
C8H	0.00	288.86	0.00	78.39
C8H2	0.00	226.15	0.00	75.94
CA	42.85	42.85	36.99	36.98
CA(A)	0.00	0.00	9.93	9.93
CA(B)	0.12	0.12	10.15	10.15
CA(L)	2.61	2.60	12.11	12.10
CA+	185.30	185.30	38.37	38.37
CA2	82.66	82.66	61.29	61.29
CABR	-11.81	-11.81	60.42	60.41
CABR2	-92.00	-92.00	75.20	75.20
CABR2(S)	-163.30	-163.30	31.00	30.99
CACL	-25.00	-25.00	57.71	57.71
CACL2	-112.70	-112.70	69.35	69.35
CACL2(S)	-190.20	-190.20	25.00	24.99
CAF	-65.00	-65.00	54.86	54.86
CAF2	-187.50	-187.50	65.41	65.42
CAH2O2	-145.98	-145.97	68.23	68.25
CAH2O2(S)	-235.68	-235.68	19.93	19.93
CAI	-1.21	-1.21	62.43	62.42
CAI2	-61.70	-61.70	78.26	78.26
CAO	10.50	10.50	52.49	52.52
CAO(S)	-151.79	-151.79	9.13	9.15
CAOH	-46.34	-46.34	56.25	56.26
CAOH+	88.21	88.21	54.92	54.93
CAS	29.54	29.52	55.56	55.55
CCL	106.10	106.10	52.46	52.45
CCL2	53.02	53.02	63.29	63.28
CCL2CCLO	-24.27	-24.27	85.06	84.97

Species	$H^o(298)\text{kcal/mole}$		$S^o(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
CCL2CCLOH	-44.66	-44.69	83.09	82.88
CCL2CH	62.30	62.29	71.95	71.93
CCL2HOO	-1.37	-1.33	78.30	79.17
CCL2OHCH2	-22.77	-22.60	79.91	80.63
CCL2OHCHCL	-31.69	-31.54	87.57	89.10
CCL3	16.58	16.58	72.20	72.20
CCL3CCLH2	-35.29	-35.28	85.57	85.59
CCL3CCLO	-56.49	-56.47	89.99	90.43
CCL3CH2	18.79	18.89	81.61	82.80
CCL3CHCL	11.06	11.09	88.40	89.03
CCL3CHO	-45.51	-45.47	83.71	85.04
CCL3OO	-0.74	-0.71	83.14	83.46
CCL4	-20.22	-20.22	78.91	78.91
CCLH2OO	1.22	1.27	71.06	71.68
CH	142.00	142.00	43.72	43.71
CH+	388.80	388.80	41.00	41.00
CH2	92.48	92.48	46.72	46.71
CH2(S)	101.50	101.50	45.10	45.10
CH2CCL	61.43	61.39	64.24	64.15
CH2CCL2	0.75	0.71	68.84	68.76
CH2CCLOH	-37.01	-36.94	69.00	69.35
CH2CHCCH	69.14	69.14	66.49	67.33
CH2CHCCH2	74.11	74.14	74.70	75.31
CH2CHCH2	38.70	38.64	64.39	64.73
CH2CHCHCH	86.13	86.09	72.75	73.06
CH2CHCHCH2	28.33	28.29	69.74	70.44
CH2CHCL	4.69	4.67	63.03	62.98
CH2CL	27.08	27.07	59.28	59.28
CH2CL2	-22.83	-22.83	64.57	64.57
CH2CLCCL2	6.02	6.05	82.70	83.32
CH2CLCCLO	-58.33	-58.30	77.51	78.10
CH2CLCH2	23.00	23.10	68.36	69.46
CH2CLCH2CL	-32.35	-32.33	72.20	72.45
CH2CLCHCL	13.10	13.14	75.92	76.80
CH2CLCHCL2	-35.23	-35.22	80.05	80.12
CH2CLCHO	-41.67	-41.66	72.11	74.04

Species	$H^{\circ}(298)\text{kcal/mole}$		$S^{\circ}(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
CH ₂ CO	0.00	-12.40	0.00	57.78
CH ₂ F ₂	-107.71	-107.71	58.94	58.91
CH ₂ HCO	0.00	6.00	0.00	63.99
CH ₂ O	-27.70	-27.70	52.26	52.24
CH ₂ OH	-4.21	-4.10	58.93	58.87
CH ₂ OHCCl ₂	-23.26	-23.21	82.18	82.65
CH ₂ OHCHCl	-16.90	-16.79	74.35	74.94
CH ₂ SiCl	45.68	45.67	69.39	69.33
CH ₂ SiCl ₃	-87.71	-87.71	90.16	91.94
CH ₂ SiH ₂ Cl	-0.90	-0.87	74.23	75.92
CH ₂ SiHCl ₂	-44.67	-44.67	83.30	85.08
CH ₃	34.82	34.82	46.38	46.37
CH ₃ C(O)Cl	-56.93	-56.86	70.60	71.87
CH ₃ CC	123.81	123.82	60.28	60.27
CH ₃ CCCH ₂	74.33	74.34	78.57	80.35
CH ₃ CCCH ₃	40.92	40.94	71.58	73.36
CH ₃ CCH ₂	61.04	61.09	69.12	69.24
CH ₃ CCL	61.68	61.73	66.18	67.81
CH ₃ CCL ₂	10.33	10.42	75.42	76.27
CH ₃ CCL ₃	-33.55	-33.51	76.48	76.61
CH ₃ CCLO	-56.93	-56.86	70.60	71.87
CH ₃ CH ₂ CCH	44.66	44.75	71.46	71.43
CH ₃ CH ₂ CH ₂ CH ₃	-30.64	-30.50	72.68	73.31
CH ₃ CH ₂ Cl	-27.17	-27.10	66.00	66.33
CH ₃ CH ₂ O	-0.51	-0.44	65.48	65.81
CH ₃ CHCH	64.70	64.75	68.49	68.74
CH ₃ CHCL	18.22	18.30	68.46	69.48
CH ₃ CHCL ₂	-32.08	-32.02	72.79	73.04
CH ₃ CHOH	-14.34	-14.17	66.73	67.77
CH ₃ CL	-20.00	-20.00	55.99	55.97
CH ₃ CO	0.00	-5.40	0.00	63.73
CH ₃ F	-56.00	-56.00	53.25	53.22
CH ₃ HCO	0.00	-39.51	0.00	63.04
CH ₃ NO	18.88	18.95	62.33	63.46
CH ₃ NO ₂	-16.83	-16.84	70.26	72.03
CH ₃ O	0.00	3.89	0.00	54.60

Species	$H^{\circ}(298)\text{kcal/mole}$		$S^{\circ}(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
CH ₃ OCH ₃	-43.80	-43.72	63.74	64.35
CH ₃ OCL	-14.06	-13.98	64.97	65.42
CH ₃ OH	0.00	-48.06	0.00	57.27
CH ₃ ONO	-15.30	-15.25	66.63	66.87
CH ₃ ONO ₂	-26.12	-26.06	71.34	71.63
CH ₃ SICL	-2.47	-2.44	70.99	72.63
CH ₃ SIH ₂ SIH	-10.12	-9.96	88.03	91.66
CH ₃ SIH ₂ SIH ₂ CH ₃	-10.92	-10.79	88.03	90.60
CH ₃ SIHCL ₂	-93.81	-93.74	79.61	80.53
CH ₄	-17.90	-17.90	44.49	44.46
CHCL	80.00	80.00	56.12	56.11
CHCL ₂	19.51	19.51	65.08	65.08
CHCL ₂ CCCL ₂	8.53	8.53	90.99	92.74
CHCL ₂ CCLO	-57.87	-57.85	84.59	85.22
CHCL ₂ CH ₂	20.23	20.24	78.03	79.99
CHCL ₂ CHCL	10.32	10.35	82.79	83.54
CHCL ₂ CHCL ₂	-36.03	-36.02	85.18	85.39
CHCL ₃	-23.25	-23.25	70.64	70.64
CHCLCCL	55.99	55.98	72.48	72.40
CHCLCCLOH	-43.59	-43.51	76.26	76.42
CHCLCH	64.77	64.81	64.47	64.48
CHCLCHCL	-1.15	-1.15	69.24	69.19
CHCLCHOH	-38.64	-38.56	68.93	69.13
CHCLOH	-16.71	-16.65	65.30	65.41
CHCLOHCH ₂	-15.20	-15.08	74.53	76.30
CHCLOHCHCL	-24.95	-24.85	82.31	83.81
CHF	30.00	30.00	53.36	53.35
CHF ₃	-166.60	-166.60	62.03	62.02
CHOHCLCCL ₂	-31.95	-31.84	88.72	90.27
CHSICL	89.13	89.13	70.30	70.30
CHSICL ₂	29.60	29.61	81.07	82.86
CHSICL ₃	-35.28	-35.27	88.41	90.19
CHSIH ₂ CL	50.52	50.55	73.11	74.85
CHSIHCL	67.86	67.93	70.62	72.26
CHSIHCL ₂	7.19	7.22	80.87	82.62
CL	28.99	28.99	39.45	39.45

Species	$H^{\circ}(298)\text{kcal/mole}$		$S^{\circ}(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
CL(CH ₃)SICH ₂	-13.11	-13.08	78.44	79.58
CL ₂	0.00	0.00	53.29	53.29
CL ₂ CCCL ₂	-5.66	-5.67	81.51	81.41
CL ₂ CCHCL	-3.95	-3.96	77.64	77.54
CL ₂ CCHO	-12.45	-12.46	77.67	77.57
CL ₂ CHOH	-66.56	-66.41	71.53	72.50
CL ₂ CO	-52.70	-52.70	67.64	67.64
CL ₂ COH	-22.80	-22.68	73.07	73.68
CL ₂ HCO	-4.12	-4.12	71.65	71.64
CL ₂ SI(CH ₃) ₂	-113.74	-113.59	88.72	90.45
CL ₂ SI(CH ₃)CH ₂	-64.26	-64.18	92.21	94.86
CL ₂ SICH ₂	-34.22	-34.25	75.18	75.10
CL ₂ SICH ₃	-52.78	-52.71	80.76	81.74
CL ₂ SISI	32.71	32.71	79.88	79.88
CL ₂ SISICL	-24.42	-24.41	92.40	92.46
CL ₂ SISICL ₂	-95.69	-95.69	102.08	102.02
CL ₃ CCO	1500.00	1500.02	-5.27	87.34
CL ₃ CO	-4.37	-4.37	78.35	78.35
CL ₃ COH	-66.33	-66.23	77.64	79.21
CL ₃ SICH ₃	-137.81	-137.74	84.47	85.28
CL ₃ SISI	-26.17	-26.17	89.43	89.43
CL ₃ SISICL	-99.56	-99.55	101.49	103.27
CLCCCL	56.20	56.20	64.28	64.28
CLCCO	42.24	42.25	68.92	68.87
CLCH ₂ OH	-55.49	-55.49	69.49	71.45
CLCO	-6.48	-6.48	64.39	64.39
CLCOH	1.17	1.13	62.43	62.37
CLH ₂ CO	-2.35	-2.35	64.42	64.41
CLHCO	-44.30	-44.30	61.80	61.79
CLO	29.20	29.19	53.00	52.99
CLOCL	19.71	19.71	63.65	63.65
CLOO	33.60	33.60	63.54	63.53
CLSI(CH ₃) ₂	-26.19	-26.06	82.72	84.80
CLSI(CH ₃) ₂ CH ₂	-37.20	-37.04	92.86	96.44
CLSI(CH ₃) ₃	-86.29	-86.08	90.84	93.65
CLSICH ₃	-2.86	-2.82	70.99	72.64

Species	$H^o(298)$ kcal/mole		$S^o(298)$ cal/(mole·K)	
	Data	Fit	Data	Fit
CLSISI	99.11	99.11	71.44	71.44
CLSISICL	33.48	33.48	81.76	81.88
CN	104.00	104.00	48.41	48.40
CN+	430.87	430.87	50.99	50.98
CN–	14.50	14.50	46.81	46.81
CN2	113.00	113.00	54.04	54.03
CNN	139.70	139.70	55.35	55.35
CNO	97.64	97.64	55.57	55.57
CO	–26.42	–26.42	47.21	47.21
CO2	–94.05	–94.05	51.07	51.07
CO2–	–105.50	–105.50	57.49	57.48
COS	–33.08	–33.08	55.32	55.33
CS	67.00	67.00	50.30	50.29
CS2	27.95	27.95	56.85	56.85
CSICL	146.05	146.06	68.07	68.07
CSICL2	89.11	89.11	76.71	76.71
CSICL3	9.05	9.05	86.79	86.79
CSIH2CL	105.85	105.85	69.88	69.88
CSIHCL	119.47	119.47	67.68	67.68
CSIHCL2	63.16	63.16	77.47	77.47
D	52.99	52.99	29.46	29.45
D2	0.00	0.00	34.62	34.62
DH	0.08	0.08	34.34	34.34
DIOXANE	–75.11	–75.12	71.76	71.72
E	0.00	0.00	0.00	4.98
F	18.90	18.90	36.15	36.14
F–	–61.08	–61.08	34.77	34.76
F2	–0.09	–0.09	48.14	48.14
F2N2(C)	16.40	16.40	62.07	62.08
F2O2	14.00	13.99	64.42	64.33
F2SINH	–146.95	–146.93	70.92	70.92
F3SIN	–200.02	–200.02	73.86	73.87
FNNF	17.88	17.88	63.07	63.47
FNO3	2.50	2.50	69.99	69.99
FO	26.00	26.00	51.77	51.76
FO2	3.00	3.00	61.90	61.90

Species	$H^{\circ}(298)\text{kcal/mole}$		$S^{\circ}(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
FONO(C)	10.18	10.16	64.43	64.34
FONO(T)	14.13	14.12	64.88	64.79
FSIN	54.37	54.37	63.67	63.67
GA	68.53	68.52	43.83	43.82
GA2H6	31.50	31.50	69.05	69.05
GAAS	88.40	88.40	63.23	63.23
GAAS(3,C)	245.75	245.75	100.00	100.00
GAAS(3,L)	256.25	256.25	127.75	127.75
GAAS(5,C)	357.75	357.75	130.50	130.50
GAAS(5,L)	420.00	420.00	193.50	193.50
GAET	17.75	17.75	81.60	81.60
GAET2	4.50	4.50	100.43	100.43
GAET3	-17.05	-17.05	112.98	112.98
GAH	54.80	54.80	49.18	49.17
GAH2	41.00	41.00	56.00	56.00
GAH3	27.00	27.00	54.50	54.50
GAME	18.53	18.53	63.80	63.80
GAME2	16.42	16.43	80.55	80.55
GAME3	-10.88	-10.87	87.88	87.88
H	52.10	52.09	27.39	27.39
H(CH3)SiCH2	26.36	26.39	70.27	71.37
H+	367.17	367.15	26.01	26.01
H-	33.23	33.19	26.02	26.01
H2	0.00	0.00	31.21	31.21
H2ALME	6.00	6.00	61.73	61.73
H2ASME	24.05	24.05	64.85	64.85
H2C4O	54.58	54.59	66.42	66.43
H2CCC	160.67	160.67	61.07	61.07
H2CCC(S)	133.42	133.42	58.50	58.49
H2CCCCCH	128.19	128.19	75.36	75.37
H2CCCCCH	111.34	111.32	72.83	72.94
H2CCCCCH2	75.53	75.49	64.77	65.12
H2CCCH	83.03	83.04	61.48	61.48
H2CCCLO	-11.53	-11.54	69.74	69.67
H2CCH(SiCL2H)	-66.26	-66.22	84.68	85.71
H2CCH2OH	-4.57	-4.46	69.01	71.17

Species	$H^o(298)\text{kcal/mole}$		$S^o(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
H2CCHO	3.55	3.51	61.95	61.87
H2CCHSI	97.77	97.77	66.01	65.94
H2CCHSIH	73.54	73.58	66.68	66.79
H2CCHSIH2	58.21	58.21	69.03	68.94
H2CCHSIH3	20.65	20.70	68.95	69.47
H2CLSICH3	-50.13	-50.06	72.04	73.01
H2CLSIISICL3	-146.58	-146.56	100.61	101.70
H2CN	59.10	59.11	53.59	53.59
H2CNCH2	56.61	56.53	61.18	61.01
H2CNCH2O	45.02	44.98	68.50	68.38
H2CNCHO	-0.52	-0.56	66.78	66.64
H2CNH	21.89	21.85	54.81	55.45
H2CNNHO	49.78	49.72	67.28	67.10
H2CNNO	58.35	58.36	66.42	66.98
H2CNNO2	33.62	33.64	72.48	73.06
H2CNO	41.46	41.42	61.08	61.01
H2CNO2	36.44	36.47	65.53	65.58
H2CONO	33.07	33.10	68.31	68.54
H2GAET	-2.30	-2.30	83.68	83.68
H2GAME	15.00	15.00	64.85	64.85
H2NF	-6.49	-6.49	54.73	54.72
H2NNO	18.25	18.21	60.27	60.18
H2NO	15.82	15.82	55.69	55.68
H2NOH	-12.23	-12.16	56.04	56.17
H2O	-57.80	-57.80	45.11	45.10
H2O(L)	0.00	-68.31	0.00	16.71
H2O(S)	0.00	-69.96	0.00	10.71
H2O2	0.00	-32.53	0.00	55.65
H2S	-4.90	-4.90	49.15	49.14
H2SI(CH3)2	-23.20	-23.08	72.44	73.83
H2SI(CH3)CH2	25.55	25.61	77.77	79.83
H2SI(NH2)2	-37.30	-37.15	71.62	72.38
H2SIC	167.19	167.19	60.31	60.21
H2SICCH	90.95	90.95	66.92	66.80
H2SICH	105.35	105.42	62.48	63.58
H2SICH2	40.75	40.72	59.94	59.85

Species	$H^{\circ}(298)\text{kcal/mole}$		$S^{\circ}(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
H2SICH3	33.05	33.11	64.52	65.41
H2SIN	149.19	149.19	59.51	59.51
H2SINH	40.99	40.95	59.90	60.09
H2SINH2	28.03	28.09	65.77	65.79
H2SINH3	23.78	23.85	66.78	66.78
H2SISIH2	62.90	62.87	66.69	66.89
H3ASGAET3	-11.00	-11.00	124.48	124.48
H3ASGAME3	-4.70	-4.70	102.50	102.50
H3CONHO	6.46	6.56	71.67	72.65
H3SIC	147.61	147.61	61.79	61.71
H3SICCH	53.02	53.02	64.11	64.02
H3SICH	92.67	92.67	65.63	66.94
H3SICH2	41.54	41.54	67.62	68.97
H3SICH3	-7.32	-7.25	61.75	62.43
H3SIN	234.59	234.60	56.93	56.93
H3SINH	51.32	51.34	65.52	66.21
H3SISIH	74.91	74.96	67.99	69.32
H3SISIH3	19.11	19.16	68.06	68.06
HALME	27.25	27.25	62.78	62.78
HALME2	-6.73	-6.72	75.32	75.33
HASALME	56.50	56.50	83.68	83.68
HASGAET	69.15	69.15	97.28	97.28
HASGAME	70.00	70.00	87.88	87.88
HASME	42.58	42.58	65.90	65.90
HASME2	18.10	18.10	78.45	78.45
HCCCHCCH	134.95	134.95	73.15	73.17
HCCCL	54.95	54.95	57.29	57.29
HCCHCCH	129.91	129.88	68.80	69.06
HCCO	42.44	42.44	60.74	60.73
HCCOH	20.42	20.43	58.69	58.70
HCCSICL2H	-31.76	-31.76	82.04	82.04
HCL	-22.06	-22.06	44.65	44.64
HCL2SICH3	-94.23	-94.16	79.61	80.53
HCL2SISICL2H	-145.25	-145.24	99.80	101.08
HCLCCLO	-19.42	-19.43	77.51	77.40
HCLCCHO	-6.02	-6.03	70.20	70.09

Species	$H^{\circ}(298)\text{kcal/mole}$		$S^{\circ}(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
HCLSI(CH ₃) ₂	-68.24	-68.09	81.59	83.53
HCLSI(CH ₃)CH ₂	-19.15	-19.06	83.79	86.52
HCLSIH ₂	2.62	2.59	68.45	68.37
HCLSIH ₃	-9.10	-9.03	72.91	74.00
HCLSI	67.05	67.05	71.34	71.34
HCN	31.89	31.89	48.21	48.21
HCNH	66.15	66.10	55.58	55.90
HCNO	38.42	38.43	53.75	53.79
HCO	10.40	10.40	53.67	53.65
HCO+	199.10	199.10	48.59	48.59
HCOOH	-92.57	-92.61	59.32	59.26
HE	0.00	0.00	0.00	30.12
HE+	0.00	568.46	0.00	31.50
HF	-65.14	-65.14	41.51	41.50
HG2BR2(S)	-48.80	-48.80	52.28	52.27
HG2CL2(S)	-63.32	-63.32	46.02	46.00
HG2F2(S)	-116.00	-116.00	38.40	38.39
HG2I2(S)	-28.46	-28.47	57.67	57.66
HGAET	22.90	22.90	83.68	83.68
HGAET2	-2.30	-2.30	100.50	100.50
HGAME	29.00	29.00	65.90	65.90
HGAME2	2.50	2.50	79.50	79.50
HGBR	24.90	24.90	64.88	64.87
HGCL2	-34.97	-34.96	70.43	70.43
HGCL2(S)	-55.00	-55.00	34.54	34.53
HGF2	-70.19	-70.18	63.55	63.55
HGF2(S)	-101.00	-101.00	27.80	27.79
HGH	57.00	57.00	52.49	52.48
HGI	31.90	31.90	67.07	67.06
HGO	10.00	10.00	57.13	57.13
HGO(S)	-21.70	-21.70	16.80	16.79
HMEGAET	4.00	4.00	88.90	88.90
HN(OH) ₂	-24.72	-24.64	61.98	62.09
HN ₃	71.87	71.87	239.08	57.14
HNC	43.85	43.85	48.93	48.93
HNCN	76.43	76.43	59.36	59.36

Species	$H^{\circ}(298)\text{kcal/mole}$		$S^{\circ}(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
HNCNH	35.61	35.71	57.31	57.42
HNCO	-28.22	-28.22	57.05	57.05
HNF	32.00	32.00	54.98	54.97
HNF2	-13.79	-13.79	60.06	60.06
HNNHO	21.91	21.86	58.70	58.63
HNNO	55.25	55.20	60.59	60.53
HNNONO	59.02	58.99	70.98	70.97
HNO	23.80	23.80	52.73	52.72
HNO2	-14.15	-14.15	56.75	56.73
HNO3	-32.10	-32.10	63.66	63.66
HNOH	21.05	21.06	55.78	55.78
HO2	2.50	2.50	54.73	54.72
HOCH2OH	-96.64	-96.53	61.14	61.31
HOCL	-18.64	-18.64	56.34	56.33
HOCN	-3.55	-3.53	57.66	59.25
HOCO	-46.31	-46.29	60.12	60.11
HONO	-18.34	-18.34	59.59	59.58
HONO2	-30.18	-30.18	63.20	63.16
HSI(CH3)2	18.27	18.38	74.81	76.56
HSI(CH3)2CH2	9.32	9.44	86.18	88.89
HSI(CH3)3	-39.40	-39.24	83.61	85.87
HSI(NH2)2	5.62	5.77	72.56	73.38
HSI(NH2)3	-64.86	-64.68	78.65	79.52
HSIC	184.85	184.85	58.24	58.13
HSICCH	104.97	104.97	64.44	64.32
HSICH2	85.83	85.81	60.64	60.53
HSICH3	48.84	48.90	62.04	63.21
HSICL	17.00	17.00	59.80	59.80
HSIN	92.99	92.99	54.76	54.75
HSINH	84.80	84.79	60.63	60.68
HSINH2	26.33	26.29	59.77	60.05
HSISICL	79.13	79.11	73.04	72.96
I*C3H7	0.00	18.20	0.00	60.09
K	21.31	21.31	38.30	38.30
K(L)	0.55	0.55	17.08	17.07
K+	122.90	122.90	36.92	36.92

Species	$H^{\circ}(298)\text{kcal/mole}$		$S^{\circ}(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
K2	30.37	30.37	59.67	59.66
K2B4O7(S)	-796.90	-796.89	49.80	49.82
K2B6O10(S)	-1107.44	-1107.50	60.00	59.87
K2B8O13(S)	-1420.92	-1420.93	70.20	70.18
K2CO3(S)	-274.90	-274.91	37.17	37.15
K2H2O2	-156.50	-156.50	78.37	78.35
K2O(S)	-86.80	-86.79	22.50	22.51
K2O2(S)	-118.50	-118.47	27.00	27.05
K2SO4	-261.50	-261.50	87.49	87.50
K2SO4(A)	-343.62	-343.62	41.96	41.94
K2SO4(B)	-340.40	-340.41	45.96	45.94
K3CL6AL(S)	-500.00	-499.97	90.00	90.08
K3CL9AL2(S)	-683.60	-683.61	112.00	111.96
K3F6AL(S)	-795.00	-794.96	68.00	68.11
KBF4	-371.00	-371.00	75.35	75.36
KBO2	-161.10	-161.10	71.06	71.06
KBO2(S)	-237.80	-237.81	19.12	19.10
KBR	-43.04	-43.04	59.85	59.85
KBR(L)	-89.98	-89.99	25.23	25.22
KBR(S)	-94.12	-94.12	22.93	22.92
KCL	-51.31	-51.31	57.12	57.11
KCL(L)	-100.81	-100.81	20.71	20.71
KCL(S)	-104.37	-104.37	19.73	19.73
KCL4AL(S)	-286.00	-286.01	47.00	46.98
KCLO4(S)	-102.80	-100.21	36.10	40.62
KCN	19.00	19.00	60.48	60.47
KCN(L)	-24.89	-24.89	32.10	32.09
KCN(S)	-27.12	-27.12	30.54	30.53
KF	-78.10	-78.10	54.14	54.13
KF(L)	-132.52	-132.52	16.17	16.16
KF(S)	-135.90	-135.90	15.91	15.91
KH	29.40	29.40	47.30	47.30
KH(S)	-13.82	-13.81	12.00	12.02
KI	-30.00	-30.00	61.70	61.70
KI(L)	-74.77	-74.77	27.27	27.26
KI(S)	-78.37	-78.37	25.43	25.42

Species	$H^{\circ}(298)\text{kcal/mole}$		$S^{\circ}(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
KO	17.00	17.00	56.86	56.86
KO–	–33.00	–33.00	54.06	54.06
KO ₂ (S)	–68.00	–68.00	29.28	29.27
KOH	–98.64	–98.65	23.09	23.07
KOH+	119.00	119.00	59.80	59.81
ME2GAET	–5.25	–5.25	97.28	97.28
MEGAET	14.25	14.25	89.95	89.95
MEGAET2	–7.33	–7.32	106.70	106.71
MG	35.28	35.28	35.50	35.50
MG(L)	2.16	2.16	10.16	10.16
MG(S)	0.00	0.00	7.81	7.81
MG+	213.09	213.09	36.88	36.88
MG ₂	68.91	68.91	58.28	58.27
MG ₂ BR ₄	–183.50	–183.50	110.24	110.23
MG ₂ C ₃ (S)	19.00	19.00	24.00	24.01
MG ₂ F ₄	–410.70	–410.69	80.52	80.55
MGAL ₂ O ₄ (S)	–549.50	–549.49	21.20	21.22
MGB ₂ (S)	–21.98	–21.99	8.60	8.59
MGBR	–8.45	–8.45	58.52	58.52
MGBR ₂	–72.40	–72.40	71.92	71.92
MGBR ₂ +	174.80	174.80	76.87	76.87
MGC ₂ (S)	21.00	21.00	13.00	13.01
MGCL	–10.40	–10.40	55.76	55.76
MGCL ₂	–93.80	–93.80	66.18	66.18
MGCL ₂ (S)	–153.35	–153.35	21.42	21.42
MGCO ₃ (S)	–265.70	–265.70	15.74	15.73
MGF	–56.60	–56.60	52.81	52.81
MGF ₂	–173.70	–173.70	61.28	61.28
MGF ₂ (S)	–268.70	–268.70	13.68	13.67
MGF ₂ +	141.49	141.49	61.67	61.68
MGH	40.40	40.40	46.15	46.14
MGH ₂ (S)	–18.20	–18.20	7.43	7.42
MGH ₂ O ₂	–136.80	–136.80	63.85	63.87
MGH ₂ O ₂ (S)	–221.00	–221.00	15.12	15.10
MGN	69.00	69.00	53.71	53.71
MGO(S)	–143.70	–143.70	6.44	6.45

Species	$H^{\circ}(298)\text{kcal/mole}$		$S^{\circ}(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
MGOH	-39.38	-39.38	54.10	54.11
MGOH+	139.68	139.68	52.75	52.76
MGS	34.71	34.71	53.87	53.84
MGS(S)	-82.63	-82.63	12.03	12.02
MGSO4(S)	-301.57	-301.58	21.84	21.83
N	112.98	112.95	36.61	36.61
N*C3H7	0.00	22.60	0.00	64.13
N2	0.00	0.00	45.77	45.76
N2F2(C)	17.88	17.88	62.26	62.24
N2F2(T)	20.08	20.07	62.14	62.06
N2F4	-2.00	-2.00	71.96	71.98
N2H2	50.90	50.90	52.22	52.20
N2H3	0.00	36.78	0.00	54.61
N2H4	22.79	22.79	57.03	57.02
N2H4(L)	12.10	12.09	29.05	29.03
N2O	19.61	19.61	52.55	52.55
N2O+	318.69	318.69	55.87	55.86
N2O4	2.17	2.17	72.72	72.72
N3	99.00	99.00	54.10	54.10
NA	25.76	25.75	36.71	36.71
NA(L)	0.58	0.57	13.83	13.82
NA+	145.76	145.75	35.34	35.33
NA2	32.87	32.87	54.99	54.99
NA2B4O7(S)	-783.16	-783.17	45.29	45.27
NA2B6O10(S)	-1094.76	-1094.79	55.50	55.43
NA2C2N2	-2.10	-2.10	82.93	82.93
NA2F2	-202.30	-202.30	68.66	68.67
NA2H2O2	-145.20	-145.20	73.44	73.43
NA2O(L)	-89.11	-89.12	21.90	21.88
NA2O(S)	-99.90	-98.48	17.94	19.10
NA2O2	-122.66	-121.57	22.66	24.05
NA2SO4	-247.04	-247.04	82.87	82.89
NA2SO4(D)	-329.66	-329.66	39.01	38.99
NA2SO4(i)	-330.04	-330.04	38.30	38.28
NA2SO4(iii)	-330.99	-330.99	37.02	37.01
NA2SO4(iv)	-331.63	-331.64	35.89	35.87

Species	$H^{\circ}(298)\text{kcal/mole}$		$S^{\circ}(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
NA2SO4(v)	-331.70	-331.70	35.75	35.74
NA3CL6AL(S)	-473.00	-472.97	83.00	83.08
NA3F6AL(S)	-792.76	-792.77	57.00	56.97
NABH4(S)	-45.85	-45.85	24.23	24.23
NABO2	-155.00	-155.00	68.63	68.63
NABO2(S)	-233.20	-233.21	17.58	17.56
NABR	-34.40	-34.40	57.63	57.63
NABR(L)	-81.11	-81.11	24.94	24.93
NABR(S)	-86.38	-86.38	20.75	20.74
NACH	22.53	22.53	58.14	58.14
NACL	-43.36	-43.36	54.90	54.90
NACL(S)	-98.26	-98.26	17.24	17.23
NACL4AL(S)	-273.00	-273.01	45.00	44.97
NACN	22.53	22.53	58.14	58.14
NACN(S)	-21.68	-21.68	28.32	28.31
NAF	-69.42	-69.42	51.98	51.98
NAF2-	-160.00	-160.00	59.89	59.89
NAF4AL	-440.00	-440.00	82.41	82.43
NAH	29.70	29.70	45.00	44.99
NAI(S)	-68.80	-68.80	23.54	23.54
NAO	20.00	20.00	54.74	54.74
NAO-	-29.00	-29.00	51.95	51.95
NAO2(S)	-62.30	-62.30	27.70	27.69
NAO2AL(S)	-270.84	-270.59	16.83	17.17
NAOH	-47.27	-47.26	54.57	54.58
NAOH(L)	-99.64	-99.64	18.13	18.12
NAOH+	162.00	162.00	57.96	57.96
NCN	107.59	107.59	54.77	54.76
NCO	31.51	31.51	54.14	54.14
NF	53.93	53.93	50.82	50.82
NF2	7.87	7.87	59.40	59.39
NF3	-27.97	-27.97	61.79	61.79
NFO	-15.70	-15.70	59.27	59.27
NFO2	-26.00	-26.00	62.18	62.18
NH	85.20	85.20	43.29	43.29
NH2	45.50	45.50	46.51	46.50

Species	$H^o(298)\text{kcal/mole}$		$S^o(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
NH3	-10.97	-10.97	46.05	46.03
NNH	58.57	58.57	53.63	53.62
NO	21.58	21.58	50.35	50.34
NO+	236.66	236.66	47.35	47.34
NO2	7.91	7.91	57.34	57.33
NO2-	-48.45	-48.45	56.52	56.51
NO2F	-23.10	-23.09	61.26	61.26
NO3	17.00	17.00	60.35	60.35
NO3F	3.34	3.34	68.94	68.85
NOF	-16.91	-16.90	58.63	58.63
NOF3	-39.00	-39.00	66.54	66.55
O	59.55	59.55	38.47	38.46
O+	374.95	374.95	37.01	37.01
O-	24.32	24.32	37.69	37.68
O2	0.00	0.00	49.01	49.00
O2-	-11.61	-11.62	50.06	50.06
O2F	22.56	22.56	60.57	60.56
O3	34.10	34.10	57.08	57.08
OC(OH)2	-147.04	-147.04	64.46	64.40
OCHCHO	-49.55	-49.53	64.82	64.98
OCHNNHO	-2.05	-2.09	69.36	69.15
OF	23.73	23.73	50.43	50.43
OF2	4.60	4.60	58.54	58.54
OH	9.32	9.32	43.88	43.87
OH+	314.80	314.80	43.66	43.65
OH-	-34.32	-34.32	41.19	41.19
ONHNHO	23.55	23.52	62.66	62.55
ONHNOH	-1.77	-1.77	65.04	64.93
P	79.80	79.80	38.98	38.98
P2	42.68	42.68	52.11	52.11
P4	30.77	30.78	66.89	66.92
S	66.20	66.20	40.09	40.09
S(L)	0.00	0.44	0.00	8.77
S(S)	0.00	0.00	0.00	7.62
S+	306.48	306.47	39.08	39.08
S-TRIAZINE	56.36	56.37	64.49	64.49

Species	$H^{\circ}(298)\text{kcal/mole}$		$S^{\circ}(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
S2	30.71	30.71	54.51	54.50
SH	33.30	33.30	46.73	46.73
SI	107.70	107.70	40.12	40.12
SI(CH3)2	32.16	32.19	74.55	77.23
SI(CH3)3	3.12	3.28	84.75	87.23
SI(CH3)3CH2	-6.88	-6.71	96.57	99.89
SI(CH3)4	-55.74	-55.51	93.08	96.05
SI(L)	11.59	11.58	10.63	10.62
SI(NH2)3	-18.77	-18.63	84.34	84.27
SI(NH2)4	-92.88	-92.67	84.54	85.38
SI(S)	0.00	0.00	4.50	4.50
SI2	145.79	145.79	54.83	54.83
SI2C	128.00	128.00	57.88	57.88
SI2CL5	-151.65	-151.64	109.12	110.10
SI2CL5H	-188.98	-188.97	108.00	108.98
SI2CL6	-232.75	-232.73	111.13	111.85
SI2F6	-569.62	-569.61	97.16	97.16
SI2H2	95.63	95.62	58.84	58.83
SI2H3	105.70	105.70	65.51	65.51
SI2H5	55.70	55.70	68.85	68.85
SI2H6	19.10	19.10	64.54	64.53
SI3	152.00	152.00	64.00	64.01
SI3H8	28.90	28.90	81.57	81.56
SI3N4(A)	-178.00	-178.00	27.00	26.99
SIC	172.00	172.01	50.89	50.93
SIC(B)	-17.50	-17.50	3.97	3.98
SIC2	147.00	147.00	56.55	56.55
SICCH	125.77	125.77	60.40	60.26
SICH	124.39	124.39	54.94	54.83
SICH2	74.15	74.15	55.99	55.92
SICH3	74.53	74.53	60.16	60.13
SICL	37.90	37.90	56.80	56.80
SICL2	-40.30	-40.30	67.20	67.20
SICL2H2	-74.50	-74.50	68.40	68.40
SICL3	-76.50	-76.50	75.50	75.50
SICL3CH2CH	-140.60	-140.59	93.99	95.65

Species	$H^{\circ}(298)\text{kcal/mole}$		$S^{\circ}(298)\text{cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
SICL3H	-118.60	-118.60	74.90	74.89
SICL4	-158.40	-158.40	79.10	79.09
SICLH3	-32.20	-32.20	59.80	59.79
SIF	-12.42	-12.42	52.71	52.71
SIF(NH2)2	-95.48	-95.33	76.93	77.70
SIF(NH2)3	-170.70	-170.55	87.97	87.91
SIF2	-149.86	-149.86	61.38	61.38
SIF2(NH2)2	-247.30	-247.19	82.82	82.77
SIF2N	-63.11	-63.11	70.51	70.51
SIF2NH2	-167.24	-167.21	77.17	77.48
SIF3	-237.42	-237.42	67.76	67.76
SIF3NH	-249.65	-249.65	82.15	83.70
SIF3NH2	-317.89	-317.89	79.98	81.03
SIF3NHSIH3	-320.19	-320.16	95.97	96.88
SIF3NSIH3	-252.84	-252.83	97.65	99.34
SIF4	-385.98	-385.98	67.55	67.54
SIFH3	-85.50	-85.50	57.00	57.00
SIFNH	-13.57	-13.49	68.88	68.95
SIFNH2	-80.01	-80.04	64.68	64.62
SIH	91.70	91.70	44.20	44.20
SIH2	64.80	64.80	49.50	49.49
SIH2CL	7.80	7.80	62.30	62.30
SIH2F	-42.16	-42.16	59.70	59.70
SIH2F2	-186.38	-186.38	62.81	62.81
SIH3	47.43	47.43	51.81	51.80
SIH3NH2	-11.45	-11.40	65.66	65.66
SIH3NHSIH3	-14.32	-14.32	83.54	85.95
SIH3NSIH3	48.90	48.90	83.75	86.69
SIH3SIH2CH3	4.03	4.14	79.43	81.90
SIH4	8.09	8.10	48.90	48.90
SIHCL2	-34.30	-34.30	70.30	70.30
SIHF	-35.70	-35.70	57.07	57.07
SIHF2	-139.57	-139.57	65.05	65.05
SIHF3	-288.63	-288.63	66.65	66.65
SIN	115.55	115.55	51.95	51.95
SINH	38.39	38.39	51.66	51.66

Species	$H^o(298)\text{ kcal/mole}$		$S^o(298)\text{ cal/(mole}\cdot\text{K)}$	
	Data	Fit	Data	Fit
SINH2	48.67	48.67	58.56	58.56
SN	63.00	63.00	53.06	53.05
SO	1.20	1.20	53.02	53.01
SO2	-70.95	-70.95	59.30	59.29
SO3	-94.59	-94.59	61.34	61.34
TI	113.20	113.20	43.07	43.06
TICL	36.90	36.90	59.54	59.54
TICL2	-56.70	-56.70	66.50	66.50
TICL3	-128.90	-128.90	75.70	75.71
TICL4	-182.40	-182.40	84.79	84.80

2.4. Input in 9-Coefficient Format (NASA9)

The format of the thermodynamic data fitted using a 9-coefficient polynomial is given in Appendix C of <https://ntrs.nasa.gov/citations/20020085330> [2] (p. 375). Specifically, the non-dimensional specific heat at constant pressure is given as

$$\frac{C_p^0}{R} = \sum_{n=2}^4 a_n T^n \quad (2.5)$$

The corresponding enthalpy and entropy are obtained by the corresponding integrations and therefore produce two additional integration constants. The data obtained from the reference above are provided with Chemkin in a file named `therm_NASA.dat` and this file is located in the `\installDir\reaction\data`, where `installDir` is the installation directory for Ansys software. The following set of rules and restrictions apply:

1. The data must be contained within a block that starts with `THERMO NASA9` and ends with `END`.
2. Comments may be added before or after the data block or *between* the data for species. However, there can be no comments *within* the data (within the fit coefficients) characters. The comment lines must begin with character `"!`.
3. Although arbitrary temperature exponents for the fitting polynomial are allowed by the NASA9 format, this is not true for Ansys Chemkin in this release. Specifically, the temperature exponents must be `{-2.0, -1.0, 0.0, 1.0, 2.0, 3.0, 4.0}`. The data at the reference website include two species, `P4010(cr)` and `P4010(L)`, that do not have the standard fit. These species are not included in the file `therm_NASA9.dat` that is distributed with the installation.
4. It is possible to use data in both 7-coefficient polynomial format and this 9-polynomial form.
 - a. In order to do so, both input data-blocks should be in the same file. One data block would be contained between `THERMO NASA9 . . . . . END` and the other would be within `THERMO . . . . . END`.
 - b. The two data-blocks can be in any order.

- c. There can be comments in-between the two blocks.
 - d. The data in 9-coefficient form take precedence. That is, when the data are included in both formats for a given species, the version in 9-coefficient form will get preprocessed and utilized for that species.
5. Some additional data input such as SMILES-strings or absorption coefficients may also be specified (with appropriately tagged comment lines) within the NASA9 data. Since it is also possible to include blocks of data in both formats, you may copy-paste the existing (7-coefficient) data that includes such additional data and append (or prepend) NASA9 data in the same file. Ansys Chemkin will then use the 9-coefficient form to compute the thermodynamic quantities while the other additional data will come from the 7-coefficient block. This capability may be useful, as it avoids copying a lot of lines and inserting them in the proper location in the NASA9 input data.
 6. The number of elements in a species is restricted to 5. Since data in both formats can be given in the input file, it is possible to specify very large molecules with an unlimited number of elements in 7-coefficient form, as mentioned in [Alphabetical Listing of Keywords \[T-Z\] \(p. 346\)](#), along with NASA9 data for other species.
 7. Note for some common gas-phase species names/symbols in combustion related mechanisms: A pair of classic examples of this are: (a) Argon is declared as Ar (and not AR); (b) for C_2H_2 , there are two different species, namely, acetylene and vinylidene. Therefore, you may have to make appropriate changes to the included `therm_NASA9.dat` file if you are using it with existing mechanisms. This situation underscores the need for an informed usage of the thermodynamic data. Note that, in general, a reaction mechanism and thermodynamic data should be considered as one consistent unit. Therefore, even though changing the data to NASA9 format should not change or invalidate the results obtained using an existing reaction mechanism, you should take care to verify the outcome.
 8. The NASA9 data can also be included in the reaction-mechanism input file. When doing so, follow these guidelines:
 - a. It must be contained within the THERMO NASA9 and END.
 - b. This block must be located before the REACTIONS block.
 - c. When given in the reaction mechanism file, it is treated as if *all* the data for the gas-phase species are included in that block. That is, there would neither be a separate data-input file for the gas-phase thermodynamic data nor would there be the 7-coefficient format input (between THERMO . . . END) block.

2.5. Liquid Species Thermodynamic Data

The liquid species thermodynamic data in Ansys Chemkin are different from their gas-phase counterparts. In addition to the heat capacity, data for liquid density ρ_l , heat of vaporization H_{vap} , vapor pressure P_{vap} , critical properties (T_c, P_c, V_c, ω) , and standard-state enthalpy H_l^0 and entropy S_l^0 are required.

2.5.1. Data Format

The property data of all liquid species must be defined in the LIQPROPERTIES ALL section of the surface mechanism file. The keyword ALL must be included on the LIQPROPERTIES line because

Ansys Chemkin does not utilize an external data file to store additional liquid species data. The LIQ-PROPERTIES section must be provided before the REACTION section (and preferably after the THERM section if there is one).

The property data of each liquid species starts with its definition (symbol and atomic compositions) on the first line, which is followed by the properties. The properties of the liquid species can appear in any order; however, each property must be given over one single, unbroken line. The liquid species symbol is limited to 16 characters and is case-sensitive. The species symbol must be unique even for the same compound in different phases. For example, if H2O is used to represent the water vapor in the gas-phase mechanism, H2O cannot be used again for the liquid water; alternative choices would be H2O(L) or simply WATER. The elemental compositions of the species are provided after the species symbol on the same line. The elemental composition data are format-free and space delimited. [Figure 2.5: Example of the liquid species property data in the Ansys Chemkin format \(p. 35\)](#) shows an example of the liquid species property block in the surface mechanism file.

Figure 2.5: Example of the liquid species property data in the Ansys Chemkin format

```
LIQPROPERTIES ALL
c2h5oh(l)      c 2 h 6 o 1      ! Ethanol
! From "The Properties of Gases and Liquids"
CriticalProperties=513.90 61.4 167.1      ! Tc(K) Pc(bar) Vc(cm3) *Required
AcentricFac=0.644      ! acentric factor *Required
! From NIST webbook
RefLiqEnthalpy=2.76E5      ! Liquid enthalpy of formation at 298.15K (J/mol) *Optional
RefLiqEntropy=159.86      ! Liquid entropy at 298.15K (J/mol-K) *Optional
! From DIPPR database
Density=(DIPPR105)1.6288 0.27469 0.23178      !DIPPR EQ #105 *Required
SpecificHeat=(DIPPR100)102640 -139.63 -0.030341 0.0020386 0      !DIPPR EQ #100 *Required
HeatVaporization=(DIPPR106)55789000 0.31245 0 0 0      !DIPPR EQ #106 *Required
VaporPressure=(DIPPR101)73.304 -7122.3 -7.1424 0.0000028853 2 !DIPPR EQ #101 *Required
! liquid water
h2o(l)      h 2 o 1
CriticalProperties = 647.37 221.2 57.1      ! Tc(K) Pc(bar) Vc(cm3)
AcentricFac = 0.3852
RefLiqEnthalpy = -2.8583E5      ! Liquid water enthalpy of formation at 298.15K (J/mol)
RefLiqEntropy = 69.95      ! Liquid water entropy at 298.15K (J/mol-K)
! From DIPPR database
Density = (DIPPR105) 3.557 0.2338 647.1 0.18721
SpecificHeat = (DIPPR100) 2.7637e5 -2090.1 8.125 -0.014116 9.3701e-6
HeatVaporization = (DIPPR106) 5.1546e7 0.28402 -0.15843 0.2375 0.0
VaporPressure = (DIPPR101) 73.649 -7258.2 -7.3037 4.1653e-6 2.0
```

[Table 2.5: List of required properties for each liquid species \(p. 35\)](#) lists the properties that must be provided for each liquid species. Detailed descriptions of the properties can be found in the corresponding sections in the Chemkin Theory Manual and the references therein. The liquid property keywords are case-insensitive.

Table 2.5: List of required properties for each liquid species

Required liquid property	Keyword	Reference in Chemkin Theory Manual
Critical Properties	criticalproperties	Liquid Standard-State Entropy
Acentric factor	acentricfac	Liquid Standard-State Entropy
Density	density	Liquid Species Density Models
Specific Heat Capacity at Const. Pressure	specificheat	Heat Capacity at Constant Pressure Cp

Required liquid property	Keyword	Reference in Chemkin Theory Manual
Heat of Vaporization	heatvaporization	Heat of Vaporization
Vapor Pressure	vaporpressure	Vapor Pressure
Standard-State Enthalpy	refliqenthalpy	Liquid Standard-State Entropy
Standard-State Entropy	refliqentropy	Liquid Standard-State Entropy

The liquid properties are given as a function of temperature. Because the liquid state for most compounds of interest exists within a narrow temperature range, the liquid property data are usually fitted by one set of parameters. Ansys Chemkin will use the property method specified to calculate the property values for temperatures below the critical temperature.

2.5.2. Cubic EOS (CuEOS) Liquid Density Models

The Cubic Equations of State (CuEOS) method uses the Cubic Equation of State for Pure Substance to calculate the density of liquid species, based on the same theory described in [Real Gas Model in the Chemkin Theory Manual](#). Ansys Chemkin uses 5 CuEOS models: Van der Waals (VW), Redlich-Kwong (RK), Soave-Redlich-Kwong (SRK), Aungier-Redlich-Kwong (ARK), and Peng-Robison (PR).

The input format for this method in the surface/liquid kinetics file is: `density = (CuEOS_<CuEOS_name>)`. The Cu_EOS_name is a required parameter and must be one of the implemented CuEOS models in Chemkin. For example: `density=(CuEOS_PR)` means the density of this liquid species would be calculated using the CuEOS method and the Peng-Robison model.

Chapter 3: Gas-phase Kinetics Input

The *Gas-phase Kinetics* input file provides a symbolic description of an elementary chemical reaction mechanism. This file is used during Pre-processing to create a *Gas-phase Kinetics* linking file (*chem.asc*) that stores pertinent information about that mechanism for access during the reactor-model simulation. The information in the Linking File is subsequently accessed by an initialization routine that copies the needed information into memory during a reacting-flow simulation. The stored information is used in calculations related to the equation of state, thermodynamic properties, and chemical production rates.

The *Gas-phase Kinetics* input file includes information on elements, species, thermodynamic data, and the reaction mechanism. Element data are read first, species data are second, followed by optional thermodynamic data, with reactions specified last. The thermodynamic data for the species may come be included in the *Gas-phase Kinetics* input file and/or from a Thermodynamic Database (for example, *therm.dat*). With the exception of the thermodynamic data, all input is free format. The required syntax for the four types of input is described in [Element Data \(p. 37\)](#) through [Reaction Mechanism Description \(p. 43\)](#). The auxiliary keywords for gas-phase reactions are described in [Table 3.7: Alphabetical Listing of Gas-phase Reaction Auxiliary Keywords \(p. 47\)](#) and the options for specifying units on the REACTIONS line are described in [Table 3.4: Alphabetical Listing of REACTIONS-line Options for Gas-phase Kinetics Data \(p. 43\)](#). [Alphabetical Listing of Project Input Keywords \(p. 139\)](#) describes the meaning and usage of each keyword entry that may be included as part of a Reactor Model input file.

Note:

Input information in the *Gas-phase Kinetics* input file must be contained within the first **100 columns, or it will be ignored.**

Note:

In the *Gas-phase Kinetics* input file, thermo data must precede reaction data.

3.1. Element Data

All chemical species in the reaction mechanism must be composed of chemical elements or isotopes of chemical elements. Each element and isotope must be declared as a one- or two-character symbol. The purpose of the element data is to associate atomic weights of the elements with their character symbol representations and to identify the order in which arrays of element information in the *Gas-phase Kinetics* Subroutine Library are referenced. For example, an array of atomic weights for the elements is in exactly the same order in which the elements were declared in the element data. In other words, if the atomic weights are stored in an array AWT, then AWT(3) is the atomic weight of the third element declared in the element data.

Element data must start with the word ELEMENTS (or ELEM), followed by any number of element symbols on any number of lines. Element symbols may appear anywhere on a line, but those on the

same line must be separated by blanks. Any line or portion of a line starting with an exclamation mark (!) is considered a comment and will be ignored. Blank lines are ignored.

If an element is on the periodic chart, then only the symbol identifying the element need appear in the element data.

Note:

The elements that Ansys Chemkin recognizes are as follows: H, HE, LI, BE, B, C, N, O, F, NE, NA, MG, AL, SI, P, S, CL, AR, K, CA, SC, TI, V, CR, MN, FE, CO, NI, CU, ZN, GA, GE, AS, SE, BR, KR, RB, SR, Y, ZR, NB, MO, TC, RU, RH, PD, AG, CD, IN, SN, SB, TE, I, XE, CS, BA, LA, CE, PR, ND, PM, SM, EU, GD, TB, DY, HO, ER, TM, YB, LU, HF, TA, W, RE, OS, IR, PT, AU, HG, TL, PB, BI, PO, AT, RN, FR, RA, AC, TH, PA, U, NP, PU, AM, CM, BK, CF, ES, FM, D, E

For the elements appearing on the periodic chart, the Ansys Chemkin pre-processors have the atomic weight (in grams per mole) stored internally. For isotopes, a one- or two- character symbol must be input by the user to identify each isotope, and a symbol and an atomic weight (in grams per mole) for each must be defined. The same symbol must be used in the thermodynamic data to identify the elemental composition of species involving the isotope. Once an isotope has been so defined, it is treated exactly as a new element. If an ionic species is used in the reaction mechanism (that is, OH⁺), an electron must be declared as the element E.

For an isotope, the atomic weight must follow the identifying symbol and be delimited by slashes (/). The atomic weight may be in integer, floating-point, or E format (for example, 2, 2.0, 0.2E1), but internally it will be converted to a floating point number. For example, the isotope deuterium may be defined as D/2.014/. If desired, the atomic weight of an element in the periodic chart may be altered by including the atomic weight as input just as though the element were an isotope.

Figure 3.1: Examples of Species Data (p. 38) shows several equivalent ways to describe element information. In this example the elements are hydrogen, oxygen, nitrogen, and the isotope deuterium.

Figure 3.1: Examples of Species Data

```
ELEMENTS  H  D /2.014/  O  N  END

ELEM                                     ! ELEM is equivalent to ELEMENTS
  H
  D / 2.014 /
  O
  N
END                                     ! an END line is optional

ELEM H
ELEM D/2.014/
ELEM O
ELEM N
```

Table 3.1: Summary of the Rules for Element Data (p. 38) summarizes the rules for element data.

Table 3.1: Summary of the Rules for Element Data

Rule	Description
1	The first element line must start with the word ELEMENTS (or ELEM).
2	Element or isotope names are either one- or two-character symbols.

Rule	Description
3	An isotope name (that is, a name not on the periodic chart) must be followed by its atomic weight (in grams per mole) delimited by slashes.
4	Each element or isotope should be declared only once; however, duplicated element symbols will be ignored.
5	An element or isotope name may appear anywhere on the line.
6	Any number of element or isotope names may appear on a line, and more than one line may be used.
7	Element or isotope names that appear on the same line must be separated by at least one blank space.
8	An element or isotope name that begins on one line may not continue to the next line.
9	Any blank spaces between an element or isotope name and the first slash are ignored and any blank spaces between slashes and an atomic weight are also ignored. However, no blank spaces are allowed within an element name or an atomic weight.
10	There may be more than one ELEMENT statement.
11	All characters following an exclamation mark are comments.
12	It is recommended that an END statement follow a group of elements.
13	Elements required by <i>Surface Kinetics</i> surface species must be declared in the <i>Gas-phase Kinetics</i> input file.

3.2. Species Data

Each chemical species in a problem must be identified on one or more species line(s). Any set of up to 16 upper or lower case characters can be used as a species name. In addition each species must be composed of elements that have been identified in the element data. As for the element data, one of the primary purposes of the species data is to identify the order in which arrays of species information are referenced in the *Gas-phase Kinetics* Subroutine Library.

Species data must start with the word SPECIES (or SPEC), followed by any number of species symbols on any number of lines. Species symbols may appear anywhere on a line, but those on the same line must be separated by blank spaces. Any line or portion of a line starting with an exclamation mark (!) is considered to be a comment and will be ignored. Blank lines are ignored. [Figure 3.2: Examples of Species Data \(p. 39\)](#) shows several equivalent ways to describe species information.

Figure 3.2: Examples of Species Data

```

SPECIES    H2  O2  H  O  OH  H2O  N2  N  NO  END

SPEC                                ! SPEC is equivalent to SPECIES
  H2  O2
  H  O  OH  H2O  N2  N  NO
END

SPEC H2
spec O2

```

The rules for species data are summarized in [Table 3.2: Summary of the Rules for Species Data](#) (p. 40).

Table 3.2: Summary of the Rules for Species Data

Rule	Description
1	Species data must start with the word SPECIES (or SPEC).
2	Species names are composed of up to 16-character upper- or lower- case symbols. The names cannot begin with the characters +, =, or a number; an ionic species name may end with one or more + 's or - 's.
3	Each species should be declared only once; however, duplicated species symbols will be ignored.
4	Each species that subsequently appears in a reaction must be declared.
5	A species name may appear anywhere on the line.
6	Any number of species names may appear on a line, and more than one line may be used.
7	Species named on the same line must be separated by at least one blank space.
8	A species name that begins on one line may not continue to the next line.
9	There may be more than one SPECIES statement.
10	All characters following an exclamation mark are comments.
11	For best results, an END statement should follow a species group.

3.3. Thermodynamic Data

All gas-phase species that appears in the reactions contained in the *Gas-phase Kinetics* input or in the *Surface Kinetics* input, must have associated thermodynamic data. The data may be extracted from a database file (for example, *therm.dat*) and/or read directly from the *Gas-phase Kinetics* input file. Details on the thermodynamic data format, whether including in the *Gas-phase Kinetics* input file or in a thermodynamic database file, are provided in [Thermodynamic Data Format](#) (p. 3).

Note:

When thermodynamic data input is included in the *Gas-phase Kinetics* input file, it must immediately follow species data.

Note:

The *therm.dat* file distributed with Ansys Chemkin represents a historical (not necessarily best) collection of data accumulated by Sandia National Laboratories over the period from 1980 to 1995. The data fits in this collection are based on a variety of sources, including JANAF Tables, NASA, and computational chemistry calculations performed at Sandia and elsewhere. This data set has been fixed and not updated in order to assure backwards compatibility and consistency with published Chemkin results.

3.4. Real Gas Data

Ansys Chemkin employs the cubic equation of state (EOS) to capture the P-T-V relationship of a real gas mixture at high pressures. For each gas species in the real gas mixture, the cubic equation of state models require additional properties that are not part of the regular thermodynamic data. These properties include the critical point, P_c , T_c , and V_c , and the acentric factor ω , and would be provided in the real gas data block of the gas-phase mechanism. The real gas data block starts with the keyword EOS_. Immediately following this keyword (no space), a phrase indicating the choice of the cubic equation of state model to be used with this gas mechanism is appended. There are five cubic EOS models available in Ansys Chemkin. (For more details, see [Real Gas Model in the Chemkin Theory Manual](#)). These cubic equation of state models, along with their key phrases, are listed in [Table 3.3: Cubic equation of state models available in Chemkin \(p. 41\)](#). For example, the keyword EOS_PR will cause the Peng-Robinson equation of state to be applied whenever this gas mechanism is used in a Ansys Chemkin simulation.

Table 3.3: Cubic equation of state models available in Chemkin

Cubic EOS Model	Key Phrase
van der Waals	VAND or VDW
Redlich-Kwong	REDL or RK
Soave-Redlich-Kwong	SOAV or SRK
Aungier-Redlich-Kwong	AUNG or ARK
Peng-Robinson	PENG or PR

The required properties of all gas species in the mechanism are given below the EOS_ keyword. Each gas species will have its properties listed in one single line. The line must start with the species name and be followed by, in the exact same order, the values of P_c , T_c , V_c , and ω for this gas species. The critical pressure P_c is in bar, the critical temperature T_c in Kelvin, and the critical molar volume V_c in cm^3/mole . All four parameters are required. If V_c or ω are not available for a species, set the value to zero.

The parameters are format-free and separated by blank space(s). If the binary interaction coefficients between this gas species and other species are known, the coefficients can be given as auxiliary keywords in the line(s) below the property data line. The interacting species name and the corresponding binary interaction coefficient should be provided in the format illustrated here with the coefficient value delimited by slashes (/):

<interacting species name>/<interaction coefficient>/

For example, the binary interaction coefficient between O2 and N2 can be given in a line below the properties data line of O2 (or N2) as N2/ -0.0078/ (or O2/ -0.0078/).

If you have multiple binary interaction coefficients to specify, they should be separated by blank space(s) and can be written in a single line or in several lines. The binary interaction coefficient is only required once for each pair of species.

All species in the mechanism must have their real gas data given in the real gas data block, and the species data lines can appear in any order. The real gas data block should be closed by the keyword END.

[Figure 3.3: Example of Real Gas data input \(p. 42\)](#) shows some examples of the real gas data input.

Figure 3.3: Example of Real Gas data input

```

! Real Gas Information
! R.C. Reid, J.M. Prausnitz, and B.E. Poling, The Properties of Gases & Liquids, 4th ED.
EOS_SRK
! Soave-Redlich-Kwong EOS
! Species symbol, TC[K], PC[bar], VC[cm3/mol], Best-fitted Acentric Factor
H      33.2      13.64      0.0      0.0
H2     33.15     13.0      65.1     -0.2324
! Binary Inteaction Coefficients
O      44.5      26.9      0.0      0.0
O2     154.6     50.4     73.4     0.0298
! Binary Inteaction Coefficients
OH     400.0     149.0      0.0      0.1
HO2    400.0     82.0      0.0      0.2
H2O    647.37    221.2     57.1     0.3443
H2O2   730.10    21.68      0.0      0.5
CH4    190.56     46.0     99.2     0.01142
! Binary Inteaction Coefficients
CO2/0.093/ N2/0.028/ CO/0.032/
CO     132.9     35.0     93.2     0.0295
! Binary Inteaction Coefficients
CH4/0.032/
CO2    304.1     73.8     93.9     0.2373
! Binary Inteaction Coefficients
N2/-0.032/
CH4/0.093/
N2     126.2     33.9     89.8     0.0358
! Binary Inteaction Coefficients
CO2/-0.032/ CH4/0.028/
END

```

3.5. Transport Data

Gas-phase species transport data is required for a collision-frequency reaction formulation, and for reactor models or other programs that require a transport linkfile. The data can be read from a database file (for example, *tran.dat*) and/or read directly from the *Gas-phase Kinetics* input file. To include transport data in the input file, the first line of the data should be the word TRANSPORT (or TRAN), and the last line should be the word END. If TRANSPORT ALL is used, it is expected that all required transport data is given in this section, or else a database file is used to supplement data not provided here.

The TRANSPORT . . . END data block's format should resemble this:

```

TRANSPORT
C2H4 2 280.800 3.971 0.000 0.000 1.500
END

```

For the collision frequency reaction, the required collision diameter of species will be obtained from the transport data and stored in the gas-phase linkfile. For reactor models or other programs that require a supplemental transport linkfile, the User Interface provides a check-box option on the Pre-Processing panel, Process Transport Properties; if this is checked, transport-data coefficient fitting is performed, and a transport linkfile written.

Details on the transport data format, whether included in the *Gas-Phase Kinetics* input file or in a transport properties database file, are provided in [Transport Data Format \(p. 97\)](#).

Note:

If the *Gas-Phase Kinetics* input file includes transport properties data input, this data must follow species data and precede reaction data.

3.6. Reaction Mechanism Description

The reaction mechanism may consist of any number of chemical reactions involving the species named in the species data. A reaction may be reversible or irreversible; it may be a three-body reaction with an arbitrary third body and/or enhanced third-body efficiencies; it may have a Lindemann [5] (p. 375), Troe [6] (p. 375) or SRI [7] (p. 375) pressure fall-off formulation; it may have an arbitrary pressure-dependence defined by special fits or interpolation; it may involve a photon; and it may depend on a species temperature other than that of the bulk gas. [Pressure-dependent Reactions](#) of the [Chemkin Theory Manual](#) provides more detailed discussion of these different formulations. In this section, we describe the rules and syntax needed to enter different types of reactions in the *Gas-phase Kinetics* input file. The keywords for controlling these reaction parameters are described in [Alphabetical Listing of Project Input Keywords](#) (p. 139) .

Reaction data must start with a line that contains the word REACTIONS (or REAC). The lines following the REACTIONS line contain reaction descriptions, together with their Arrhenius rate coefficients. The reaction description is composed of a reaction path, reaction rate coefficients, and (optionally) some auxiliary information or keywords.

3.6.1. REACTIONS Line Options

On the same line as the REACTIONS word, you may specify units of the Arrhenius rate coefficients ([Equation 3.5](#) of the [Chemkin Theory Manual](#)) followed by the word CAL/MOLE, KCAL/MOLE, JOULES/MOLE, KJOULES/MOLE, KELVINS, or EVOLTS for E_i , and/or MOLES or MOLECULES for A_i . If MOLECULES is specified, then the units for A_i are cm, molecules, sec, and K.

Note:

If units are not specified, A_i and E_i must be in cm, mole, sec, K, and cal/mole, respectively. Note that T is always in Kelvin. Ansys Chemkin uses the thermal calorie, 4.184 Joules.

Table 3.4: Alphabetical Listing of REACTIONS-line Options for Gas-phase Kinetics Data

Keyword	Definition
CAL/[MOLE]	Reiterates the default units for all gas-phase reactions that follow the REACTIONS header line for parameters with energy units such as E_i . Notes - Default units for E_i are cal/mole.
EVOL[TS]	Supersedes the default units for all gas-phase reactions which follow the REACTIONS header line for parameters with energy units such as E_i . Notes - Default units for E_i are cal/mole.
JOUL[ES/MOLE]	Supersedes the default units for all gas-phase reactions which follow the REACTIONS header line for parameters with energy units such as E_i . Notes - Default units for E_i are cal/mole.

Keyword	Definition
KCAL[/MOLE]	Supersedes the default units for all gas-phase reactions which follow the REACTIONS header line for parameters with energy units such as E_i. Notes - Default units for E_i are cal/mole.
KELV[INS]	Supersedes the default units for all gas-phase reactions which follow the REACTIONS header line for parameters with energy units such as E_i. Notes - Default units for E_i are cal/mole.
KJOU[LES/MOLE]	Supersedes the default units for all gas-phase reactions which follow the REACTIONS header line for parameters with energy units such as E_i. Notes - Default units for E_i are cal/mole.
MOLEC[ULES]	Supersedes the default units for all gas-phase reactions which follow the REACTIONS header line for pre-exponential factors A_i. Notes - Default units for A_i are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.
MAXSP	Increases the maximum number of reactants or products allowed in a reaction. The number given by this keyword must be greater than the default limit of 6. For example, REACTIONS MAXSP=11. Notes -This keyword is available to both the gas-phase and surface reaction mechanism.
MOLE[S]	Supersedes the default units for all gas-phase reactions which follow the REACTIONS header line for pre-exponential factors A_i. Notes - Default units for A_i are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.
USRPROD	Indicates that the user will provide a user-written rate routine that will supply all of the species net rates of production, overriding any other reaction input in the <i>Gas-phase Kinetics</i> input file. The net rate-of-production for all species will be obtained by calling the user-supplied subroutine, CKUPROD. An optional slash(/)-delimited integer parameter allows the user to select from more than one type of rate formulation. Wherever the species production rates are required, they will be obtained by calling the user-written subroutine called CKUPROD. A template of CKUPROD is provided in the Ansys Chemkin installation, in the file <i>cklib_user_routines.f</i> located in the directory <i>user_subroutines</i>. Information about how to compile and link user routines into Chemkin is included in Chemkin Application Programming Interface Manual.

Keyword	Definition
	Notes - USRPROD cannot be used in conjunction with USRPROG (p. 60) (entered after a particular reaction).

Note:

This API does not support user-written programming, so you are cautioned to use the CKUPROD user-routine feature at your own risk. Also, there are some features in Ansys Chemkin that will be incompatible with the global replacement of species rates of production, such as sensitivity analysis and rate-of-production analysis. Such features will return zero values when user-rate programming is encountered.

3.6.2. Reaction Data

Reaction Data follows the REACTIONS line and precedes an END statement that concludes the Reactions Data section. Each reaction entry line is divided into two fields. The first contains the symbolic description of the reaction path for that reaction while the second contains the Arrhenius rate coefficients. Both fields are format-free and blank spaces are ignored. Any line or portion of a line starting with an exclamation mark (!) is considered a comment and is ignored. Blank lines are also ignored.

The reaction description, given in the first field, must be composed of the species symbols, coefficients, delimiters, and any special symbols defined in [Table 3.5: Reaction Data Criteria \(p. 45\)](#).

Table 3.5: Reaction Data Criteria

Species Symbols	
	Each species in a reaction is described with the unique sequence of characters as they appear in the species data and the thermodynamic data (e.g., H2).
Coefficients	
	A species symbol may be preceded by an integer or real coefficient. The coefficient has the meaning that there are that number of moles of the particular species present as either reactants or products; e.g. 20H, is equivalent to OH + OH. Non-integer coefficients are allowed in <i>Gas-phase Kinetics input</i> , but the element balance in the reaction must still be maintained.
Delimiters	
+	A plus sign is the delimiter between each reactant species and each product species.
=	An equality sign is the delimiter between the last reactant and the first product in a reversible reaction.
<=>	An equality sign enclosed by angle brackets can also be used as the delimiter between the last reactant and the first product in a reversible reaction.
=>	An equality sign with an angle bracket on the right is the delimiter between the last reactant and the first product in an irreversible reaction.
Special Symbols	
+M	An M as a reactant and product stands for an arbitrary third body. An M in the reaction description indicates that a third body is participating in the reaction. In a reaction containing an M, species can be specified to have enhanced third

Species Symbols	
	body efficiencies, in which case auxiliary information (described below) must follow the reaction line. If no enhanced third body efficiencies are specified, then all species act equally as third bodies and the effective concentration of the third body is the total concentration of the mixture.
(+M)	An M as a reactant and product surrounded by parentheses indicates that the reaction is a pressure-dependent reaction, in which case auxiliary information line(s) (described below) must follow the reaction to identify the fall-off formulation and parameters. A species may also be enclosed in parenthesis. Here, for example, (+H2O) indicates that water is acting as the third body in the fall-off region, not the total concentration M.
E	The symbol E as a reactant and/or product is used to represent an electron. An electron is treated just like any other species, and is composed of the element E, which must be declared as element data. If an E appears in any reaction, then it must also be declared as a species in the species data.
!	An exclamation mark means that all following characters are comments on the reaction. For example, the comment may be used to give a reference to the source of the reaction and rate data.

The second field of the REACTIONS line is used to define the Arrhenius rate coefficients A_i , β_i , and E_i in that order, as given by Equation 3.5 of the [Chemkin Theory Manual](#). At least one blank space must separate the first number and the last symbol in the reaction. The three numbers must be separated by at least one blank space, be stated in either integer, floating point, or "E" format (for example, 123, 123.0 or 123E1), and have units associated with them.

Note:

Unless modified by options specified on the REACTIONS line or in Auxiliary Reaction Keywords, the default units for A_i are in cgs (cm, sec, K, mole), the exact units depending on the reaction. The factor β_i is dimensionless. The default units for the activation energies are cal/mole.

Examples of reaction data are shown in [Figure 3.4: Examples of Reaction Data \(p. 46\)](#).

Figure 3.4: Examples of Reaction Data

```

REACTIONS
H2 + O2 = 2OH
! H2 + O2 = OH + H
H + O2 + M = HO2 + M
! H + O2 + M = HO2
! H + O2 = HO2 + M
OH+ + H + E = H2O
O = O(*)
0.5H2 + 0.5O2 = OH
END
CAL/MOLE ! these are the default units for the reaction rates
1.7E13 0 47780. ! Ref. 21
1.7E13 0 47780. ! same as previous reaction,
! commented to prevent a duplication error
2.0E15 0.000 -870.
2.0E15 0.000 -870.
2.0E15 0.000 -870.
1.E19 0 0.0
1.3E5 0 0
! photoactive reaction, represented without HV
! example of real coefficients
! END statement is optional; ! <eof> condition is equivalent

```


Table 3.6: Summary of the Rules for Reaction Data (p. 47) is a summary of the reaction data rules.

Table 3.6: Summary of the Rules for Reaction Data

Rule	Description
1	The first reaction line must start with the word REACTIONS (or REAC), and may include units definition(s).
2	The reaction description can begin anywhere on the line. All blank spaces, except those between Arrhenius coefficients, are ignored.
3	Each reaction description must have =, <=> or => between the last reactant and the first product.
4	Each reaction description must be contained on one line.
5	Three Arrhenius coefficients must appear in order (A_i , β_i , and E_i) on each Reaction line, separated from each other and from the reaction description by at least one blank space; no blanks are allowed within the numbers themselves.
6	There cannot be more than six reactants or six products in a reaction.
7	Comments are any and all characters following an exclamation mark.
8	For best results an END statement should follow the reaction input.

3.6.3. Auxiliary Reaction Data

Auxiliary Reaction Data is entered in lines immediately following the Reaction Data for a specific reaction path. The format of an auxiliary information line is a character-string keyword followed by a slash-delimited (/) field, which begins and ends with a slash (/), and which contains an appropriate number of parameters (either integer, floating point, or "E" format).

These data or keywords are used to indicate different reaction-rate expressions, units, pressure-dependency, and other ways in which the reaction behavior may be modified. Table 3.8: Summary of the Rules for Auxiliary Reaction Data (p. 62) provides detailed information about the meaning and usage of each auxiliary keyword entry option for gas-phase reactions. Also, Figure 3.5: Examples of Auxiliary Reaction Data (p. 60) provides some additional examples of reaction data.

Table 3.7: Alphabetical Listing of Gas-phase Reaction Auxiliary Keywords

Keyword	Definition			
<SpeciesName>	Neutral Third Body Efficiency - If a reaction contains M as a reactant and/or product, auxiliary information lines may follow the reaction line to specify enhanced third-body efficiencies of certain species (that is, a_{kir} , Equation 3.19 of the Chemkin Theory Manual). To define an enhanced third body efficiency, the keyword is the species name of the third body, and its one parameter is its enhanced efficiency factor. A species that acts as an enhanced third body must be declared as a species. Examples of third body efficiencies are shown in the first three reactions in Figure 3.5: Examples of Auxiliary Reaction Data (p. 60) .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Species name</i>	Required	--	CO /1.87/

Keyword	Definition			
	Stoichiometric coefficient ν_{ki}	Required	--	CO/1.87/
	Reaction Example	REACTIONS CAL/MOLE HCO+M=H+CO+M 0.250E+15 0.000 16802.000 ! Warnatz CO/1.87/ H2/1.87 CH4/2.81/ CO2/3./ H2O/5./		
CHEB	Chebyshev Polynomial Rate Expressions - Supersedes the default reaction rate expression by a Chebyshev polynomial evaluation (see Equation 3.43 of the Chemkin Theory Manual). CHEB must be followed by (slash delimited) parameters; for the first CHEB, the first value is N , the number of basis functions along the temperature axis; the second is M , the number of basis functions along the pressure axis; and the remainder are the $N \times M$ coefficients a_{nm} from Equation 3.41 in the order of $a_{11}, a_{12}, ..., a_{1M}, a_{21}, a_{22}, ..., a_{NM}$, in this or additional CHEB declarations.			
	Parameters	Optional/Reqd.	Units	Examples
	Number of temperature functions N	Required	--	CHEB / 7 3 -4.1624 .9394 -.18563 12.438/
	Number of pressure functions M	Required	--	CHEB / 7 3 -4.1624 .9394 -.18563 12.438/
	Chebyshev coefficients a	Required	--	CHEB / 7 3 -4.1624 .9394 -.18563 12.438/
	Reaction Example	C2H5 + O2 (+M) <=> C2H4E + H02 (+M) 1.00E+00 .000 0. ! mecon 7/97 CHEB/ 7 3 1.0216E+01 - 1.1083E+00 -1.9807E-01 7.8325E-01/ CHEB/ 1.1609E+00 1.1762E-01 - 9.5707E-02 1.0928E-01 1.1551E-01/ CHEB/ -8.0290E-02 -1.0978E-01 3.7074E-04 -1.4830E-02 -6.0589E-02/ CHEB/ -2.8056E-02 6.9203E-03 - 9.7259E-03 -1.3556E-02 7.6648E-03/ CHEB/ 6.6865E-03 -8.8244E-04/		
	Notes	More than one set of CHEB data can appear for a given reaction, as many as required to input exactly $N \times M + 2$ values.		

Keyword	Definition	
		- Pressure limits of the Chebyshev polynomial for this reaction may be provided by keyword PCHEB (p. 54) . - Temperature limits of the Chebyshev polynomial for this reaction may be provided by keyword TCHEB (p. 57) .
COLLEFF	Efficiency of Collision Frequency Expression - If a reaction is bimolecular and the approximate collision diameters are known, then the collision frequency efficiency expression can be used to calculate the reaction rate constant. The Arrhenius parameters for the correction factor are specified on the reaction line. On the line following, the keyword COLLEFF is required to tell the interpreter the type of reaction. A+B<=>Products a b c COLLEFF In addition to the parameters for the correction factor <i>a</i>, <i>b</i>, and <i>c</i>, the diameters for each reacting species must be specified. Ansys Chemkin uses the Lennard-Jones diameter as an approximation for the spherical diameter of a species. The Lennard-Jones diameter is one of the inputs read by the <i>Transport</i> Pre-Processor that are specified as outlined in Transport Data Format (p. 97) .	
	Reaction Ex-ample	<pre>C6H6 + C6H6 => C12H10 + H2 0.02 0 0 COLLEFF</pre>
DUP	Duplicate Reactions - Two or more reactions can involve the same set of reactants and products, but proceed through distinctly different processes. In these cases, it may be appropriate to state a reaction mechanism that has two or more reactions that are the same, but have different rate parameters. However, duplicate reactions are normally considered errors by the <i>Gas-phase Kinetics</i> Pre-Processor. If the user requires duplication (for example, the same reactants and products with different Arrhenius parameters), the keyword DUP must follow the reaction line of each duplicate reaction, including the first occurrence of the reaction that is duplicated. For example, if the user wishes to specify different rate expressions for each of two identical reactions, there must be two occurrences of the DUP keyword, one following each of the reactions. No auxiliary parameters are required. Examples are shown in Figure 3.5: Examples of Auxiliary Reaction Data (p. 60) .	
	Reaction Ex-ample	<pre>H02+H02=H2O2+O2 4.20E14 0.0 11982 DUP</pre>

Keyword	Definition														
		H02+H02=H2O2+O2 1.3E11 0.0 -1629 DUP													
EXCI	Energy Loss Parameter - Auxiliary data may be used to specify the energy loss per reaction event by specifying the keyword EXCI, followed by the value of the energy loss per event, in units of electron volts. This option overrides the calculation of energy loss from the change in enthalpy determined by the reaction description and the thermodynamic data of the reactants and products. The option is useful in describing electron-impact excitation reactions, for example, where the user does not wish to keep track of the excited-species density, but wants to include the energy loss to the electrons due to the excitation process. An example of the use of EXCI is given in Figure 3.5: Examples of Auxiliary Reaction Data (p. 60) . The EXCI keyword represents the ΔH_r parameter that is used to describe inelastic collisions in Equation 8.144 of the Chemkin Theory Manual for the electron balance in plasma simulations. <table><tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr><tr><td>Energy loss per event</td><td>Required</td><td>electron-volts</td><td>TDEP/E/ EXCI/11.60/</td></tr><tr><td>Reaction Example</td><td colspan="3">E + AR => AR + E </td></tr></table>			Parameters	Optional/Reqd.	Units	Examples	Energy loss per event	Required	electron-volts	TDEP/E/ EXCI/ 11.60 /	Reaction Example	E + AR => AR + E		
Parameters	Optional/Reqd.	Units	Examples												
Energy loss per event	Required	electron-volts	TDEP/E/ EXCI/ 11.60 /												
Reaction Example	E + AR => AR + E														

Keyword	Definition			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	FORD /Pt(S) 1.0/
	Stoichiometric coefficient ν_{ki}	Required	--	FORD /Pt(S) 1.0/
	Reaction Example	JP10+1402 => 10C02 + 8H2O 6.454323E+13 0.0 29188.8 FORD / JP10 1.153923 / FORD / 02 0.738210 /		
	Notes	Multiple occurrences of the FORD (p. 50) construct may appear on the auxiliary line.		
HIGH	Defines the high-pressure limit for pressure-dependent chemically activated bimolecular reactions (see Equation 3.26 of the Chemkin Theory Manual). HIGH must be followed by the three slash-delimited high-pressure limit Arrhenius parameters A_∞ , β_∞ , and E_∞ , and the Arrhenius coefficients on the reaction line represent the low-pressure limit Arrhenius parameters A_0 , β_0 , and E_0 .			
	Parameters	Optional/Reqd.	Units	Examples
	Pre-exponential factor A_∞	Required	Depends on reaction	HIGH /6.85E-12 6.53 -834./
	Temperature exponent β_∞	Required	--	HIGH /6.85E-12 6.53 -834./
	Activation energy E_∞	Required	cal/mole	HIGH /6.85E-12 6.53 -834./
	Reaction Example	C2H5+O2(+M)= C2H4+H02(+M) 1.41E7 1.09 -1975. HIGH/6.85E-12 6.53 -834./ TROE/0.45 1.E-10 1.E10/ H2/2/ C0/2/ C02/3/ H2O/5/		
	Notes	- Required when SRI (p. 57) or TROE (p. 58) is present - Additional pressure-dependency parameters may be provided by keywords SRI (p. 57) or TROE (p. 58).		

Keyword	Definition			
		If no additional parameters, the Lindemann formulation is applied.		
JAN	Optional Rate Fit Expressions - Supersedes the default reaction rate expression by a Janev-Langer reaction rate (see Equation 3.49 of the Chemkin Theory Manual). JAN must be followed by the nine slash-delimited Janev-Langer rate parameters, b_{ni} .			
	Parameters	Optional/Reqd.	Units	Examples
	Janev-Langer parameters b_1 - b_9	Required	eV	JAN / -19.73476 3.992702 -1.773436 0.5331949 -0.1 0.02 -0.002 8.E-5 -2.E-6/
	Reaction Example	$\text{H}^* + \text{E} = \text{H} + 2\text{E} \qquad 1.0$ $0.0 \quad 0.0$ $\text{JAN} / -19.73476 \ 3.992702 \ -1.773436$ $0.5331949 \ -0.1 \ 0.02 \ -0.002 \ 8.E-5 \ -$ $2.E-6/$		
	Notes	- If fewer than 9 parameters are required for the fit, the user must provide zeros for the remainder of the parameters. - The Janev rate expression was originally designed for usage with plasmas, and the temperature unit is eV (that is, electron-volt). When the rate is calculated, the system temperature is first converted to eV. For temperatures in kelvin, it will be $T/11595$ in eV. Therefore the temperature needs to be in eV when fitting the JAN rate coefficients, while other reactions in the mechanism still use temperature in K.		
LOW	Defines the low-pressure limit for pressure-dependent unimolecular fall-off reactions (see Equation 3.25 of the Chemkin Theory Manual). LOW must be followed by the slash-delimited low-pressure limit Arrhenius parameters A_0 , β_0 , and E_0 , and the Arrhenius coefficients on the reaction line represent the three high-pressure limit Arrhenius parameters A_∞ , β_∞ , and E_∞ .			
	Parameters	Optional/Reqd.	Units	Examples
	Pre-exponential factor A_0	Required	depends on reaction	LOW /1.73E69 -15.07 60491./
	Temperature exponent β_0	Required	--	LOW /1.73E69 -15.07 60491./
	Activation energy E_0	Required	cal/mole	LOW /1.73E69 -15.07 60491./

Keyword	Definition			
	Reaction Ex-ample	O+CO(+M)<=>CO2(+M) 1.800E+10 .000 2385.00 LOW/ 6.020E+14 .000 3000.00/		
	Notes	- Required when SRI (p. 57) or TROE (p. 58) is present - Supplemental pressure-dependency parameters may be provided by keywords SRI (p. 57) or TROE (p. 58). - If no additional parameters, the Lindemann formulation is applied.		
LT	Landau-Teller Reactions - Supersedes the default reaction rate expression by the Landau-Teller reaction rate (see Equation 3.47 of the Chemkin Theory Manual). LT must be followed by the two slash-delimited Landau-Teller reaction rate parameters <i>Bi</i> and <i>Ci</i> .			
	Parameters	Optional/Reqd.	Units	Examples
	Landau-Teller parameter <i>B_i</i>	Required	--	LT /-67 62.1/
	Landau-Teller parameter <i>C_i</i>	Required	--	LT /-67 62.1/
	Reaction Ex-ample	H2(1)+H2O(000)=H2(0)+H2O(001) 2.89E15 0 0 LT / -67 62.1/		
	Notes	If explicit REV (p. 55) parameters are given for the reaction, then explicit reverse Landau-Teller parameters must also be given by keyword RLT (p. 56) .		
MOME	Plasma Momentum-Transfer Collision Frequency Options - Indicates that the reaction parameters describe the momentum-transfer collision frequency for electrons. This keyword requires no supplemental data, but changes the treatment of the reaction-rate coefficients. The option causes the reaction to be flagged as an electron momentum-transfer reaction, and assumes that the reaction rate constant is in units of cm ³ /mole-s or cm ³ /molecule-s, depending on the units specified in the REACTIONS statement. These reactions are treated as special cases when <i>Gas-phase Kinetics</i> subroutines evaluate reaction rates-of-progress, as described in Rates of Creation and Destruction of Species of the Chemkin Theory Manual .			
	Reaction Ex-ample	E + AR* => E + AR* 1.0502E-08 2.5929E-01 1.7464E+04 TDEP/E/		

Keyword	Definition			
		MOME		
	Notes	These options would generally not be used (or would be ignored) with any of the standard Ansys Chemkin reactor models; they are there for users who may be incorporating Chemkin into a multi-dimensional plasma simulation user program.		
PCHEB	Supersedes the default pressure limits for a Chebyshev polynomial rate expression (see Equation 3.42 of the Chemkin Theory Manual). PCHEB must be followed by the two slash-delimited values Pmin and Pmax.			
	Parameters	Optional/Reqd.	Units	Examples
	Minimum pressure Pmin	Required	atm	PCHEB / 1.0 100.0/
	Maximum pressure Pmax	Required	atm	PCHEB / 1.0 100.0/
	Reaction Example	C2H5+O2(+M)=C2H4E+H02 (+M) 1.0 0.0 0.0 LOW / 1.0 0.0 0.0 / PCHEB / 1.0 100.0/ CHEB/ 7 3 10.216 -1.1083 -0.19807 0.78325/ CHEB/ 1.1609 0.1.1762 -0.095707 0.10928 0.11551/ CHEB/ -0.08029 -0.10978 3.7074E- 04 -0.01483 -0.060589/ CHEB/ -0.028056 6.9203E-03 - 9.7259E-03 -0.013556 7.6648E-03/ CHEB/ 6.6865E-03 -8.8244E-04/		
	Notes	• The default Chebyshev polynomial pressure limits are Pmin=0.001, Pmax=100. • Chebyshev polynomial parameters must be provided by use of keyword CHEB (p. 48). • Default Chebyshev polynomial temperature limits may be superseded by keyword TCHEB (p. 57).		
	PLOG	Pressure Dependence Through Logarithmic Interpolation - Provides a general-purpose way of describing pressure-dependent reaction rates. Using the PLOG keywords, you can enter any number of sets of Arrhenius reaction-rate coefficients at different reactor pressures. The PLOG data will		

Keyword	Definition																				
	override the Arrhenius coefficients provided on the reaction line. The PLOG keyword must be followed by the slash-delimited values for the pressure at which the reaction rates are given and the three Arrhenius parameters, A_i, β_i, and E_i, for that pressure. Multiple PLOG entries can be provided, but they must be included in ascending order of pressure. See the Ansys Chemkin Theory Manual, General Pressure Dependence Using Logarithmic Interpolation , General Pressure Dependence Using Logarithmic Interpolation . <table><tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr><tr><td>Pressure</td><td></td><td>atm</td><td>PLOG /0.03947 2.9512E+09 1.28 13474./</td></tr><tr><td>Pre-exponential factor A_i</td><td></td><td>Depends on reaction</td><td>PLOG /0.03947 2.9512E+09 1.28 13474./</td></tr><tr><td>Temperature exponent β_i</td><td></td><td>--</td><td>PLOG /0.03947 2.9512E+09 1.28 13474./</td></tr><tr><td>Activation energy E_i</td><td></td><td>cal/mole</td><td>PLOG /0.03947 2.9512E+09 1.28 13474./</td></tr></table> Reaction Ex-ample <pre>H2CCCH+H=C3H2(S)+H2 2.9512E+09 1.28 13474. PLOG /0.03947 2.9512E+09 1.28 13474./ PLOG /1. 1.0965E+10 1.13 13929./ PLOG /10. 3.3113E+13 0.195 17579./ PLOG /100. 3.3113E+13 0.195 17579./</pre> Notes There should not be more than one PLOG entry for the same pressure for a reaction. However, you can use the DUPLICATE option to have two reactions that are the same and that both use PLOG entries; in this case the resulting reaction-rates will be summed as is the usual case for DUPLICATE reactions.	Parameters	Optional/Reqd.	Units	Examples	Pressure		atm	PLOG /0.03947 2.9512E+09 1.28 13474./	Pre-exponential factor A_i		Depends on reaction	PLOG /0.03947 2.9512E+09 1.28 13474./	Temperature exponent β_i		--	PLOG /0.03947 2.9512E+09 1.28 13474./	Activation energy E_i		cal/mole	PLOG /0.03947 2.9512E+09 1.28 13474./
Parameters	Optional/Reqd.	Units	Examples																		
Pressure		atm	PLOG /0.03947 2.9512E+09 1.28 13474./																		
Pre-exponential factor A_i		Depends on reaction	PLOG /0.03947 2.9512E+09 1.28 13474./																		
Temperature exponent β_i		--	PLOG /0.03947 2.9512E+09 1.28 13474./																		
Activation energy E_i		cal/mole	PLOG /0.03947 2.9512E+09 1.28 13474./																		
REV	Reverse Rate Parameters - Supersedes the reverse rates that would normally be computed through the equilibrium constant, Equation 3.6 of the Chemkin Theory Manual . REV must be followed by the three slash-delimited Arrhenius coefficients (A_i, β_i, and E_i) to specify the reverse rate.																				

Keyword	Definition			
	Parameters	Optional/Reqd.	Units	Examples
	Pre-exponential factor A_i		depends on reaction	REV / 6.61E-14 0.0 9561./
	Temperature exponent β_i		--	REV / 6.61E-14 0.0 9561./
	Activation energy E_i		cal/mole	REV / 6.61E-14 0.0 9561./
	Reaction Example	C2F4 + M = CF2 + CF2 + M 1.126E-07 0. 27528.0 REV / 9.381E-14 0. 31404.1 /		
RLT	Supersedes the default reverse reaction rate expression by the Landau-Teller reaction rate (see Equation 3.47 of the Chemkin Theory Manual). RLT must be followed by the two slash-delimited Landau-Teller reaction rate parameters B_i and C_i .			
	Parameters	Optional/Reqd.	Units	Examples
	Landau-Teller parameter B_i	Required	--	RLT /-67 62.1/
	Landau-Teller parameter C_i	Required	--	RLT /-67 62.1/
	Reaction Example	H2(1)+H2O(000)=H2(0)+H2O(001) 2.89E15 0 0 RLT / -67 62.1/		
	Notes	- Required when the combination of LT (p. 53) and REV (p. 55) keywords is present. - If explicit REV (p. 55) parameters are given for the reaction, then explicit reverse Landau-Teller parameters must also be given by keyword RLT.		
RORD	Reverse Reaction Order Parameter - Supersedes the reverse reaction order for any species in the mechanism (with respect to species concentration), regardless of whether the species appears as a reactant or a product in the reaction. RORD must be followed by the slash-delimited species name and the new reaction order, and supersedes the values of ν''_{ki} in Equation 3.4 of the Chemkin Theory Manual pertaining to the particular species named on the line; the reaction order for all other species maintain their default values. Multiple occurrences of the RORD construct may appear on the auxiliary line.			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	RORD /OH 2.0/

Keyword	Definition			
	<i>Stoichiometric coefficient ν''_{ki}</i>	Required	--	RORD /OH 2.0/
	Reaction Ex-ample	H2+O2=2OH 0.170E+14 0.00 47780 RORD /OH 2.0/		
	Notes	See also FORD (p. 50).		
	SRI	Defines the SRI pressure-dependent reaction rate (see Equation 3.34 of the Chemkin Theory Manual). SRI must be followed by either three, or five, slash-delimited parameters <i>a</i> , <i>b</i> , <i>c</i> , <i>d</i> , and <i>e</i> . The fourth and fifth parameters are optional and if omitted, they are by default <i>d</i> =1 and <i>e</i> =0.		
	Parameters	Optional/Reqd.	Units	Examples
	<i>SRI reaction rate parameters a - e</i>	Required	--	SRI /0.45 797. 979. 1.0 0.0/
	Reaction Ex-ample	CH3+H(+M) = CH4(+M) 6.0E16 -1.0 0 LOW/8.0E26 -3.0 0/ SRI/0.45 797.0 979.0/ H2/2/ C0/2/ C02/3/ H2O/5/		
	Notes	• Additional SRI parameters are required, by use of keywords LOW (p. 52) or HIGH (p. 51).		
TCHEB	Supersedes the default temperature limits for a Chebyshev polynomial rate expression (see Equation 3.41 of the Chemkin Theory Manual). TCHEB must be followed by the slash-delimited values, <i>Tmin</i> and <i>Tmax</i> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Minimum temperature Tmin</i>	Required	K	TCHEB / 300.0 2500./
	<i>Maximum temperature Tmax</i>	Required	K	TCHEB / 300.0 2500./
	Reaction Ex-ample	C2H5+O2(+M)=C2H4E+HO2 (+M) 1.0 0.0 0.0 LOW / 1.0 0.0 0.0 / TCHEB / 300. 2500./ CHEB/ 7 3 10.216 -1.1083 -0.19807 0.78325/ CHEB/ 1.1609 0.1.1762 -0.095707 0.10928 0.11551/		

Keyword	Definition			
		CHEB/ -0.08029 -0.10978 3.7074E-04 -0.01483 -0.060589/ CHEB/ -0.028056 6.9203E-03 -9.7259E-03 -0.013556 7.6648E-03/ CHEB/ 6.6865E-03 -8.8244E-04/		
	Notes	- The default Chebyshev polynomial temperature limits are $T_{min}=300, T_{max}=2500$. - Required Chebyshev polynomial parameters must be provided by use of keyword CHEB (p. 48). - Supplemental Chebyshev polynomial pressure limits may be provided by use of keyword PCHEB (p. 54).		
TDEP	Species Temperature Dependence - Causes the reaction rate constant to be evaluated using the specified species temperature and the rate parameters given in the reaction data. In the case when there is more than one temperature defined in the system, the Application must call the <i>Gas-phase Kinetics</i> subroutine CKKTFL to indicate which temperature in the temperature array corresponds to each species. Examples of the TDEP input are shown in Figure 3.5: Examples of Auxiliary Reaction Data (p. 60).			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	TDEP/E/
	Keyword Usage	E + CL2 => CL- + CL 5.8901E-09 - 2.5619E-01 1.5834E+04 TDEP/E/		
TROE	Defines the Troe pressure-dependent reaction rate (see Equation 3.33 of the Chemkin Theory Manual). TROE must be followed by the slash-delimited 3 or 4 parameters α, T^{***}, T^* , and T^{**} ; the fourth parameter is optional and if omitted, the last term in Equation 3.33 is not used.			
	Parameters	Optional/Reqd.	Units	Examples
	α	Required	Depends on reaction	TROE /0.5336 629.2 2190. 626.5/
	T^{***}	Required	K	TROE /0.5336 629.2 2190. 626.5/
	T^*	Required	K	TROE /0.5336 629.2 2190. 626.5/
	T^{**}	Optional	K	TROE /0.5336 629.2 2190. 626.5/

Keyword	Definition			
	Reaction Ex-ample	C2H5+O2(+M)= C2H4+H2O(+M) 1.41E7 1.09 -1975. HIGH/6.85E-12 6.53 -834./ TROE/0.45 1.E-10 1.E10/ H2/2/ CO/2/ CO2/3/ H2O/5/		
	Notes	Other required TROE parameters must be provided by use of keywords LOW (p. 52) or HIGH (p. 51).		
UNITS	Reaction Units - Supersedes the current units for a particular reaction rate fit that may differ from the default units specified for other reaction expressions in the chemistry mechanism. UNITS must be followed by the slash-delimited character-string string , where string is one of the following: EVOL[TS], KELV[INS], CAL/[MOLE], KCAL[/MOLE], JOUL[ES/MOLE], or KJOU[LES/MOLE] for parameters with energy units such as E_i , or MOLES or MOLEC[ULES] for pre-exponential factors A_i , where the letters in brackets are optional. The inclusion of MOLEC[ULES] would indicate that the reaction rate expression is in units of molecules/cm ³ rather than mole/cm ³ . The UNITS auxiliary keyword allows only one string parameter, but the user can repeat the UNITS as many times as needed for a given reaction.			
	Parameters	Optional/Reqd.	Units	Examples
	Reaction units character string	Required	--	UNITS /MOLECULES/
	Reaction Ex-ample	CF3+ + E + #WSIO2(B) => #SIO2 + CF3 0.33 0.0 0.0 BOHM ! YIELD /0.01 20. 0.5 1.0/ UNITS/EVOLTS/		
	Notes	• Default units for A_i are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction. • Default units for E_i are (cal/mole). • If any of the units strings are given on the REACTIONS header line, it applies to all reactions, but may be superseded for a particular reaction by the auxiliary UNITS keyword • Even if the default energy units are changed by giving the UNITS keyword, the temperature appearing in the Arrhenius expression of Equation 3.5 of the Chemkin Theory Manual is still in Kelvins.		

Keyword	Definition								
USRPROG	Optional User Rate Subroutine CKUPROG - The net rate-of-progress for the reaction will be obtained by calling a user-supplied subroutine, CKUPROG. An optional slash(/)-delimited integer parameter allows the user to select from more than one type of rate formulation. Wherever the net reaction rate is required, it will be obtained by calling the user-written subroutine. A template of CKUPROG is provided in the Ansys Chemkin installation, in the file cklib_user_routines.f located in the directory user_routines . Information about how to compile and link user routines into Chemkin is included in Chemkin Application Programming Interface Manual .								
	<table><tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr><tr><td><i>Rate formulation type</i></td><td>Optional</td><td>--</td><td>USRPROG /1/</td></tr></table>	Parameters	Optional/Reqd.	Units	Examples	<i>Rate formulation type</i>	Optional	--	USRPROG /1/
	Parameters	Optional/Reqd.	Units	Examples					
	<i>Rate formulation type</i>	Optional	--	USRPROG /1/					
	Reaction Ex-ample	H2+O2=>2OH 1.7E13 0.0 47780 . USRPROG/1/							
Notes	USRPROG applies only to irreversible reactions, and cannot be used in conjunction with USRPROD (entered on the REACTIONS header line).								
XSMT	Flags a reaction as representing collision cross-section information for the determination of ion momentum-transfer collision frequencies in a plasma simulation. No auxiliary parameters are required. The evaluated rate-constant is assumed to be in cm ² , and is left as such when <i>Gas-phase Kinetics</i> subroutines evaluate rates of progress for other reactions. For more detail, see Rates of Creation and Destruction of Species of the Chemkin Theory Manual . Examples are given in Figure 3.5: Examples of Auxiliary Reaction Data (p. 60) .								
	Reaction Ex-ample	CL+ + CL => CL+ + CL 1.03E-13 -0.5 0.0 TDEP/CL+/ XSMT !momentum-transfer x-sec							
	Notes	These options would generally not be used (or would be ignored) with any of the standard Ansys Chemkin reactor models; they are there for users who may be incorporating Chemkin into a multi-dimensional plasma simulation user program.							

Figure 3.5: Examples of Auxiliary Reaction Data

```

REACTIONS          CAL/MOLE  ! these are the default units for the reaction rates
HCO+M=H+CO+M      0.250E+15  0.000  16802.000          ! Warnatz
CO/1.87/  H2/1.87  CH4/2.81/  CO2/3./  H2O/5./

H+C2H4(+M)=C2H5(+M)  0.221E+14  0.000  2066.000          ! Michael

```

```

LOW / 6.369E27 -2.76 -54.0 /
H2/2/ C0/2/ C02/3/ H20/5/
!Lindemann fall-off reaction
! enhanced third-body efficiencies

CH3+CH3(+M)=C2H6(+M) 9.03E16 -1.18 654.
LOW / 3.18E41 -7.03 2762 /
TROE / 0.6041 6927. 132. /
H2/2/ C0/2/ C02/3/ H20/5/
! TROE fall-off reaction, with 3 parameters
! enhanced third-body efficiencies

CH3+H(+M)=CH4(+M) 6.0E16 -1.0 0.0
LOW / 8.0E26 -3.0 0.0/
SRI / 0.45 797. 979. /
H2/2/ C0/2/ C02/3/ H20/5/
! SRI fall-off reaction
! enhanced third-body efficiencies

CH3+CH3(+M)=H + C2H5(+M) 4.989E12 0.099 10600.0 ! Stewart
HIGH/ 3.80E-7 4.838 7710. /
SRI / 1.641 4334 2725 /
! Chemically activated reaction
! SRI pressure dependence

CH4+H=CH3+H2 1.25E14 0 1.190E4
REV / 4.80E12 0 1.143E4 /
! Westbrook

! The following two reactions are acceptable duplicates:

H2+O2 = 2OH 1.7E13 0 47780
DUPLICATE
H2+O2 = 2OH 1.0E13 0 47000.
DUPLICATE

H2(1)+H2O(000)=H2(0)+H2O(001) 2.89E15 0 0
LT / -67 62.1/
! Landau-Teller reaction

! The following is a Chebyshev polynomial rate description

C2H5 + O2 (+M) <=> C2H4E + H02 (+M) 1.00E+00 .000 0. ! Bozzelli
TCHEB/ 300 2500/ PCHEB/1 100/
CHEB/ 7 3 1.0216E+01 -1.1083E+00 -1.9807E-01 7.8325E-01/
CHEB/ 1.1609E+00 1.1762E-01 -9.5707E-02 1.0928E-01 1.1551E-01/
CHEB/ -8.0290E-02 -1.0978E-01 3.7074E-04 -1.4830E-02 -6.0589E-02/
CHEB/ -2.8056E-02 6.9203E-03 -9.7259E-03 -1.3556E-02 7.6648E-03/
CHEB/ 6.6865E-03 -8.8244E-04/

! The following reactions allow plasma kinetics descriptions
E + E + AR+ <=> AR + E 1.414E+39 -4.500 0.00 ! Mansbach & Keck
TDEP/E/ REV/6.807E+31 -3.0 364218./ !electron temperature dependence

E + AR => AR + E 4.9E-7 0.162 8.7634E3
TDEP/E/ MOME !Momentum-transfer collision frequency
UNITS/KELVIN/

AR+ + AR => AR+ + AR 1.E-16 0.0 0.0 !units of cm^2
XSMI !Ion momentum-transfer collision cross-section

E + AR => AR + E 2.235E16 0.0 3.47E5
TDEP/E/ EXCI/11.60/ ! metastable excitation reaction
DUP

H2O+H = OH+H2 0.117E+10 1.30 3626
FORD /H2O 1.1/

END !END line is optional

```

3.6.3.1. Problems Having No Reactions

In some problems only information about the elements and species is needed (for example, chemical equilibrium computations). For these it is not necessary to include reaction data. The *Gas-phase Kinetics* Pre-processor will create the Linking File (for example, *chem.asc*), but it will not contain any reaction information. Therefore, no subroutines in the *Gas-phase Kinetics* Subroutine Library that deal with chemical reactions (for example, chemical production rates) may be used.

Table 3.8: Summary of the Rules for Auxiliary Reaction Data (p. 62) summarizes the rules for auxiliary reaction data.

Table 3.8: Summary of the Rules for Auxiliary Reaction Data

Rule	Description
1	Auxiliary information lines may follow reaction lines that contain an M to specify enhanced third-body efficiencies, a reversible reaction to specify the reverse rate parameters explicitly, or any reaction that specifies Landau-Teller parameters. Auxiliary information must follow any duplicate reactions as well as all reactions that indicate pressure-dependent behavior by (+M) (that is, provide fall-off parameters).
2	A species may have only one enhanced third body efficiency associated with it in any one reaction.
3	Only one radiation wavelength may be declared in a reaction.
4	The order in which the enhanced third body declarations are given is the order in which arrays of enhanced third body information are referenced in the subroutine package.
5	There cannot be more than ten enhanced third bodies in a reaction.
6	Keyword declarations may appear anywhere on the line, in any order.
7	Any number of keywords may appear on a line and more than one line may be used; however, a keyword and its parameter(s) must appear on the same line.
8	Keyword declarations that appear on the same line must be separated by at least one blank space.
9	Any blank spaces between a keyword and the first slash are ignored and any blanks between the slashes and parameter(s) are also ignored. However, no blank spaces are allowed within a keyword or a parameter.
10	All characters following an exclamation mark are comments.
11	In ion momentum-transfer collision cross-section reactions there must be exactly two reactant species, one of which must be an ion.
12	In electron momentum-transfer collision frequency reactions, there must be exactly two reactant species, one of which must be the electron.

3.6.4. Error Checks

The *Gas-phase Kinetics* Pre-processor checks each input line for proper syntax and writes diagnostic messages on logical file LOUT if errors are encountered. If an error condition occurs, the Pre-processor continues to read and diagnose the input, but an error flag is written to the Linking File and the *Gas-phase Kinetics* subroutine CKINIT will not initialize the work arrays. Therefore, the input must be error

free before any of the *Gas-phase Kinetics* subroutines can be called. The possibilities for an error condition are listed [Table 3.9: Error Checks \(p. 63\)](#).

Table 3.9: Error Checks

Data Type	Possible Errors
Element Data	Atomic weight for an element or isotope is not declared, and the element is not found in the Pre-processor's database.
	Atomic weight has been declared, but not enclosed by two slashes (/).
	If an element is declared twice, a diagnostic message is printed, but the duplicate is simply eliminated from consideration and is not considered a fatal error.
Species Data	If a species is declared twice, a diagnostic message is printed, but the duplicate is eliminated from consideration and is not considered a fatal error.
	No thermodynamic data have been found for a declared species.
Thermodynamic Data	Thermodynamic data are format sensitive and therefore provide possibilities for error if not formatted exactly as described by Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4) .
	An element in the thermodynamic data for a declared species has not been included in the element data.
	With the THERMO ALL option, line 2 (Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4)) is not found.
Reaction Data	A delimiter =>, <=>, or = between the reactants and the products is not found.
	Three Arrhenius parameters are not found.
	Reactants and/or products have not been properly delineated by a plus sign (+).
	A species as a reactant or product has not been declared in the species data.
	The reaction does not balance in elements.
	The reaction does not balance in electronic charge.
	A reaction is a duplicate not declared by the auxiliary data keyword DUP.
	A third-body species enclosed in parentheses in a fall-off reaction appears as reactant or product, but not both.
	A species is a third-body in a fall-off reaction, and +M also appears in the reaction.
	More than one +M or third body appear as reactants and/or products.
	There are more than six reactants or six products.

Data Type	Possible Errors
Auxiliary Reaction Data	There is an unknown or misspelled keyword or enhanced third-body species name.
	Parameters for a keyword are not enclosed in slashes.
	The wrong number of parameters appear for a keyword.
	There are duplicate keywords for a reaction.
	LOW, HIGH, TROE, SRI, PCHEB, TCHEB, or CHEB are found after a reaction that did not have a species or M in parentheses.
	LOW, HIGH, or CHEB is not found after a pressure-dependent reaction.
	A combination of TROE, SRI, CHEB and/or PLOG is found.
	LT and REV are found for a Landau-Teller reaction, but RLT is not found.
	LT is given for a fall-off reaction.
	There are more than ten enhanced third bodies.
	There are more than or less than two reactants specified with XSMI or MOME keywords.
	An ionic species is not specified as a reactant with the XSMI keyword.
	The electron is not a reactant when using the MOME keyword.
	USRPROG given for a USRPROD mechanism.
	USRPROG given for a reversible reaction.

Chapter 4: Surface Kinetics Input

The *Surface Kinetics* input file provides symbolic description of a surface reaction mechanism. Pre-processing this file requires obtaining information stored in the *Gas-phase Kinetics* linking file (for example, *chem.asc*) that was created from the gas-phase mechanism associated with the chemistry set. Pre-processing the *Surface Kinetics* input file results in the creation of an additional linking file (for example, *surf.asc*) that contains information about the surface mechanism and the species it involves. The information in the *Surface Kinetics* Linking File is subsequently accessed by the initialization routine in the *Surface Kinetics* Subroutine Library to store information in memory during a reacting-flow simulation. This stored information is then used to call other routines in the *Surface Kinetics* Subroutine Library to provide information on thermodynamic properties and chemical production rates.

The *Surface Kinetics* input includes information on surface sites (phases), surface species, bulk phases, bulk species, thermodynamic data, and the reaction mechanism. The order of data entry in the *Surface Kinetics* input file is: material name, site data, bulk data, thermodynamic data, reaction data, and a material-end statement. All input data is optional, but species included in reaction strings must be declared as site or surface species (or as gas species in the Gas Kinetics input file) and must have associated thermodynamic data included either directly in the *Surface Kinetics* input file or in a thermodynamic database file (for example, *therm.dat*). Such sets of information can be repeated for any number of different materials within the same *Surface Kinetics* input file. With the exception of the thermodynamic data, all input is format free. The syntax and rules for all of the data input is described in this chapter. The auxiliary keywords for surface reactions are described in [Table 4.6: Alphabetical Listing of Surface Reaction Auxiliary Keywords \(p. 78\)](#) and the options for specifying units on the REACTIONS line are described in [Table 4.3: Alphabetical Listing of REACTIONS-line Options for Surface Reaction Data \(p. 71\)](#). [Alphabetical Listing of Project Input Keywords \(p. 139\)](#) describes the meaning and usage of each keyword entry that may be included as part of a Reactor Model input file.

Note:

The *Surface Kinetics* Input File allows **259** columns for the presentation of the input data.

4.1. Material Declaration

Entirely different surface reaction mechanisms (that is, with different surface and bulk phases and species, and different surface reactions) can be specified in the same *Surface Kinetics* input file through the use of multiple materials. For multiphase chemistry, a material may contain liquid phase components. Both solids and liquid phase components can be included in the same material. At the beginning of each separate portion of the input file corresponding to a given material, you give an input line with the keyword MATERIAL followed by an optional space-delimited material name. If no name for the material is supplied, a default name MATERIAL **n** is provided, where **n** is the number of the material (for example, MATERIAL2 for the second material given in an input file). An example of the usage of multiple materials is given in [Figure 4.1: Examples of Material Declarations \(p. 66\)](#).

Figure 4.1: Examples of Material Declarations

```

!-----GAS-PHASE KINETICS PRE-PROCESSOR INPUT-----
ELEMENTS  SI CL E AL
SPECIES   E CL2+ CL+ SICL4 SICL2 CL

NOTE THAT ABOVE IS A CHEM.INP FILE, WHILE BELOW IS A SURF.INP FILE.

!-----SURFACE KINETICS PRE-PROCESSOR INPUT-----
MATERIAL WAFER
SITE/POLY/ SDEN/2.25e-9/
  SI(S)  SICL(S) SICL2(S) SICL3(S)
END
BULK SI(B)/2.33/
REACTIONS  MWOFF
  CL + SI(S)      => SICL(S)                1.0    0.0    0.0
  STICK
  E + CL2+ + 2SI(S) => 2SICL(S)            0.4    0.0    0.0
  BOHM
  E + CL+ + SICL3(S) + SI(B) => SICL4 + SI(S) 0.50   0.0    0.0
  BOHM
  ENRGDEP/1. 0.5 1.0/ UNITS/EVOLT/
  E + CL+ + #SICL3(S) + #SI(B) + SICL(S) &
    => SICL2(S) + #SICL2 + #SICL(S)        0.50   0.0    0.0
  BOHM
  YIELD/0.0712 1.21 0.5 1.0/ UNITS/EVOLT/
!      /A  Eth[eV] a b /  for #=A(Ei^a-Eth^a)^b
END
MATERIAL WALL
SITE/METAL/ SDEN/2.25E-9/
  AL(S)  ALCL(S)
END
REACTIONS  MWOFF
  CL+ + E        => CL                    0.6    0.0    0.0
  BOHM
  CL + AL(S)     => ALCL(S)              1.0    0.0    0.0
  STICK
END

```

4.2. Site Data

Surface-phase species exist on sites, and a site and its species must be identified on one or more lines of site data. The first line in a set of site data must start with the word **SITE** ; an optional name may be associated with a site if it immediately follows **SITE** and is delimited by slashes (/). If no name for the site is supplied, a default name **SITE n** is provided, where **n** is the number of a site (for example, **SITE2** for the second site type listed). Following **SITE** and/or the site name, the word **SDEN** and a slash-delimited density (the standard state site density for this site, in mole/cm²) for the site is required.

The optional keyword **INTERFACE** can be used to specify the phases (homogeneous phases such as the gas phase and the bulk phases) that share the surface site phase (see the example in [Figure 4.2: Examples of Site Data \(p. 67\)](#)). The **INTERFACE** keyword is slash (/)-limited and must follow immediately after the **SDEN** keyword. A list of at least one but no more than two interfacing phases can be assigned to a surface site phase. The first phase of the list is the primary neighbor phase; if the temperature of the surface site phase is not given explicitly, the temperature of the primary neighbor phase will be assigned to the site phase. The **INTERFACE** keyword is utilized only by the multiphase reactor models.

The species that can reside on the site type are declared by a list of species symbols (names) on the same line or on additional lines.

Note:

The name of a site species must not duplicate the name of a gas-phase species or a bulk species, and must be unique among the site species for all materials.

An optional slash-delimited site occupancy number may follow a species name, that is, the number of individual sites that this species occupies. (For example, a large chemical species might cover two or more sites.) The default site occupancy for a surface species is 1. The sets of SITE data input can continue for as many site types as are needed.

Any set of up to sixteen upper- or lower-case characters can be used as a site name or species symbol. In addition, each species must be composed of elements that have been identified in the *Gas-phase Kinetics* Pre-processor and thus contained in the *Gas-phase Kinetics* Linking File. One of the purposes of the site data is to define the order in which arrays of site species information are referenced in the *Surface Kinetics* Subroutine Library.

Note:

Species symbols may not begin with a number, a plus sign (+), a pound sign (#), or an equality sign (=), have imbedded blanks, or include a slash (/). An ionic species may end with any number of plus or minus signs; an imbedded plus sign must be enclosed in parentheses.

Any line starting with or any portion of a line following an exclamation mark (!) is considered a comment and will be ignored. Blank lines are also ignored. [Figure 4.2: Examples of Site Data \(p. 67\)](#) shows sample site data. The rules for site data are summarized in [Table 4.1: Summary of the Rules for Site Data \(p. 68\)](#).

For multiphase chemistry, sites can be defined for the liquid surface using the same format used for the solid surface, as described in the preceding paragraphs.

Figure 4.2: Examples of Site Data

```

SITE / PLANE /          SDEN/1.04E-9/  ! PLANAR SITE
  ASH(V)                ! FIRST SPECIES ON PLANE SITE
  ASH2(V) ASH3(V) H(S) CH3(V) AS(V) AS2(V)/2/
  V                      ! EMPTY PLANAR SITE
END                      ! AN END STATEMENT IS OPTIONAL
SITE / LEDGE /          SDEN/1.66E-10/  ! LEDGE SITE
  GACH(L)               ! FIRST SPECIES ON LEDGE
  DMG(L)/2/             ! THIS SPECIES OCCUPIES 2 SITES
  L                      ! EMPTY LEDGE SITE
SITE SDEN/1.0E-10/ GA(S) ! SITE WITH ONLY ONE SPECIES
                        ! SITE NAME NOT INCLUDED

SITE/ANODE_GAS/ SDEN/0.00004062194/  INTERFACE/ANODE Gas/ ! INTERFACE SITE SPECIFIED
                                           ! SITE "ANODE_GAS" IS THE INTERFACE
                                           ! BETWEEN THE BULK PHASE "ANODE" AND
                                           ! THE "Gas" PHASE

H(*)/1/
PT(*)/1/
END

```

```

BULK /ANODE/
PT(B)
END

```

Table 4.1: Summary of the Rules for Site Data

Rule	Description
1	Site data must start with a line containing the word SITE, followed by an optional slash-delimited name (that is, SITE/ name /).
2	The standard state site density is required as a slash-delimited number (in mole/cm ²) following the word SITE and/or the site name, and preceded by the word SDEN.
3	The site density is followed by one or more site species name declarations. Declaring a site with no site species is an error.
4	Site and species names are composed of up to sixteen upper- or lower-case character symbols. The names cannot begin with the characters +, =, #, or a number; an ionic species name may end with one or more + or - signs; an embedded plus sign must be enclosed in parentheses (+). Names cannot include a slash (/).
5	All species names should be unique; duplicate species names will be ignored and a warning issued. A species name may not duplicate a name of a gas-phase species, another surface species, or a bulk species.
6	A site name must not duplicate the name of any other phase (gas, surface site, or bulk phase).
7	Each surface species that subsequently appears in a surface reaction must have been declared in this section.
8	A site species name may appear anywhere on the line.
9	A site species may have a slash-delimited site occupancy (the number of sites that this species occupies on the surface) following the species name.
10	A species name declaration that begins on one line may not continue to the next line (that is, do not break a species name into two lines).
11	There may be more than one set of SITE data.
12	All characters on a line following an exclamation mark are considered comments.
13	SITE data are not required.

4.3. Bulk Data

A set of bulk data may consist of one or more condensed-phase species. The first line in a set of bulk data must start with the word BULK and may be followed by an optional slash-delimited name for the bulk phase. If a name is not supplied for bulk phase n , then the name BULK n is supplied. Bulk species are declared by a list of unique species symbols (names) on the same line or on additional lines. An optional slash-delimited density (in g/cm³) may follow a species name. If no density is supplied, the unphysical value of -1.0 is stored as a flag. The rules for bulk species symbols (names) are essentially

the same as those for site species. [Figure 4.3: Examples of Bulk Data \(p. 69\)](#) shows sample bulk data. The rules for bulk data are summarized in [Table 4.2: Summary of the Rules for Bulk Data \(p. 69\)](#).

For multiphase chemistry, the liquid phase is defined by including the keyword LIQUID in the bulk definition. An example is shown in [Figure 4.4: Examples of Bulk Data for Liquid Phase \(p. 70\)](#). Unlike the solid phase, the density for liquid is obtained from the properties data in the LIQPROPERTIES block. The properties are described in [Liquid Species in the Chemkin Theory Manual](#).

Table 4.2: Summary of the Rules for Bulk Data

Rule	Description
1	Bulk data must start with a line containing the word BULK, and may be followed by a slash-delimited name for the bulk phase (that is, BULK/ name /).
2	The BULK declaration and/or bulk name must be followed by one or more bulk species declarations. Declaring a bulk phase with no bulk species is an error.
3	Bulk and bulk species names are composed of up to sixteen upper- or lower-case character symbols. The names cannot begin with the +, =, #, or a number; an ionic species name may end with one or more + or - signs; an embedded plus sign must be enclosed in parentheses (+). Names cannot include a slash (/).
4	All species names should be unique; duplicate species names will be ignored and a warning issued. A species name may not duplicate a name of a gas-phase species, a surface species, or another bulk species.
5	All phase names must be unique. For example, a bulk phase name may not duplicate the name of any other phase (gas, surface site, or bulk phase).
6	Each bulk species that subsequently appears in a surface reaction must have been declared in this section.
7	A bulk species declaration may start anywhere on the line.
8	A bulk species name may be followed by an optional slash-delimited mass density (in g/cm ³).
9	A bulk species declaration that begins on one line may not continue to the next line (that is, do not break species names into two lines).
10	There may be more than one set of BULK data.
11	All characters on a line following an exclamation mark are considered comments and are ignored.
12	BULK data are not required.

Figure 4.3: Examples of Bulk Data

```

BULK / GA_RICH / GA2AS(1)/3.0/ GA3AS(1)/3.0/      END
                                           !an END statement is optional

BULK / GA_RICH /
GA2AS(1)/3.0/
GA3AS(1)/3.0/
GA2AS(1)/2.0/      !THIS NAME IS A DUPLICATE AND WILL BE IGNORED
BULK AS(B)          !BULK PHASE WITH NO NAME SUPPLIED
                   !ONLY ONE BULK SPECIES AND NO DENSITY SUPPLIED
END

```

Figure 4.4: Examples of Bulk Data for Liquid Phase

```
BULK /jetFuel/ LIQUID      !Keyword LIQUID specifies the phase. Bulk name here is jetFuel
nc12h26(l) c6h12-1(l) nc6h14(l) !species included in this liquid phase
END
```

4.4. Thermodynamic Data

Any chemical species that appears in a problem must have thermodynamic data associated with it. This data is used in evaluation of thermodynamic properties (entropy, enthalpy, heat capacity) and reverse reaction rate constants through the equilibrium constant. Often thermodynamic data for a species, for instance a surface species, is unknown. Such data can sometimes be calculated via theoretical techniques. However, the user can work around the need for actual thermodynamic data for all species by making the reactions irreversible. In this case, the user can supply " placeholder" thermodynamic data for the surface species to satisfy the requirement.

Note:

If every reaction in the mechanism is either irreversible, or if Arrhenius rate parameters are given explicitly for the reverse reaction, then the thermodynamic data for species are not actually used for anything related to the kinetics. They may, however, be used in surface heat balances if such are enabled for a particular reacting-flow problem.

The data may be extracted from a database file (for example, *therm.dat*) and/or read directly from the *Surface Kinetics* input file. Details on the thermodynamic data format, whether including in the *Surface Kinetics* input file or in a thermodynamic database file, are provided in [Thermodynamic Data Format \(p. 3\)](#) .

For multiphase chemistry, thermodynamic data are given in a different form described in [Liquid Species in the Chemkin Theory Manual](#) . Properties for all the liquid species defined in SITE and BULK must have corresponding data in the LIQPROPERTIES block.

Note:

When thermodynamic data is included in the *Surface Kinetics* Input file, it must immediately follow phase (SITE and BULK) data.

4.5. Reaction Mechanism Description

The surface reaction mechanism may consist of any number of chemical reactions involving the solid species named in the site and bulk data, as well as the gas-phase species declared in the *Gas-phase Kinetics* input file. A reaction may be reversible or irreversible. Reaction data must start with a line containing the word REACTIONS (or REAC). The lines following the REACTIONS line contain reaction descriptions together with their Arrhenius rate coefficients. The reaction description is composed of reaction data and perhaps optional auxiliary reaction data.

4.5.1. REACTIONS Line Options

On the same line as the REACTIONS word, you may define certain options that will apply globally to all surface reactions. In some cases, Auxiliary Reaction Keywords given for a specific reaction may override these global settings. A summary of the REACTIONS -line options are provided in [Table 4.3: Alphabetical Listing of REACTIONS-line Options for Surface Reaction Data \(p. 71\)](#).

Note:

Even if the default energy units are changed by giving one of these keywords, the temperature appearing in the Arrhenius expression of [Equation 3.5](#), that is, in T raised to the β power and in the denominator of the activation energy term, is still in Kelvins.

Note:

If units are not specified, A_i and E_i are assumed to be in (cm, mole, sec, K) and cal/mole, respectively.

Table 4.3: Alphabetical Listing of REACTIONS-line Options for Surface Reaction Data

Keyword	Definition
ATM	Supersedes the default units for all surface reactions that follow the REACTIONS header line for pre-exponential factors A_i ; the units of gas species are partial pressures in atm.
	Notes Default units for A_i are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.
BAR	Supersedes the default units for all surface reactions that follow the REACTIONS header line for pre-exponential factors A_i ; the units of gas species are partial pressures in bar.
	Notes Default units for A_i are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.
CAL/[MOLE]	Re-iterates the default units for all surface reactions that follow the REACTIONS header line for parameters with energy units such as E_i .
	Notes Default units for E_i are cal/mole.

Keyword	Definition
DYN[ES]	Supersedes the default units for all surface reactions which follow the REACTIONS header line for pre-exponential factors A_i ; the units of gas species are partial pressures in dyne/cm ² .
	Notes Default units for A_i are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.
EVOL[TS]	Supersedes the default units for all surface reactions which follow the REACTIONS header line for parameters with energy units such as E_i .
	Notes Default units for E_i are cal/mole.
JOUL[ES/MOLE]	Supersedes the default units for all surface reactions which follow the REACTIONS header line for parameters with energy units such as E_i .
	Notes Default units for E_i are cal/mole.
KCAL[/MOLE]	Supersedes the default units for all surface reactions which follow the REACTIONS header line for parameters with energy units such as E_i .
	Notes Default units for E_i are cal/mole.
KELV[INS]KCAL/MOLE	Supersedes the default units for all surface reactions which follow the REACTIONS header line for parameters with energy units such as E_i .
	Notes Default units for E_i are cal/mole.
KJOU[LES/MOLE]	Supersedes the default units for all surface reactions which follow the REACTIONS header line for parameters with energy units such as E_i .

Keyword	Definition
	Notes Default units for E_i are cal/mole.
MAXSP	Increases the maximum number of reactants or products allowed in a reaction. The number given by this keyword must be greater than the default limit of 6. For example, REACTIONS MAXSP=11. Notes This keyword is available to both the gas-phase and surface reaction mechanism.
MOLEC[ULES]	Supersedes the default units for all surface reactions which follow the REACTIONS header line for pre-exponential factors A_i . Notes Default units for A_i are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.
MOLE[S]	Re-iterates the default units for all surface reactions which follow the REACTIONS header line for pre-exponential factors A_i . Notes Default units for A_i are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.
MWOFF	Turns off the Motz-Wise correction of Equation 4.15 of the Chemkin Theory Manual for all sticking-coefficient reactions which follow the REACTIONS header line. Notes By default, the Motz-Wise correction is off for all sticking coefficient reactions; the default may be superseded for a particular sticking-coefficient reaction by use of the auxiliary reaction keyword MWOFF (p. 84) or MWON (p. 84) .
MWON	Turns on the Motz-Wise correction of Equation 4.15 of the Chemkin Theory Manual for all sticking-coefficient reactions which follow the REACTIONS header line. Notes By default, the Motz-Wise correction is off for all sticking coefficient reactions; the default may be superseded for a particular

Keyword	Definition
	sticking-coefficient reaction by use of the auxiliary reaction keyword MWOFF (p. 84) or MWON (p. 84) .
NONCON	Allows non-conservation of sites in any surface reaction which follows the REACTIONS header line. Normally, any reaction that does not conserve the number of surface sites in each surface phase is considered to be in error; the inclusion of NONCON on the REACTIONS line supersedes that rule.
PAS[CA]LS]	Supersedes the default units for all surface reactions that follow the REACTIONS header line for pre-exponential factors A_i ; the units of gas species are partial pressures in pascals.
	Notes Default units for A_i are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.
SITE[FR]	Supersedes the default units for all surface reactions which follow the REACTIONS header line for pre-exponential factors A_i ; the units of surface species are site fraction and the reaction rate unit is 1/sec.
	Notes Default units for A_i are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.
TOR[R]	Supersedes the default units for all surface reactions which follow the REACTIONS header line for pre-exponential factors A_i ; the units of gas species are partial pressures in torr.
	Notes Default units for A_i are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.
USRPROD	The net rate-of-production for all species will be obtained by calling a user-supplied subroutine, SKUPROD. An optional slash(/)-delimited integer parameter allows the user to select from more than one type of rate formulation. Wherever the net rates of production of species are required, they will be obtained by calling the user-written subroutine. A template of SKUPROD is provided in the Ansys Chemkin installation, in the file <i>sklib_user_routines.f</i> located in the directory <i>user_subroutines</i> . Information about how to compile and link user routines into Chemkin is included in Chemkin Application Programming Interface Manual .

Keyword	Definition
	Notes USRPROD cannot be used in conjunction with USRPROG (p. 87) (entered after a particular reaction).

Note:

Chemkin does not support user-written programs, so you are cautioned to use the SKUPROD user routine feature at your own risk. Also, there are some features in the program executables that will be incompatible with the global replacement of species rates of production, such as sensitivity analysis and rate-of-production analysis. Such features will return zero values when user-rate programming is encountered.

4.5.2. Reaction Data

Each reaction entry is divided into two fields, (an entry may use multiple lines if it is more than 80 characters long). A reaction data entry is continued on the next line using the special character "& " at the end of the line; any information following the & symbol on the same line is ignored. The first field in the reaction entry contains the symbolic description of the reaction, while the second contains the Arrhenius rate coefficients. Both fields are format free, and blank spaces are ignored. All characters on a line following an exclamation mark (!) are considered comments and are ignored. Blank lines are also ignored.

The reaction description, given in the first field, must be composed of the species symbols, coefficients, and delimiters as summarized below.

Note:

Ansys Chemkin 2021 R2 supports limited choice of rate formulations. All liquid and gas-liquid reactions are assumed to be volumetric. Inter-phase reactions involving liquid and solid surface are not supported in 2021 R2.

Reactions for multiphase chemistry follow the same format as described in this section for solid surface reactions. Like solid surface reactions, liquid species can react with gas species, species from the same bulk, and species from other bulks from the same material defined in the kinetics input.

Table 4.4: Surface Reaction Data Criteria

Species Symbols	
	Each species in a reaction is described with the unique sequence of characters as they appear in the species data and the thermodynamic data.
Coefficients	
	A species symbol may be preceded by an integer or real coefficient. The coefficient has the meaning that there are that many moles of the particular species present as either reactants or products; for example, 2OH is equivalent to OH +OH. The "# " symbol is used to mark stoichiometric coefficients that

Species Symbols	
are additionally multiplied by a YIELD coefficient. This is explained in Auxiliary Reaction Data (p. 78) .	
Delimiters	
+	A plus sign is the delimiter between each reactant species and each product species.
=	An equality sign is the delimiter between the last reactant and the first product in a reversible reaction.
<=>	An equality sign enclosed by angle brackets can also be used as the delimiter between the last reactant and the first product in a reversible reaction.
=>	An equality sign with an angle bracket on the right is the delimiter between the last reactant and the first product in an irreversible reaction.

The second field of the reaction line is used to define the Arrhenius rate coefficients A_i , β_i , and E_i in that order, as given by [Equation 3.5](#) of the [Chemkin Theory Manual](#) . At least one blank space must separate the last species name in the reaction and first number. The three numbers must be separated by at least one blank space, be stated in either integer, floating point, or "E" format (for example, 123 or 123 . 0 or 12 . 3E1), and have units associated with them (although the units do not appear on the input line). Unless modified by the REACTIONS line or by the UNITS auxiliary keyword, the default units for A_i are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction. The factor β_i is dimensionless. The default units for the activation energies are cal/mole.

The second field of the reaction line may optionally be used to specify the coefficients a_i , b_i , and c_i of [Equation 4.10](#) of the [Chemkin Theory Manual](#) for a sticking coefficient. In order for the second field to apply to sticking coefficient parameters, the next line of input must contain the auxiliary keyword STICK.

Examples of some reaction data are shown in [Figure 4.5: Examples of Reaction Data \(p. 76\)](#) . [Table 4.5: Summary of the Rules for Reaction Data \(p. 76\)](#) summarizes the reaction data rules.

Figure 4.5: Examples of Reaction Data

```

REACTIONS  KCAL/MOLE  NONCON
ASH3 + AS(P) <=> ASH3(P) + AS(D)      4.0E11   0 25   ! Ref. 21
! ASH3 + AS(P) <=> ASH3(P) + AS(D)      4.0E11   0 0   ! same as previous
ASH <=> AS(D) + H(S)      1.0   0 0
      STICK
GA(CH3)3(L) + GA2AS(A) <=> AS + GA(CH3)(L) + 2 GAME & ! continued on next line
                                1.0E13   0 4000.

```

Table 4.5: Summary of the Rules for Reaction Data

Rule	Description
1	The first reaction line must start with the word REACTIONS (or REAC), and may be followed by units definition(s), the word MWON, MWOFF, NONCON, or the word USRPROD.
2	The word MWOFF can be used to turn off the Motz-Wise correction of Equation 4.15 of the Chemkin Theory Manual , for all sticking-coefficient reactions, or the word MWON can be used to specify that the Motz-Wise

Rule	Description
	correction is to be used for all sticking-coefficient reactions (the default). Including MWOFF or MWON as an auxiliary keyword for an individual reaction (discussed later) will override the setting given on the REACTIONS line.
3	Valid unit declarations are EVOLTS, KELVINS, CAL/MOLE, KCAL/MOLE, JOULES/MOLE, KJOULES/MOLE, MOLES, MOLECULES, SITEFR, ATM, BAR, DYN, TOR, and PASCAL.
4	The word NONCON is required on the first reaction line if any of the reactions do not conserve the number of surface sites of a given type.
5	The reaction description can begin anywhere on this line. All blank spaces, except those separating the Arrhenius coefficients, are ignored.
6	Each reaction description must have =, <=>, or => between the last reactant and the first product.
7	Each species in a reaction is described with a unique sequence of characters (name) as they appear in the species data and the thermodynamic data. However, if a species name is not unique (because it is duplicated in another phase), the name must be modified by appending its slash-delimited phase name: as name / phase /.
8	Stoichiometric coefficients are represented by an integer or real number preceding a species name. The default is to assume a stoichiometric coefficient of 1. The "# " symbol preceding the stoichiometric coefficient denotes a coefficient which is additionally multiplied by a "yield" multiplier.
9	A reaction description may be contained on more than one line. If a line contains the symbol &, all information following the & symbol will be ignored and the next line will be considered a continuation of the first.
10	Three Arrhenius coefficients must appear in order (A_i , β_i , and E_i) on each Reaction line, separated from each other and from the reaction description by at least one blank space; no blanks are allowed within a number.
11	There cannot be more than six reactants or six products in a reaction.
12	To specify a sticking coefficient rather than a rate constant the three numbers after the reaction description have the meaning a_i , b_i , and c_i (see Equation 4.10 of the Chemkin Theory Manual) and the auxiliary reaction data word STICK must appear on the next line of input. To use this option the reaction must have only one gas-phase species as a reactant and its stoichiometric coefficient must be 1.
13	All characters on a line following an exclamation mark are comments.
14	For best results, an END statement should follow reaction input.

4.5.2.1. Vapor-Liquid Phase Transfer

For liquid species to participate in the vapor-liquid phase transfer process, they must be mapped one-to-one. This mapping is provided in the form of a unimolecular reaction, as shown in [Figure 4.6: Examples of Reaction Data for Liquid Phase \(p. 78\)](#). Each reaction must be followed by the auxiliary data line VLE. The model for handling the vapor-liquid equilibrium (VLE) levels is defined by the keyword IDEAL or HENRY on the same line. Additional auxiliary inputs are described next. The three parameters specified as the reaction rate coefficients follow the Arrhenius form. However,

they are used as a multiplier to the actual rate of mass transfer between the phases. We recommend using the value of 1.0 0.0 0.

Figure 4.6: Examples of Reaction Data for Liquid Phase

```
REACTION
nc12h26(l) = c6h12-1(l) + nc6h14(l)          5.4E+13  0  57907. !volumetric reaction in liquid bulk
! Vapor Liquid transfer steps - must have one species from liquid and gas on either side of the reaction step.
! Keyword VLE provides equilibrium model; KMASS can be used to explicitly provide mass transfer rate constant.
! Rates of phase change are controlled by mass transfer models in Chemkin reactor.
nc12h26(l) = nc12h26      1.0  0.0  0.  !Mass transfer rate multiplier
VLE / IDEAL/                      !IDEAL = Raoult's law, HENRY = Henry's law
nc6h14(l) = nc6h14      1.0  0.0  0.
VLE / IDEAL/
c6h12-1(l) = c6h12-1      1.0  0.0  0.
VLE / IDEAL/
END
```

4.5.3. Auxiliary Reaction Data

Auxiliary information appears on one or more separate lines after the reaction data line is read, and serves to modify or give additional parameters needed to evaluate that reaction's rate expression. The format in an auxiliary information line is a character string keyword followed by a slash-delimited (/) field containing an appropriate number of parameters (either integer, floating point, E format, or character). Examples of many of the auxiliary options described in this section are shown in [Figure 4.7: Examples of Auxiliary Reaction Data \(p. 90\)](#). [Table 4.6: Alphabetical Listing of Surface Reaction Auxiliary Keywords \(p. 78\)](#) provides detailed information on the meaning and usage of each auxiliary keyword entry that may be included as part of the Surface Reaction Data.

Auxiliary reactions for multiphase chemistry follow the similar format as specified above. Liquid-phase-specific data are described in [Table 4.7: Auxiliary Keywords for Liquid Phase Reactions \(p. 88\)](#). An example of the use of these data in a multiphase kinetics input file is shown in [Figure 4.8: Examples of Auxiliary Reaction Data for Liquid Phase \(p. 90\)](#).

Table 4.6: Alphabetical Listing of Surface Reaction Auxiliary Keywords

Keyword	Definition				
BOHM	Bohm Velocity Limit for Ions - Applies the Bohm velocity correction for a reaction involving a positive ionic species (see Equation 4.29 of the Chemkin Theory Manual). No auxiliary parameters are required.				
	Reaction Example	CL+ + E	=> CL	0.4	0.0
		0.0			
	BOHM				
	Notes	• The three coefficients given in the second field of the reaction line are interpreted as the parameters a_i, b_i, c_i, in Equation 4.29 of the Chemkin Theory Manual). • The reaction can have only one gas-phase reactant species, which must be a positive ion, and its stoichiometric coefficient must be 1.			

Keyword	Definition			
COV	Coverage Dependent Reactions - Modifies the expression for the forward rate constant by coverage parameters (see Equation 4.7 of the Chemkin Theory Manual). Must be followed by (slash delimited) surface species name and the three parameters η_{ki} , μ_{ki} and ε_{ki} .			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	COV /Pt(S) 0.0 0.0 0.9/
	Coverage parameter η_{ki}	Required	--	COV /Pt(S) 0.0 0.0 0.9/
	Coverage parameter μ_{ki}	Required	--	COV /Pt(S) 0.0 0.0 0.9/
	Coverage parameter ε_{ki}	Required	cal/mole	COV /Pt(S) 0.0 0.0 0.9 /
	Reaction Example	O(S) +O(S) =>Pt(S) +Pt(S) +O2 3.700E+23 0.0 213.0 COV/O(S) 0.0 0.0 -93.3/		
	Notes	More than one set of COV data can appear for a given reaction, and these would be applied multiplicatively as in Equation 4.7 of the Chemkin Theory Manual .		
DCOL	The reaction rate is proportional to the collision frequency between a gas molecule and a particle surface (see Equation 19.79 of the Chemkin Theory Manual). Must be followed by the (slash delimited) collision-diameter of the gas-phase reactant.			
	Parameters	Optional/Reqd.	Units	Examples
	Collision diameter	Required	cm	DCOL / 2.45E-8 /
	Reaction Example	A1 + 8H(se) => 5H(se) + 6C(B) + 3open(se) + 4H2 + H 0.1 0.0 0.0 FORD/H(se) 2.0/ DCOL/2.46E-8/ STICK		
	Notes	- The reaction must be irreversible. - The reaction may have only one gas-phase.		
	DUP	Duplicate Reactions - Two or more reactions can involve the same set of reactants and products, but proceed through distinctly different processes. In these cases, it may be appropriate to state a reaction mechanism that has two or more reactions that are the same, but have different rate parameters. However, duplicate reactions are normally considered errors by the <i>Surface Kinetics</i> Pre-Processor. If the user requires duplication (for example, the same reactants and products with different Arrhenius parameters), keyword DUP must follow the reaction line of		

Keyword	Definition			
	each duplicate reaction (including the first occurrence of the reaction that is duplicated). For example, if the user wishes to specify different rate expressions for each of two identical reactions, there must be two occurrences of the DUP keyword, one following each of the reactions. No auxiliary parameters are required.			
	Reaction Example	02 + 2PT(S) => 20(S) 1.80E+21 -0.5 0.0 DUP 02 + 2PT(S) => 20(S) 0.023 0.00 0.00 DUP		
	Notes	DUP is required for each of any duplicated reaction in the mechanism.		
ENRGDEP	Ion-energy Dependent Rates - Allows the rate constant to depend on ion energy according to Equation 4.30 of the Chemkin Theory Manual . ENRGDEP must be followed by the three (slash delimited) $E_{ion,0}$, f_i , and g_i .			
	Parameters	Optional/Reqd.	Units	Examples
	Threshold energy $E_{ion,0}$	Required	cal/mole	ENRGDEP / 1.0 0.5 1.0/
	Exponential constant f_i	Required	--	ENRGDEP /1.0 0.5 1.0/
	Exponential constant g_i	Required	--	ENRGDEP /1.0 0.5 1.0 /
	Reaction Example	E + CL+ + SICL3(S) + SI(B) => SICL4 + SI(S) 0.50 0.0 0. BOHM ENRGDEP/1. 0.5 1.0/ UNITS/EVOLT/		
	Notes	- There must be exactly one positive ionic reactant species in the reaction. - Only irreversible reactions are allowed with this option.		
FORD	Arbitrary Reaction Orders - Supersedes the forward reaction order for any species in the mechanism (with respect to species concentration), regardless of whether the species appears as a reactant or a product in the reaction. FORD is followed, in slash-delimited format, by the species name and the new reaction order. This option overrides the values of ν_{ki} in Equation 3.4 of the Chemkin Theory Manual pertaining to the particular species named on the line; the reaction order for all other species is maintained at the default values.			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	FORD / Pt(S) 1.0/

Keyword	Definition			
	<i>Stoichiometric coefficient</i>	Required	--	FORD /Pt(S) 1.0/
	Reaction Example	A1 + 8H(se) => 5H(se) + 6C(B) + 3open(se) + 4H2 + H 0.1 0.0 0.0 FORD/H(se) 2.0/ DCOL/2.46E-8/ STICK		
	Notes	• Multiple occurrences of the FORD construct may appear on the auxiliary line.		
KPRODUCT	K-Product - K-product for reversible ionization reaction in liquid/aqueous phase – specifies the value of K-product as a function of temperature on which the reaction takes place. The definition of the K-product can be found in Given K-Product for Ion Dissociation Reactions in the Liquid Phase in the Chemkin Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	Temperature polynomial coefficient a_0	Required	--	KPRODUCT/ 1.0E-14 0.0 0.0 0.0/
	Temperature polynomial coefficient a_1	Required	--	KPRODUCT/1.0E-14 0.0 0.0 0.0/
	Temperature polynomial coefficient a_2	Required	--	KPRODUCT/1.0E-14 0.0 0.0 0.0/
	Temperature polynomial coefficient a_3	Required	--	KPRODUCT/1.0E-14 0.0 0.0 0.0/
	Reaction Example	HOCHO(aq) = H+ + HC02- 3.6E06 0.0 0.0 KPRODUCT /1.77e-04 0.2 0.003 -0.0001 /		
	Notes	• The ionization reaction must be a liquid-phase reversible reaction and the product species must belong to the same phase. When more than one KPRODUCT keyword is given for a reaction, the parameters from the last one will be applied.		
LANG	Langmuir-Hinshelwood Reaction Parameters - Indicates the use of the Langmuir-Hinshelwood rate expression. One auxiliary line should be supplied for each species appearing in the denominator of Equation 4.21 of the Chemkin Theory Manual . The keyword is followed, in slash delimited format, by the species name, the pre-exponential multiplier, the temperature factor, the enthalpy for			

Keyword	Definition			
	the equilibrium constant, and the reaction order for that species (usually equal to one). The equilibrium constant is defined as $K=AT^{\beta}\exp(-H/RT)$, similar to the standard expression for rate constants.			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	LANG /C6H6 1.26 0.0 0.0 1.0/
	Pre-exponential factor A	Required	Depends on reaction	LANG /C6H6 1.26 0.0 0.0 1.0/
	Temperature exponent β	Required	--	LANG /C6H6 1.26 0.0 0.0 1.0/
	Equilibrium enthalpy H	Required	cal/mole	LANG /C6H6 1.26 0.0 0.0 1.0/
	Reaction order	Required	--	LANG /C6H6 1.26 0.0 0.0 1.0 /
	Reaction Example	C6H5CH3 + H2 => C6H6 + CH4 2.507E-8 0.0 0.0 ! rate at 600C LANG /C6H6 1.26 0.0 0.0 1.0/ LANG /C6H5CH3 1.01 0.0 0.0 1.0/ LHDE /1/ LHNU /C6H5CH3/ LHPR /atm/		
	Notes	- Only irreversible reactions are allowed with this option. - Each species listed in a LHNU (p. 83) statement must have a LANG statement. - Additional keywords LHDE (p. 82) , LHNU (p. 83) , and LHPR (p. 83) provide more flexibility in the form of the Langmuir-Hinshelwood or Eley-Rideal rate expressions.		
	LHDE	Langmuir-Hinshelwood Denominator Exponent Parameter - Allows the default value of 2 for the overall exponent for the denominator (m) to be overridden when LANG (p. 81) is used to specify a Langmuir-Hinshelwood rate expression. To specify an Eley-Rideal reaction, this keyword would be used and m set to 1. The use of any positive number is permitted, including real or fractional numbers.		
	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition					
	<i>Denominator exponent m</i>	Required	--	LHDE /1/		
	Reaction Example	C6H5CH3 + H2 => C6H6 + CH4 2.507E-8 0.0 0.0 ! rate at 600C LANG /C6H6 1.26 0.0 0.0 1.0/ LANG /C6H5CH3 1.01 0.0 0.0 1.0/ LHDE /1/ LHNU /C6H5CH3/ LHPR /atm/				
LHNU	Allows the explicit inclusion of equilibrium constants in the numerator of the LANG (p. 81) rate expression (the use of <i>k</i> rather than <i>k'</i> , see Langmuir-Hinshelwood and Eley-Rideal Reactions of the Chemkin Theory Manual) when LANG (p. 81) is used to specify a Langmuir-Hinshelwood rate expression. This keyword is followed by a slash delimited list of species names. For each species in the list, a multiplier of <i>K</i> will be applied to the rate constant.					
	Parameters	Optional/Reqd.	Units	Examples		
	<i>Species name</i>	Required	--	LHNU /C6H5CH3/		
	Reaction Example	C6H5CH3 + H2 => C6H6 + CH4 2.507E-8 0.0 0.0 ! rate at 600C LANG /C6H6 1.26 0.0 0.0 1.0/ LANG /C6H5CH3 1.01 0.0 0.0 1.0/ LHDE /1/ LHNU /C6H5CH3/ LHPR /atm/				
	Notes	• Each species listed in a LHNU statement must have a LANG (p. 81) statement.				
LHPR	Indicates that the equilibrium constants are given in pressure units when LANG (p. 81) is used to specify a Langmuir-Hinshelwood rate expression. The LHPR (p. 83) keyword will affect the equilibrium constants for the specified reaction only; the reaction rate will still be assumed to be in the units specified on the REACTIONS line, or in the default moles, cm, and sec. The keyword is followed by the slash-delimited name of the pressure unit being used: ATM, BAR, TORR, PASC (for Pascals), or DYNE (for dynes per square cm), where the names are not case sensitive.					

Keyword	Definition					
	Parameters	Optional/Reqd.	Units	Examples		
	Pressure units character string	Required	--	LHPR /atm/		
	Reaction Example	C6H5CH3 + H2 => C6H6 + CH4 2.507E-8 0.0 0.0 ! rate at 600C LANG /C6H6 1.26 0.0 0.0 1.0/ LANG /C6H5CH3 1.01 0.0 0.0 1.0/ LHDE /1/ LHNU /C6H5CH3/ LHPR /atm/				
MWOFF	Motz-Wise Correction - Turns off the Motz-Wise correction of Equation 4.15 of the Chemkin Theory Manual for a sticking-coefficient reaction.					
	Reaction Example	AR* => AR 1.0 0.0 0.0 STICK MWOFF				
	Notes	By default, the Motz-Wise correction will be off for all sticking coefficient reactions; the default may be changed by including the keyword MWON (p. 73) on the REACTIONS line.				
MWON	Motz-Wise Correction - Turns on the Motz-Wise correction of Equation 4.15 of the Chemkin Theory Manual for a sticking-coefficient reaction, superseding the default. By default the Motz-Wise will be off for all reactions using sticking coefficients unless the MWON keyword is given on the REACTIONS line, in which the new default will be to include the correction term.					
	Reaction Example	ALMe3 + 0(S) => ALMe2(S) + 0.5C2H6 0.1 0.0 0.0 STICK MWON				
	Notes	By default, the Motz-Wise correction will be off for all sticking coefficient reactions; the default may be changed by including the keyword MWON on the REACTIONS line.				
NATIVE	Indicates the native species of a particle; see Native Surface Sites of the Chemkin Theory Manual .					
	Reaction Example	OPEN(S) /NATIVE/				

Keyword	Definition			
NUCL	Supersedes the default rate calculation with the nucleation reaction rate expression; see Nucleation Reaction Data of the Chemkin Theory Manual .			
	Reaction Example	2A4 => 32C(B) + 20 H(se) + 28.72 open(se) 1.0E10 0.5 0.0 NUCL		
REV	Reverse Reaction Parameters - Supersedes the reverse rates that would normally be computed through the equilibrium constant, Equation 3.6 of the Chemkin Theory Manual . REV must be followed by the three slash-delimited Arrhenius coefficients (A_i , β_i , and E_i) to specify the reverse rate.			
	Parameters	Optional/Reqd.	Units	Examples
	Pre-exponential factor A_i		Depends on reaction	REV / 1.0E13 0.0 15000./
	Temperature exponent β_i		--	REV /1.0E13 0.0 15000./
	Activation energy E_i		cal/mole	REV /1.0E13 0.0 15000 ./
	Reaction Example	C(S, R) + CH3 <=> D + CH3(S) 4.0E12 0.0 1200.0 REV /1.0E13 0.0 15000./		
RORD	Arbitrary Reaction Orders - Supersedes the reverse reaction order for any species in the mechanism (with respect to species concentration), regardless of whether the species appears as a reactant or a product in the reaction. RORD must be followed by the slash-delimited species name and the new reaction order, and supersedes the values of ν''_{ki} in Equation 3.4 of the Chemkin Theory Manual pertaining to the particular species named on the line; the reaction order for all other species maintain their default values. Multiple occurrences of the RORD construct may appear on the auxiliary line.			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	RORD /OH 2.0/
	Stoichiometric coefficient ν''_{ki}	Required	--	RORD /OH 2.0/
	Reaction Example	H2+O2=2OH		

Keyword	Definition			
	constant). There can be only one gas-phase reactant species in a sticking-coefficient reaction; moreover, its stoichiometric coefficient must be 1.			
	Reaction Example	A1 + 8H(se) => 5H(se) + 6C(B) + 3open(se) + 4H2 + H 0.1 0.0 0.0 FORD/H(se) 2.0/ DCOL/2.46E-8/ STICK		
UNITS	Unit Specifications for Reactions - Supersedes the current units for a particular reaction rate fit that may differ from the default units specified for other reaction expressions in the chemistry mechanism. UNITS must be followed by the slash-delimited character-string string , where string is one of the following (letters in brackets are optional): Parameters with energy units such as E_i : EVOL[TS] (p. 72), KELV[INS] (p. 72), CAL/[MOLE] (p. 71), KCAL/[MOLE] (p. 72), JOUL[ES/ MOLE] (p. 72), or KJOU[LES/MOLE] (p. 72). Pre-exponential factors A_i : MOLE[S] (p. 73) or MOLEC[ULES] (p. 73), where the inclusion of MOLEC would indicate that the reaction rate expression is in units of molecules/cm ³ rather than mole/cm ³ . ATM (p. 71), BAR (p. 71), PAS[CALS] (p. 74), DYN[ES] (p. 72), TOR[R] (p. 74) for pre-exponential factors a_i , where the units of gas species are partial pressures. SITE[FR] (p. 74), where the units of surface species are site fractions and the rate units are 1/sec.			
	Parameters	Optional/Reqd.	Units	Examples
	Reaction units character string	Required	--	UNITS /MOLECUES/
	Reaction Example	CF3+ + E + #WSI02(B) => #SI02 + CF3 0.33 0.0 0.0 BOHM ! YIELD /0.01 20. 0.5 1.0/ UNITS/EVOLTS/		
	Notes	• Default units for A_i are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction. • Default units for E_i are cal/mole. • Even if the default energy units are changed by giving the UNITS keyword, the temperature appearing in the Arrhenius expression of Equation 3.5 of the Chemkin Theory Manual, that is, in T raised to the β power and in the denominator of the activation energy term, is still in Kelvins. • If any of the units strings are given on the REACTIONS header line, it applies to all reactions, but		

Keyword	Definition																		
		may be superseded for a particular reaction by the auxiliary UNITS keyword. • UNITS allows only one string parameter, but the user can repeat UNITS as many times as needed for a given reaction.																	
USRPROG	Optional User Rate Subroutine SKUPROG - The net rate-of-progress for the reaction will be obtained by calling a user-supplied subroutine, SKUPROG. An optional slash(/)-delimited integer parameter allows the user to select from more than one type of rate formulation. Wherever the net reaction rate is required, it will be obtained by calling the user-written subroutine. A template of SKUPROG is provided in the Ansys Chemkin installation, in the file sklib_user_routines.f located in the directory user_subroutines . Information about how to compile and link user routines into Chemkin is included in Chemkin Application Programming Interface Manual . <table><tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr><tr><td><i>Rate formulation type</i></td><td>Optional</td><td>--</td><td>USRPROG /1/</td></tr><tr><td>Reaction Example</td><td colspan="3">CH3OH +H2O ==> CO2 + 3H2 1.0 0.00 0.0 USRPROG/3/</td></tr><tr><td>Notes</td><td colspan="3">• USRPROG applies only to irreversible reactions, and cannot be used in conjunction with USRPROD (p. 74) (entered on the REACTIONS header line).</td></tr></table>			Parameters	Optional/Reqd.	Units	Examples	<i>Rate formulation type</i>	Optional	--	USRPROG /1/	Reaction Example	CH3OH +H2O ==> CO2 + 3H2 1.0 0.00 0.0 USRPROG/3/			Notes	• USRPROG applies only to irreversible reactions, and cannot be used in conjunction with USRPROD (p. 74) (entered on the REACTIONS header line).		
Parameters	Optional/Reqd.	Units	Examples																
<i>Rate formulation type</i>	Optional	--	USRPROG /1/																
Reaction Example	CH3OH +H2O ==> CO2 + 3H2 1.0 0.00 0.0 USRPROG/3/																		
Notes	• USRPROG applies only to irreversible reactions, and cannot be used in conjunction with USRPROD (p. 74) (entered on the REACTIONS header line).																		
YIELD	Ion-energy-dependent Yield - Ion-enhanced reaction yield can be applied to a reaction using the following two steps. First, place a pound sign (#) in front of the species symbol (or stoichiometric coefficient if given) for each species that is subject to the ion-energy yield enhancement. The "sub-reaction" of species and coefficients demarcated with the # sign must satisfy mass, elemental, charge and site balance. Second, the auxiliary keyword YIELD must appear after the reaction, followed by the four parameters, h_{yield} , $E_{\text{yield},0}$, t_i , and u_i (as described in Equation 4.33 of the Chemkin Theory Manual). These parameters are included as a slash-delimited set following the YIELD auxiliary keyword. An example of a YIELD reaction is shown in Figure 4.7: Examples of Auxiliary Reaction Data (p. 90) . <table><tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr><tr><td><i>Multiplicative factor h_{yield}</i></td><td>Required</td><td>Depends on reaction</td><td>YIELD /0.053 4.0 0.5 1.0/</td></tr><tr><td><i>Energy threshold $E_{\text{yield},0}$</i></td><td>Required</td><td>cal/mole</td><td>YIELD /0.053 4.0 0.5 1.0/</td></tr><tr><td><i>Exponential constant t_i</i></td><td>Required</td><td>--</td><td>YIELD /0.053 4.0 0.5 1.0/</td></tr></table>			Parameters	Optional/Reqd.	Units	Examples	<i>Multiplicative factor h_{yield}</i>	Required	Depends on reaction	YIELD /0.053 4.0 0.5 1.0/	<i>Energy threshold $E_{\text{yield},0}$</i>	Required	cal/mole	YIELD /0.053 4.0 0.5 1.0/	<i>Exponential constant t_i</i>	Required	--	YIELD /0.053 4.0 0.5 1.0/
Parameters	Optional/Reqd.	Units	Examples																
<i>Multiplicative factor h_{yield}</i>	Required	Depends on reaction	YIELD /0.053 4.0 0.5 1.0/																
<i>Energy threshold $E_{\text{yield},0}$</i>	Required	cal/mole	YIELD /0.053 4.0 0.5 1.0/																
<i>Exponential constant t_i</i>	Required	--	YIELD /0.053 4.0 0.5 1.0/																

Keyword	Definition			
	Exponential constant u_i	Required	--	YIELD /0.053 4.0 0.5 1.0/
	Reaction Example	$\text{CF}_3^+ + \text{E} + \text{\#WSIO}_2(\text{B}) \Rightarrow \text{\#SIO}_2 + \text{CF}_3$ $0.33 \quad 0.0 \quad 0.0$ BOHM ! YIELD /0.01 20. 0.5 1.0/ UNITS/EVOLTS/		
	Notes	A reaction declared with ion-enhanced yield must contain one (and only one) positive ionic reactant species.		

Note:

Even if the default energy units are changed by giving one of the UNITS keyword, the temperature appearing in the Arrhenius expression of [Equation 3.5](#) of the [Chemkin Theory Manual](#), that is, in T raised to the β power and in the denominator of the activation energy term, is still in Kelvins.

Table 4.7: Auxiliary Keywords for Liquid Phase Reactions

Keyword	Definition	
HENRY	Henry's law for calculating equilibrium concentration levels in gas and liquid phases. Default form is dimension less. This can be changed by optional keyword UNITS.	
	Reaction Example	$\text{CO}_2 = \text{CO}_2(\text{aq}) \quad 1.0 \quad 0.0 \quad 0.$ VLE/HENRY 1 3.34e-05 2400 298.15 /
	Notes	- Four or five parameters may be provided following HENRY. The first parameter with an integer value of 1 or 2 indicates the type of temperature dependence for Henry's law. - Value of 1, use the form: $\text{Henry's Constant} = A * \exp[-B(1/T - 1/C)]$ Here, A, B, C are the three parameters input from following the first parameter. T represents temperature in K. - Value of 2, use the form: $1/\text{Henry's Constant} = \exp[A + B/T + C * \ln(T) + D * T]$

Keyword	Definition	
		<i>D</i> is the fifth parameter on the input line. This form is available only when pressure units are used specified for Henry's law using the keyword UNITS.
IDEAL	Raoult's law for calculating equilibrium concentrations in gas and liquid phases.	
	Reaction Example	C02 = C02(aq) 1.0 0.0 0. VLE/ IDEAL/
KMASS	Mass transfer coefficient used to calculate rate of mass exchange between two phases involving gas-liquid or liquid-liquid. This optional keyword follows the line with VLE inputs. Separate KMASS for product and reactant phase are specified. Units mass transfer coefficient are cm/s. The KMASS line can read in up to five parameters depending on the choice of model. The model is specified by the following keywords as the first parameter. CONK: Constant value of mass transfer coefficient. CONDL: Use two-film theory with constant diffusivity and length scale. CONDT: Use penetration theory with constant diffusivity and time scale. For CONK, mass transfer coefficient for that phase is specified by one value. Units are cm/s. For two-film and penetration theories, diffusivity is the first parameter with units of cm²/s. The last parameter is either film thickness (in cm) or contact time (in s). .	
	Reaction Example	o2(l) = o2 1.0 0.0 0.0 VLE/ IDEAL/ KMASS/ o2(l) CONDL 1.0e-4 0.01/ KMASS/ o2 CONK 1.0e-3/ REFSP/ o2/ REFSP/ o2(l) /
UNITS for Henry's Law	Form of the Henry's law can be changed using this additional keyword on the same line as HENRY. Units allowed are gas partial pressure in atm and pascal. In absence of this word, dimensionless form of Henry's law is used.	
	Reaction Example	c6h12-1(l) = c6h12-1 1.0 0.0 0. VLE / HENRY 2 3.55e-5 2400. 298.15 / UNITS/MOLAR_ATM/
	Notes	Allowed units for the gas phase concentrations are MOLAR_PA, MOLAR_ATM, ATM, PA. The first two form sconsider the units in (mole/m ³)/Pa and (mole/m ³)/atm,

Keyword	Definition	
		respectively. The latter two consider the partial pressure units in atm and Pa.
VLE	Vapor Liquid Equilibrium model for use with the phase transfer process. This requires additional parameters, IDEAL or HENRY, that specifies the model.	
	Reaction Example	c6h12-1(l) = c6h12-1 1.0 0.0 0. VLE / IDEAL /
	Notes	Only one species on reactant and product side should be provided. This mapping is unique; a species may participate in only one VLE reaction.

4.5.3.1. Summary of Auxiliary Reaction Data

Any number of auxiliary information lines may follow a reaction line, in any order, and any number of keywords may appear on an auxiliary information line; however, an auxiliary keyword and its parameter(s) must appear on the same line.

Examples of auxiliary information are shown in [Figure 4.7: Examples of Auxiliary Reaction Data \(p. 90\)](#). The above rules are summarized in [Table 4.8: Summary of the Rules for Auxiliary Reaction Data \(p. 91\)](#).

Figure 4.7: Examples of Auxiliary Reaction Data

```

REACTIONS      KCAL/MOLE
! THE FOLLOWING ARE *CONTRIVED* EXAMPLES OF AUXILIARY KEYWORD USAGE
  SICL(S) <=> CL + SI(S)                                1.0E-3 0.0 2.
                                                         REV/1.0E13 0.0 37./
  CL + SICL(S) <=> CL2 + SI(S)                            0.1 1.1 20.
    DUPLICATE STICK
    RORD /SI(S) 0/
  CL + SICL(S) <=> CL2 + SI(S)                            1.4E11 0.0 15.
    DUPLICATE COV/SICL(S) -1.2 0.5 32./ FORD/CL+ 1.0/
  CL*          => CL                                       1.0 0.0 0.
    STICK        MWOFF
  E + CL+ + SICL3(S) + SI(B) => SICL4 + SI(S)            0.50 0.0 0.
    BOHM
    ENRGDEP/1. 0.5 1.0/ UNITS/EVOLT/
  AR+ + E + #SI02(D) => #SI02 + AR                        1.0 0.0 0.0
    BOHM
    YIELD /0.023052 35. 0.5 1.0/ UNITS/EVOLTS/
  E + CL2+ + SICL3(S) + SI(B) => SICL4 + SICL(S)          0.50 0.0 0.0 FORD/ CL2+ 2.43/
  C6H5CH3 + H2 => C6H6 + CH4                             1.4E-8 0.0 0.0 ! rate at 600C
    LANG /C6H6 1.26 0.0 0.0 1.0/
    LANG /C6H5CH3 1.01 0.0 0.0 1.0/
    LHDE /1/
    LHNU /C6H5CH3/
    LHPR /atm/

```

Figure 4.8: Examples of Auxiliary Reaction Data for Liquid Phase

```

nc12h26(l) = nc12h26 1.0 0.0 0.
  VLE / IDEAL/ !Use Raoult's law for ideal liquid
  KMASS/ nc12h26 (l) CONDL 1.0e-4 0.01/
  KMASS/ nc12h26 CONK 1.0e-3/

```

```

co2(1) = co2      1.0  0.0  0.
VLE / HENRY  2  3.55e-05  2400.  298.15/

```

Table 4.8: Summary of the Rules for Auxiliary Reaction Data

Rule	Description
1	Auxiliary information lines may follow a reversible reaction to specify the reverse rate parameters explicitly; auxiliary information must follow any reactions that are duplicated.
2	Auxiliary keyword declarations may appear anywhere on the line, in any order.
3	Any number of auxiliary keywords may appear on a line, and more than one line may be used, but a keyword and its parameter(s) must appear on the same line.
4	Multiple keywords appearing on the same line must be separated by at least one blank space.
5	Any blank spaces between a keyword and the first slash are ignored and any blanks between the slashes and parameter(s) are also ignored. However, no blank spaces are allowed within a keyword or parameter.
6	The keyword REV followed by three slash-delimited Arrhenius coefficients may be used to specify the reverse rate parameters.
7	The keyword DUPLICATE (or DUP) must follow every occurrence of a duplicated reaction.
8	The keyword STICK indicates that the three coefficients on the reaction line are to be interpreted as the parameters a_i , b_i , and c_i in Equation 4.10 of the Chemkin Theory Manual . There must be exactly one gas-phase reactant species; its stoichiometric coefficient must be 1.
9	The keyword COV is used to modify the forward rate constant by the expression in Equation 4.7 of the Chemkin Theory Manual . The word COV is followed by a surface species name and the three coverage parameters η_{ki} , μ_{ki} and ε_{ki} . The four entries after the word COV are slash-delimited.
10	The keyword BOHM indicates that the three coefficients on the reaction line are to be interpreted as the parameters a_i , b_i , and c_i in Equation 4.29 of the Chemkin Theory Manual ; the Bohm velocity correction is applied. There must be exactly one gas-phase reactant species and that species must be a positive ionic species; its stoichiometric coefficients must be 1. Only irreversible reactions are allowed with this option. The electron must be declared in the list of species names in the <i>Gas-phase Kinetics</i> Pre-processor input.
11	The keyword ENRGDEP allows the rate constant to depend on ion energy according to Equation 4.30 of the Chemkin Theory Manual . The keyword is followed by the three parameters $E_{ion,0}$, f_i , and g_i which are slash-delimited. There must be exactly one positive ionic reactant species in the reaction. Only irreversible reactions are allowed with this option.
12	The keywords FORD and RORD can be used to change the reaction order (with respect to species concentration) of the forward or reverse reaction, respectively, for any species in the mechanism, regardless of whether the

Rule	Description
	species appears as a reactant or a product in the reaction. The species name and the new reaction order (slash-delimited) follow the keyword.
13	The YIELD keyword allows modification of the stoichiometric coefficients in a sub-reaction using the ion-yield option. The usage requires preceding each species in the sub-reaction (or its stoichiometric coefficient) with the pound sign (#). Following the reaction line, declare the YIELD keyword, then the four parameters h_{yield} , $E_{\text{yield},0}$, t_{ir} , and u_i of Equation 4.33 of the Chemkin Theory Manual , between slashes. There must be exactly one positive ionic reactant species in the reaction. Only irreversible reactions are allowed with this option. The sub-reaction demarcated with the # symbols must satisfy mass, elemental, charge and site balance. An example of the YIELD keyword appears in Figure 4.7: Examples of Auxiliary Reaction Data (p. 90) .
14	The UNITS keyword can be used to override the current default units for parameters with energy units or the pre-exponential factor for a given reaction. The usage is UNITS/ string /, where string is one of the following: EVOLTS, KELVINS, CAL/MOLE, KCAL/MOLE, JOULES/MOLE, or KJOULES/MOLE (for parameters with energy units), or MOLES or MOLECULES (for pre-exponential factors).
15	The string MWON can be used to turn on the Motz-Wise correction of Equation 4.15 of the Chemkin Theory Manual or the string MWOFF can be used to turn off this correction for a sticking coefficient reaction. Using the MWOFF or MWON keyword overrides the default option set up on the REACTIONS line or the default supplied by <i>Surface Kinetics</i> (which is MWOFF).
16	The LANG keyword can be used to input a Langmuir-Hinshelwood rate expression. The keyword is followed by a species name, three parameters giving the equilibrium constant, and a fourth parameter giving the order of that species in the reaction. Additional keywords LHDE, LHNU, and LHPR provide more flexibility in the form of the Langmuir-Hinshelwood or Eley-Rideal rate expressions.
17	The keyword LHDE allows the default value of 2 for the overall exponent for the denominator (m) to be overridden when LANG is used to specify a Langmuir-Hinshelwood rate expression. To specify an Eley-Rideal reaction, this keyword would be used to set m to 1. The use of any positive number is permitted, including real or fractional numbers.
18	The keyword LHNU allows the explicit inclusion of equilibrium constants in the numerator of the LH rate expression (the use of k rather than k' , see Langmuir-Hinshelwood and Eley-Rideal Reactions of the Chemkin Theory Manual) when LANG is used to specify a Langmuir-Hinshelwood rate expression. This keyword is followed by a slash delimited list of species names. For each species in the list, a multiplier of K will be applied to the rate constant. Each species listed in a LHNU statement must have a LANG statement.
19	The keyword LHPR indicates that the equilibrium constants are given in pressure units when LANG is used to specify a Langmuir-Hinshelwood rate expression. The LHPR keyword will affect the equilibrium constants for the specified reaction only; the reaction rate will still be assumed to be in the units specified on the REACTIONS line, or in the default moles, cm, and sec.

Rule	Description
	The keyword is followed by the name of the pressure unit being used: atm, bar, torr, Pasc (for Pascals), or dyne (for dynes per square cm), where the names are not case sensitive.

4.5.4. Problems Having No Reactions

In some problems only information about the surface and bulk species is needed (for example, chemical equilibrium computations). For these cases it is not necessary to include reaction data. The Pre-processor will create the linking file *surf.asc*, but it will not contain any reaction information. Therefore, no subroutines in the *Surface Kinetics* Subroutine Library that deal with chemical reactions (for example, chemical production rates) will be used (although doing so would not generate an error; the production rates of all species would be returned as zero).

4.5.5. Error Checks

Each input line is checked for proper syntax and diagnostic messages are written to the pre-processor output file if errors are encountered. If an error occurs, the pre-processor continues to read and diagnose the input, but an error flag is written to the Linking file and *Surface Kinetics* subroutine SKINIT will not initialize the work arrays. Therefore, the input must be error free before a Reactor Model can be run or before any of the *Surface Kinetics* subroutines can be called in a Reactor Model.

Possibilities for an error condition are as follows:

Table 4.9: Error Checks

Data Type	Possible Errors
Site and Bulk Species Data	A duplicated species symbol (name) is not considered a fatal error, but is eliminated from consideration and a warning diagnostic message is printed.
	No site density is found for a declared site, or the site density is negative.
	No thermodynamic data are found for a declared species.
	A site or bulk phase name duplicates another phase name (gas surface site, or bulk phase name).
	A phase or species name contains an illegal character.
	Site occupancy number is negative.
	Bulk density for a bulk species is negative.
Thermodynamic Data	Thermodynamic data are format sensitive and therefore provide possibilities for error if not formatted exactly as described by Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4) .
	An element in the thermodynamic data for a declared species is not included in the <i>Gas-phase Kinetics</i> Pre-processor input element data.
	With the THERMO ALL option, line 2 (of Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4)) is not found.

Data Type	Possible Errors
Reaction Data	A delimiter =>, <=>, or = between the reactants and the products is not found.
	Three Arrhenius parameters are not found.
	Reactants and/or products species names are not properly delineated by a plus sign (+).
	A species listed as a reactant or product is not declared in the species data.
	A reaction does not satisfy elemental balance.
	The number of sites in a reaction does not balance and the word NONCON was not included on the first REACTIONS line.
	The charge of the reaction does not balance.
	A reaction is a duplicate not declared by the auxiliary data keyword DUP.
	There are more than six reactants or six products in a reaction.
Auxiliary Reaction Data	An unknown or misspelled keyword occurs.
	Parameters for a keyword are not enclosed in slashes.
	There are the wrong number of parameters for a keyword.
	REV is declared for an irreversible reaction.
	Pre-exponential factor for a sticking coefficient is negative.
	For a sticking-coefficient reaction, there is more than one gas-phase species, or the stoichiometric coefficient for the gas-phase species is not 1.
	More than one BOHM declaration appeared for a given reaction.
	BOHM keyword is given for a reversible reaction.
	A positive ionic species did not appear as a reactant or its stoichiometric coefficient was not 1 in a Bohm reaction.
	More than 1 positive ionic species was a reactant in a Bohm reaction.
	The electron species was not declared in the list of species in the <i>Gas-phase Kinetics</i> Pre-processor input.
	Invalid string given with the UNITS auxiliary keyword.
	More than one ENRGDEP declaration appeared for a given reaction.
	A positive ionic species did not appear as a reactant or its stoichiometric coefficient was not 1 in a ENRGDEP reaction.
	Wrong number of ENRGDEP parameters given.
	Invalid species name given for FORD or RORD auxiliary keywords.
	A reaction order value was not found with the FORD or RORD keyword.
	RORD given for an irreversible reaction.

Data Type	Possible Errors
	No species coefficients were demarcated with a # symbol for a YIELD reaction.
	YIELD keyword given for a reversible reaction.
	A positive ionic species did not appear as a reactant or its stoichiometric coefficient was not 1 in a YIELD reaction.
	Wrong number of YIELD parameters given.
	More than 1 positive ionic species was a reactant in a YIELD reaction.
	LANG is declared for a reversible reaction, or for the same reaction as STICK, COV, BOHM, YIELD, or ENRGDEP.
	USRPROG given for a USRPROD mechanism.
	USRPROG given for a reversible reaction.

Chapter 5: Transport Database

In this section we list the database file that is currently included with the *Transport* software. While this database file is more of a historical record, we expect that users will want to add their own collection of data to suit their own needs.

The database file included with Ansys Chemkin should not be viewed as the last word in transport properties. Instead, it is a good starting point from which a user will provide the best available data for their particular application. Some of the numbers in the database have been determined by computing "best fits" to experimental measurements of a macroscopic transport property (for example, viscosity). In other cases the Lennard-Jones parameters have been estimated following the methods outlined in Svehla.[8] (p. 375) In still other cases they have been determined by computational chemistry techniques.

5.1. Transport Data Format

The first 16 columns in each line of the database are reserved for the species name. Presently Ansys Chemkin is programmed to allow no larger than 16-character names. Columns 17 through 80 are free-format, and they contain the molecular parameters for each species. They are, in order:

1. An index indicating whether the molecule has a monatomic, linear or nonlinear geometrical configuration. If the index is 0, the molecule is a single atom. If the index is 1 the molecule is linear, and if it is 2, the molecule is nonlinear.
2. The Lennard-Jones potential well depth ε/k_B in Kelvins.
3. The Lennard-Jones collision diameter σ in angstroms.
4. The dipole moment μ in Debye.
5. The polarizability α in cubic angstroms.
6. The rotational relaxation collision number Z_{rot} at 298 K.
7. A "comment" line is one that has either a period (.), slash (/), or exclamation mark (!) as the first non-blank character. In addition, on any line, any input that follows an exclamation mark is taken as a comment.

Note:

A Debye is $10^{-18} \text{ cm}^{3/2} \text{ ergs}^{1/2}$.

5.2. Including Transport Data in the Gas-phase Kinetics Input File

Ansys Chemkin allows you to optionally include transport data within the *Gas-phase Kinetics* Input File. This is similar to the options available for thermodynamic data. This option can be used to supplement or replace transport data that may be provided in a separate file (for example, *tran.dat*). In addition, this option may be particularly useful when reaction-rate constants are given in terms of the collision frequency (see the description of the COLLEFF keyword in [Table 3.7: Alphabetical Listing of Gas-phase Reaction Auxiliary Keywords \(p. 47\)](#)). In such cases, the Lennard-Jones diameter, which is obtained from the transport data, is required for calculation of the collision frequency that is used to derive the reaction rate for those reactions. These are cases when transport data might not otherwise be required but the necessary data for specific species needed in the collision-frequency reactions may be included in the *Gas-phase Kinetics* Input File.

A full description of the syntax of this option is included in [Transport Data \(p. 42\)](#).

5.3. Transport Data Included with CHEMKIN

[Table 5.1: Species in Transport Database \(p. 98\)](#) lists the species contained in the Ansys Chemkin *tran.dat* file, which is included in every installation, as the corresponding data for each species.

Table 5.1: Species in Transport Database

Species Name	Geometry	ϵ/k_B	σ	μ	α	Z_{rot}
Al2Me6	2	471.	6.71	0.0	0.0	1.0
AlMe3	2	471.	5.30	0.0	0.0	1.0
AR	0	136.500	3.330	0.000	0.000	0.000
AR*	0	136.500	3.330	0.000	0.000	0.000
AS	0	1045.5	4.580	0.000	0.000	0.000
AS2	1	1045.5	5.510	0.000	0.000	1.000
ASH	1	199.3	4.215	0.000	0.000	1.000
ASH2	2	229.6	4.180	0.000	0.000	1.000
ASH3	2	259.8	4.145	0.000	0.000	1.000
AsH3	2	259.8	4.145	0.000	0.000	1.000
BCL3	2	337.7	5.127	0.000	0.000	1.000
C	0	71.400	3.298	0.000	0.000	0.000
C-Si3H6	2	331.2	5.562	0.000	0.000	1.000
C2	1	97.530	3.621	0.000	1.760	4.000
C2F4	2	202.6	5.164	0.000	0.000	1.000
C2F6	2	194.5	5.512	0.000	0.000	1.000
C2H	1	209.000	4.100	0.000	0.000	2.500
C2H2	1	209.000	4.100	0.000	0.000	2.500
C2H2OH	2	224.700	4.162	0.000	0.000	1.000
C2H3	2	209.000	4.100	0.000	0.000	1.000

Species Name	Geometry	ε/k_B	σ	μ	α	Z_{rot}
C2H4	2	280.800	3.971	0.000	0.000	1.500
C2H5	2	252.300	4.302	0.000	0.000	1.500
C2H5OH	2	362.6	4.53	0.000	0.000	1.000
C2H6	2	252.300	4.302	0.000	0.000	1.500
C2N	1	232.400	3.828	0.000	0.000	1.000
C2N2	1	349.000	4.361	0.000	0.000	1.000
C2O	1	232.400	3.828	0.000	0.000	1.000
C3H2	2	209.000	4.100	0.000	0.000	1.000
C3H3	1	252.000	4.760	0.000	0.000	1.000
C3H4	1	252.000	4.760	0.000	0.000	1.000
C3H4P	1	252.000	4.760	0.000	0.000	1.000
C3H6	2	266.800	4.982	0.000	0.000	1.000
C3H7	2	266.800	4.982	0.000	0.000	1.000
C3H8	2	266.800	4.982	0.000	0.000	1.000
C4H	1	357.000	5.180	0.000	0.000	1.000
C4H2	1	357.000	5.180	0.000	0.000	1.000
C4H2OH	2	224.700	4.162	0.000	0.000	1.000
C4H3	1	357.000	5.180	0.000	0.000	1.000
C4H4	1	357.000	5.180	0.000	0.000	1.000
C4H6	2	357.000	5.180	0.000	0.000	1.000
C4H8	2	357.000	5.176	0.000	0.000	1.000
C4H9	2	357.000	5.176	0.000	0.000	1.000
C4H9	2	357.000	5.176	0.000	0.000	1.000
C5H2	1	357.000	5.180	0.000	0.000	1.000
C5H3	1	357.000	5.180	0.000	0.000	1.000
C5H5OH	2	450.000	5.500	0.000	0.000	1.000
C6H2	1	357.000	5.180	0.000	0.000	1.000
C6H5	2	412.300	5.349	0.000	0.000	1.000
C6H5(L)	2	412.300	5.349	0.000	0.000	1.000
C6H5O	2	450.000	5.500	0.000	0.000	1.000
C6H6	2	412.300	5.349	0.000	0.000	1.000
C6H7	2	412.300	5.349	0.000	0.000	1.000
CF	1	94.2	3.635	0.000	0.000	1.000
CF2	2	108.0	3.977	0.000	0.000	1.000
CF3	2	121.0	4.320	0.000	0.000	1.000
CF4	2	134.0	4.662	0.000	0.000	1.000
CH	1	80.000	2.750	0.000	0.000	0.000

Species Name	Geometry	ε/k_B	σ	μ	α	Z_{rot}
CH2	1	144.000	3.800	0.000	0.000	0.000
CH2(S)	1	144.000	3.800	0.000	0.000	0.000
CH2(SING)	1	144.000	3.800	0.000	0.000	0.000
CH2CHCCH	2	357.000	5.180	0.000	0.000	1.000
CH2CHCCH2	2	357.000	5.180	0.000	0.000	1.000
CH2CHCH2	2	260.000	4.850	0.000	0.000	1.000
CH2CHCHCH	2	357.000	5.180	0.000	0.000	1.000
CH2CHCHCH2	2	357.000	5.180	0.000	0.000	1.000
CH2CO	2	436.000	3.970	0.000	0.000	2.000
CH2F2	2	318.0	4.080	0.000	0.000	1.000
CH2HCO	2	436.000	3.970	0.000	0.000	2.000
CH2O	2	498.000	3.590	0.000	0.000	2.000
CH2OH	2	417.000	3.690	1.700	0.000	2.000
CH3	1	144.000	3.800	0.000	0.000	0.000
CH3CC	2	252.000	4.760	0.000	0.000	1.000
CH3CCCH2	2	357.000	5.180	0.000	0.000	1.000
CH3CCCH3	2	357.000	5.180	0.000	0.000	1.000
CH3CCH2	2	260.000	4.850	0.000	0.000	1.000
CH3CH2CCH	2	357.000	5.180	0.000	0.000	1.000
CH3CHCH	2	260.000	4.850	0.000	0.000	1.000
CH3CHO	2	436.000	3.970	0.000	0.000	2.000
CH3CO	2	436.000	3.970	0.000	0.000	2.000
CH3O	2	417.000	3.690	1.700	0.000	2.000
CH3OH	2	481.800	3.626	0.000	0.000	1.000
CH4	2	141.400	3.746	0.000	2.600	13.000
CH4O	2	417.000	3.690	1.700	0.000	2.000
CHF3	2	240.0	4.330	0.000	0.000	1.000
CL	0	130.8	3.613	0.000	0.000	1.000
CL-	0	130.8	3.613	0.000	0.000	1.000
CL2BNH2	2	337.7	5.127	0.000	0.000	1.000
CN	1	75.000	3.856	0.000	0.000	1.000
CN2	1	232.400	3.828	0.000	0.000	1.000
CNC	1	232.400	3.828	0.000	0.000	1.000
CNN	1	232.400	3.828	0.000	0.000	1.000
CO	1	98.100	3.650	0.000	1.950	1.800
CO2	1	244.000	3.763	0.000	2.650	2.100
DMG	2	675.8	5.22	0.000	0.000	1.000

Species Name	Geometry	ε/k_B	σ	μ	α	Z_{rot}
E	0	850.	425.	0.000	0.000	1.000
F	0	80.000	2.750	0.000	0.000	0.000
F2	1	125.700	3.301	0.000	1.600	3.800
GA	0	2961.8	4.62	0.000	0.000	0.000
GACH3	2	972.7	4.92	0.000	0.000	1.000
GAH	1	335.5	4.24	0.000	0.000	1.000
GAME	2	972.7	4.92	0.000	0.000	1.000
GAME2	2	675.8	5.22	0.000	0.000	1.000
GAME3	2	378.2	5.52	0.000	0.000	1.000
GaMe3	2	378.2	5.52	0.000	0.000	1.000
H	0	145.000	2.050	0.000	0.000	0.000
H2	1	38.000	2.920	0.000	0.790	280.000
H2ASCH3	2	408.0	4.73	0.000	0.000	1.000
H2C4O	2	357.000	5.180	0.000	0.000	1.000
H2CCCCH	2	357.000	5.180	0.000	0.000	1.000
H2CCCCH2	2	357.000	5.180	0.000	0.000	1.000
H2CCCH	2	252.000	4.760	0.000	0.000	1.000
H2CN	1	569.000	3.630	0.000	0.000	1.000
H2NO	2	116.700	3.492	0.000	0.000	1.000
H2O	2	572.400	2.605	1.844	0.000	4.000
H2O2	2	107.400	3.458	0.000	0.000	3.800
H2S	2	301.000	3.600	0.000	0.000	1.000
H2SISIH2	2	312.6	4.601	0.000	0.000	1.000
H3SISIH	2	312.6	4.601	0.000	0.000	1.000
HC2N2	1	349.000	4.361	0.000	0.000	1.000
HCCHCCH	2	357.000	5.180	0.000	0.000	1.000
HCCO	2	150.000	2.500	0.000	0.000	1.000
HCCOH	2	436.000	3.970	0.000	0.000	2.000
HCL	1	344.7	3.339	0.000	0.000	1.000
HCN	1	569.000	3.630	0.000	0.000	1.000
HCNO	2	232.400	3.828	0.000	0.000	1.000
HCO	2	498.000	3.590	0.000	0.000	0.000
HCO+	1	498.000	3.590	0.000	0.000	0.000
HE	0	10.200	2.576	0.000	0.000	0.000
HF	1	330.000	3.148	1.920	2.460	1.000
HF0	1	352.000	2.490	1.730	0.000	5.000
HF1	1	352.000	2.490	1.730	0.000	5.000

Species Name	Geometry	ε/k_B	σ	μ	α	Z_{rot}
HF2	1	352.000	2.490	1.730	0.000	5.000
HF3	1	352.000	2.490	1.730	0.000	5.000
HF4	1	352.000	2.490	1.730	0.000	5.000
HF5	1	352.000	2.490	1.730	0.000	5.000
HF6	1	352.000	2.490	1.730	0.000	5.000
HF7	1	352.000	2.490	1.730	0.000	5.000
HF8	1	352.000	2.490	1.730	0.000	5.000
HNCO	2	232.400	3.828	0.000	0.000	1.000
HNNO	2	232.400	3.828	0.000	0.000	1.000
HNO	2	116.700	3.492	0.000	0.000	1.000
HNOH	2	116.700	3.492	0.000	0.000	1.000
HO2	2	107.400	3.458	0.000	0.000	1.000
HOCN	2	232.400	3.828	0.000	0.000	1.000
HSO2	2	252.000	4.290	0.000	0.000	1.000
I*C3H7	2	266.800	4.982	0.000	0.000	1.000
I*C4H9	2	357.000	5.176	0.000	0.000	1.000
K	0	850.	4.25	0.000	0.000	1.000
K+	0	850.	4.25	0.000	0.000	1.000
KCL	1	1989.	4.186	0.000	0.000	1.000
KH	1	93.3	3.542	0.000	0.000	1.000
KO	1	383.0	3.812	0.000	0.000	1.000
KO2	2	1213.	4.69	0.000	0.000	1.000
KOH	2	1213.	4.52	0.000	0.000	1.000
N	0	71.400	3.298	0.000	0.000	0.000
N*C3H7	2	266.800	4.982	0.000	0.000	1.000
N2	1	97.530	3.621	0.000	1.760	4.000
N2H2	2	71.400	3.798	0.000	0.000	1.000
N2H3	2	200.000	3.900	0.000	0.000	1.000
N2H4	2	205.000	4.230	0.000	4.260	1.500
N2O	1	232.400	3.828	0.000	0.000	1.000
NCN	1	232.400	3.828	0.000	0.000	1.000
NCNO	2	232.400	3.828	0.000	0.000	1.000
NCO	1	232.400	3.828	0.000	0.000	1.000
NH	1	80.000	2.650	0.000	0.000	4.000
NH2	2	80.000	2.650	0.000	2.260	4.000
NH3	2	481.000	2.920	1.470	0.000	10.000
NNH	2	71.400	3.798	0.000	0.000	1.000

Species Name	Geometry	ε/k_B	σ	μ	α	Z_{rot}
NO	1	97.530	3.621	0.000	1.760	4.000
NO2	2	200.000	3.500	0.000	0.000	1.000
O	0	80.000	2.750	0.000	0.000	0.000
O(Si(OC2H5)3)2	2	522.7	5.25	0.000	0.000	1.000
O2	1	107.400	3.458	0.000	1.600	3.800
O3	2	180.000	4.100	0.000	0.000	2.000
OH	1	80.000	2.750	0.000	0.000	0.000
OSi(OC2H5)2	2	522.7	7.03	0.000	0.000	1.000
PH3	2	251.5	3.981	0.000	0.000	1.000
S	0	847.000	3.839	0.000	0.000	0.000
S*C4H9	2	357.000	5.176	0.000	0.000	1.000
S2	1	847.000	3.900	0.000	0.000	1.000
SH	1	847.000	3.900	0.000	0.000	1.000
Si	0	3036.	2.910	0.000	0.000	0.000
Si(OC2H5)4	2	522.7	7.03	0.000	0.000	1.000
Si(OC2H5)4	2	522.7	7.03	0.000	0.000	1.000
Si(OH)(OC2H5)3	2	522.7	7.03	0.000	0.000	1.000
Si(OH)(OC2H5)3	2	522.7	7.03	0.000	0.000	1.000
Si(OH)2(OC2H5)2	2	522.7	6.35	0.000	0.000	1.000
Si(OH)2(OC2H5)2	2	522.7	6.35	0.000	0.000	1.000
Si(OH)3(OC2H5)	2	522.7	5.75	0.000	0.000	1.000
Si(OH)4	2	522.7	5.25	0.000	0.000	1.000
Si2	1	3036.	3.280	0.000	0.000	1.000
Si2H2	2	323.8	4.383	0.000	0.000	1.000
Si2H3	2	318.2	4.494	0.000	0.000	1.000
Si2H4	2	312.6	4.601	0.000	0.000	1.000
Si2H5	2	306.9	4.717	0.000	0.000	1.000
Si2H6	2	301.3	4.828	0.000	0.000	1.000
Si3	2	3036.	3.550	0.000	0.000	1.000
Si3H8	2	331.2	5.562	0.000	0.000	1.000
SiF	1	585.0	3.318	0.000	0.000	1.000
SiF3	2	309.6	4.359	0.000	0.000	1.000
SiF3NH2	2	231.0	4.975	0.000	0.000	1.000
SiF4	2	171.9	4.880	0.000	0.000	1.000
SiH	1	95.8	3.662	0.000	0.000	1.000
SiH2	2	133.1	3.803	0.000	0.000	1.000
SiH2(3)	2	133.1	3.803	0.000	0.000	1.000

Species Name	Geometry	ε/k_B	σ	μ	α	Z_{rot}
SIH3	2	170.3	3.943	0.000	0.000	1.000
SIH3SIH2SIH	2	331.2	5.562	0.000	0.000	1.000
SIH4	2	207.6	4.084	0.000	0.000	1.000
SIHF3	2	180.8	4.681	0.000	0.000	1.000
SO	1	301.000	3.993	0.000	0.000	1.000
SO2	2	252.000	4.290	0.000	0.000	1.000
SO3	2	378.400	4.175	0.000	0.000	1.000
TMG	2	378.2	5.52	0.000	0.000	1.000

Chapter 6: Description and Properties of Particles

Use of Particle Tracking to determine particle size distributions in a gas-particle flow requires identification of a condensed-phase material that may exist in a form that is dispersed within the gas-flow. In addition, you must specify certain properties of the particle "cloud" that will be tracked. This section describes the necessary input to the chemistry-set files, which are needed to establish these properties. Further discussions, of how kinetics rates may be specified to control the particle nucleation, growth, and transformation, are available in Chapter [Particle Size-Distribution Tracking](#) of the [Chemkin Theory Manual](#) .

Examples are available in the Ansys Chemkin Tutorials Manual to illustrate how required information is presented to the Particle Tracking feature.

6.1. Description and Properties of the Particle Material

6.1.1. Dispersed Material

Within a reactor model that enables Particle Tracking, the simulation treats a particle population as a collection of tiny solid or liquid material pieces suspended in bulk gas. This dispersed material concept represents the fact that particles are in a condensed phase and also allows use of existing surface-kinetics capabilities to handle gas-particle interactions.

Since the particles represent a condensed-phase material, all particle-related definitions are included in the surface chemistry input file. To declare a dispersed material, the Surface Kinetics keyword MATERIAL must be provided at the top of the Surface Kinetics Input file. This allows assignment of a name to the surface material. This material can then be designated as a dispersed material (that is, it will be tracked in particle form), using the keyword DISPERSED that follows the MATERIAL statement. For example,

Figure 6.1: Example of Dispersed Material Declaration

```
MATERIAL soot
DISPERSED
END
```

With this entry, the material "soot" will be recognized by Ansys Chemkin as a dispersed material. Note that an END keyword is needed to close the DISPERSED keyword block, although at this time there is no additional information included in the block.

It is possible to have more than one type of particle co-exist in the same system, although currently the Particle Tracking equations do not consider interactions between different types of particles. Different types of particles are defined as different dispersed materials. Definitions of multiple dispersed or non-dispersed materials are separated by the MATERIAL keywords. For example, if a chemical system contains two types of particles, such that one is called soot and the other is called silicon,

they should be declared in two separate MATERIAL blocks as illustrated in [Figure 6.2: Example of Two Material Blocks \(p. 106\)](#).

Figure 6.2: Example of Two Material Blocks

```
MATERIAL soot
DISPERSED
END
REACTIONS
...
END
MATERIAL silicon
DISPERSED
END
REACTIONS
...
END
```

6.1.2. Particle Composition

One of the properties differentiating one type of particle from another is the chemical composition of the particle. The chemical composition of the particles is determined by the chemical composition of the sole bulk species specified for the dispersed material. There can only be one bulk species specified. This determines the "chemical unit" of the particle and this "chemical unit" for the initially formed condensed "species" in the material. This "chemical unit" can be a single atom, a group of atoms, or a chemical compound. Ansys Chemkin identifies the "chemical unit" of the particle by the sole bulk species on the dispersed material. For example, [Figure 6.3: Dispersed Graphite Material Declaration With Chemical Composition \(p. 106\)](#) defines a particle type called "soot".

Figure 6.3: Dispersed Graphite Material Declaration With Chemical Composition

```
MATERIAL soot
DISPERSED
END
BULK/GRAPHITE/ C(B) /1.8/
END
THERMO
C(B)          121286C    1          S    0300.00    5000.00    1000.00          1
0.14901664E+01 0.16621256E-02-0.06687204E-05 0.12908796E-09-0.09205334E-13    2
-0.07074018E+04-0.08717785E+02-0.06705661E+01 0.07181499E-01-0.05632921E-04    3
0.02142298E-07-0.04168562E-11-0.07339498E+03 0.02601595E+02          4
END
REACTIONS
...
END
```

The BULK declaration line indicates that the core of the "soot" particles consists of units of bulk species C(B) and the bulk density ρ_B of the particle core is 1.8 [gm/cm³]. The actual chemical composition of C(B), the core of the "soot" particle, is a single carbon atom as it is defined in the Thermodynamic Data section that follows the BULK declaration.

Another example is given in [Figure 6.4: Dispersed Silicon Dioxide Material Declaration With Chemical Composition \(p. 107\)](#), for a compound particle composed of silicon dioxide.

Figure 6.4: Dispersed Silicon Dioxide Material Declaration With Chemical Composition

```

MATERIAL silicon
DISPERSED
END
BULK/OXIDE/ SI02(B) /2.533/
END
THERMO
SI02(B)          72391SI  10    2          S    298.00    2000.00 1000.00      1
0.48925619E+01  0.41191629E-02-0.94570083E-07-0.80073115E-09 0.25433412E-12      2
-0.11005530E+06-0.23469570E+02 0.22325585E+01 0.12478522E-01-0.28715690E-05      3
-0.96847970E-08 0.62160411E-11-0.10962063E+06-0.10594849E+02      4
END
REACTIONS
...
END

```

6.1.3. Particle Class

Since the Particle Tracking feature employs the method of moments to solve the size distribution, it is important to understand the concept of particle class and how this class concept is connected to surface reactions that describe particle nucleation and mass growth. We define the class of a particle by the number of bulk species in its core. The "soot" particle declared in [Figure 6.4: Dispersed Silicon Dioxide Material Declaration With Chemical Composition \(p. 107\)](#) provides an example. A "soot" particle of class 100 has a core consisting of 100 C(B) species regardless of whether or not other species and atoms might exist on the surface of the particle.

When a particle nucleus is created from gas-phase precursors, its class, that is, the inception class, is determined by the stoichiometric coefficient of the bulk species in the nucleation reaction. For example, the nucleation reaction in [Figure 6.5: Nucleation Reaction Creating Particle Nuclei of Class 32 \(p. 107\)](#) creates particle nuclei of class 32:

Figure 6.5: Nucleation Reaction Creating Particle Nuclei of Class 32

```

2A4 => 32C(B) + 20 H(se) + 28.72 open(se)      1.0E10    0.5    0.0
          NUCL

```

The syntax of the nucleation reaction will be discussed in a later section. A surface reaction resulting in a net gain in the number of bulk species increases the size of the particle and vice-versa.

6.1.4. Mass and Volume of an Individual Particle

The mass of a particle is computed by summing the masses of all bulk species molecules in the core. According to the particle class definition, the mass of a class j particle becomes

$$m_p(j) = j \times m_0 \quad (6.1)$$

The mass of a single bulk species molecule m_0 is assumed to be constant and can be calculated from

$$m_0 = W_B / N_{avo} \quad (6.2)$$

where W_B is the molar weight of the bulk species and $N_{avo} = 6.022 \times 10^{23} [\text{mole}^{-1}]$ is the Avogadro number. The volume of a class j particle can be calculated from its mass and bulk density of the particle core as

$$V_p(j) = m_p(j) / \rho_B = j \times m_0 / \rho_B \quad (6.3)$$

The bulk density of the particle core ρ_B has implicitly accounted for the effect of molecule packing inside the core and its value is given when the bulk species is declared. It thus can be seen that both particle mass and volume are proportional to its class. Up to this point, there is no assumption regarding the shape of the particles so Equation 6.1 (p. 107) to Equation 6.3 (p. 108) are generally applicable to particles of all shapes.

6.1.5. Diameter and Surface Area of an Individual Particle

However, in order to derive a characteristic length scale of a particle, it is necessary to make assumption about its geometric shape. Currently, we assume that all particles are spherical. Accordingly, the representative diameter of a class j particle can be written as

$$d_p(j) = d_j = \left(\frac{6}{\pi} \times V_p(j) \right)^{1/3} = \left(\frac{6m_0}{\pi\rho_B} \right)^{1/3} j^{1/3} = d_0 \times j^{1/3} \quad (6.4)$$

The sphere-equivalent surface area of a class j particle is then given as

$$A_{s,p}(j) = \pi d_p^2(j) = \pi d_0^2 \times j^{2/3} = A_{s,0} \times j^{2/3} \quad (6.5)$$

In the above equations,

$$d_0 = \left(\frac{6m_0}{\pi\rho_B} \right)^{1/3} \quad (6.6)$$

and

$$A_{s,0} = \pi d_0^2 \quad (6.7)$$

are respectively the "unit" diameter and the "unit" surface area of the bulk species in particle core.

Chapter 7: Using Utilities

7.1. Mechanism Conversion Utility

A utility to convert a third-party mechanism to Chemkin-compatible format is available. The utility is provided as a Python 3.8-compatible code, under the installation location `\<version>\reaction\chemkinpro.<platform>\utility` folder. Instructions are available in the readme file in the same folder.

7.2. Using the FITDAT Utility

FITDAT is a utility that produces the polynomial fitting coefficients required as input for each species defined in a Gas-phase Kinetics or Surface Kinetics input file. The program accepts a molecule description in the form of character-string keywords, followed by thermodynamic data in a variety of formats. It then performs a least-squares fitting procedure for thermodynamic data, and writes an output file (e.g., *fitdat.out*) that contains the fit results and information about the quality of the fit. The file may also contain error diagnostics. The default format for the fit results is polynomial fitting coefficients for each of two temperature-ranges, as expected by the Gas-phase Kinetics and Surface Kinetics Pre-processors. An optional output format is also available if more than two temperature-ranges are desired.

Details of the various input formats for the thermodynamic data are described in [FITDAT Examples \(p. 115\)](#). The first option is to input a table of specific heat, enthalpy, and entropy values as functions of temperature. Several formats are accepted, corresponding to those used by standard references for thermodynamic data. The second option is to input thermodynamic data in the form of polynomial fitting coefficients, which FITDAT will convert to the format used by Ansys Chemkin. Again, several formats are accepted, corresponding to those used by standard compilations of thermodynamic data. The third option is to input the molecule's standard enthalpy, standard entropy, and vibrational frequencies, which are then used to estimate the thermodynamic properties.

The fit results can be cut and pasted directly into a thermodynamics data file, or a *Gas-phase Kinetics* or *Surface Kinetics* input file for use with Ansys Chemkin. In addition to this output, FITDAT creates file(s) named *species_name.csv* (e.g., *H2.csv*) containing a table of comma-delimited data for each input species. These files facilitate visualization of evaluated fit results compared to the user's input data.

7.3. Running FITDAT from the User Interface

In the Ansys Chemkin Interface, FITDAT is run from the Utility tab or menu. To open the FITDAT panel, select the **Utility > Run 'FitDat' Polynomial Equation Fitting Utility...** option. The panel shown in [Figure 7.1: Utilities—'Fitdat' Polynomial Equation Fitter \(p. 110\)](#) will be displayed in the Working Area of the User Interface.

Figure 7.1: Utilities—‘Fitdat’ Polynomial Equation Fitter

The user must first assemble an input file that describes the fitting operation desired for the *FITDAT* session. The syntax of that input file is described in [Keyword Syntax and Rules \(p. 111\)](#) . Once the input file is assembled, *FITDAT* can be run by completing the following steps:

1. Use the **Working Dir** browse or pull-down menu tools to select a working directory. This is the directory where output files from the *FITDAT* run will be created.
2. Use the **Input File** browse or pull-down menu tools to select an input file. The syntax of the input file is described in [Keyword Syntax and Rules \(p. 111\)](#) .
3. Select an **Output File** name. Type a new name in the text box if you want to modify it from the default.
4. Use the **Run FitDat** button to execute the *FITDAT* utility.
5. Use the **View Results** button to examine the output file.
6. The user can import a *FITDAT species_name.csv* file into the Ansys Chemkin Post-Processor to plot the fitting results. For more information about the Post-Processor, see the [Chemkin Visualization Manual](#) .

7.4. Programming with FITDAT

The *FITDAT* Utility is written as a FORTRAN subroutine that is called from a driver routine, and is part of the Ansys Chemkin library. We provide both C++ and FORTRAN driver routines. The driver routine performs the function of allocating total memory usage through definition of array sizes, as well as opening input and output files. *FITDAT* checks internally to ensure that the allocated work arrays are sufficiently large to process the input data. Users modifying the programs should be experienced with

compiling and linking program files on their operating system and must have either a C++ or FORTRAN compiler installed.

7.5. Keyword Syntax and Rules

The *FITDAT* Utility input is in a Keyword format. On each input line, an identifying Keyword must appear first. For some Keywords only the Keyword itself is required, while for others, additional information is required. The order of the Keyword input is generally unimportant. The rules governing the syntax of the Keyword images are listed below:

Table 7.1: Summary of Rules for Keywords

Rule	Description
1	The first character-string in the line must be a keyword; the length of the character-string depends on keyword descriptions.
2	Any further input associated with the keyword can appear anywhere after the keyword, through column 100. The specific starting column is not important, as long as there is at least one space after the keyword.
3	When more than one piece of information is required, the order in which the information appears is unimportant.
4	When numbers are required as input, they may be stated in either integer, floating point, or scientific "E" format. The utility converts the numbers to the proper type. The double precision specifier is not recognized; however, conversion to double precision is done internally as necessary.
5	When more than one piece of information is required, the pieces are delimited by one or more blank spaces.

7.6. FITDAT Keywords

Table 7.2: FITDAT Keywords

Keyword	Definition			
SPEC	A species character-string symbol, to be used in the thermodynamic data and in an Ansys Chemkin reaction mechanism, and in the name of the post-processing data file.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Species</i>	Required	--	SPEC OH
	Keyword Usage	Optional keyword. By default, this keyword is not used unless it can be determined from the data source.		
ELEM	The elemental composition of the species.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Element</i>	Required	--	ELEM O 1 ELEM H 1
	<i>Number of elements</i>	Required	--	ELEM O 1

Keyword	Definition			
				ELEM H 1
	Keyword Usage	Optional keyword. By default, this keyword is not used unless it can be determined from the data source		
DIAG	The level of fitting procedure diagnostics printed to the output file. DIAG or DIAG 1 will print a summary of data vs. polynomial evaluation relative errors. DIAG 2 will print tables of input table vs. polynomial evaluations, as well as the summary of relative error.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Diagnostic level</i>	Optional	--	DIAG 2
	Keyword Usage	Optional keyword. By default, no diagnostics are printed.		
NOTE	Print a 6-character legend to columns 19-24 of the output thermodynamic data. For example, NOTE 101602 notes the date of October 16, 2002, while NOTE Jan888 notes a JANAF data source.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Legend</i>	Required	--	NOTE 101602 NOTE Jan888
	Keyword Usage	Optional keyword. By default, no notes are printed.		
PHAS	The phase of the species, G (gas), L (liquid), or S (solid).			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Phase</i>	Required	--	PHAS G
	Keyword Usage	Optional keyword. By default, the phase G is used unless it can be determined from data source.		
LINR	The linearity of the molecule; Y (molecule is linear) or N (no).			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Linearity</i>	Required	--	LINR Y
	Keyword Usage	Optional keyword. By default, this keyword is not used unless it can be determined from the data source.		
TMIN	The minimum temperature requirement for the polynomial; if TMIN is lower than the starting temperature of input data, thermodynamic properties will be extrapolated at this point.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Temperature</i>	Required	K	TMIN 300
	Keyword Usage	Optional keyword. By default, the minimum temperature is 300 K unless it can be determined from data source.		

Keyword	Definition			
TMAX	The maximum temperature requirement for the polynomial; if TMAX is greater than the ending temperature of input data, thermodynamic properties will be extrapolated at this point.			
	Parameters	Optional/Reqd.	Units	Examples
	Temperature	Required	K	TMAX 5000
	Keyword Usage	Optional keyword. By default, the maximum temperature is 5000 K unless it can be determined from data source.		
TEMP	One or more temperatures dividing the ranges of the polynomial, at which the functional values are constrained; all TEMP values must be between TMIN and TMAX. Each TEMP given will result in a set of polynomial coefficients. If no TEMP is given, there will be one set of coefficients.			
	Parameters	Optional/Reqd.	Units	Examples
	Temperature or temperature range	Required	K	TEMP 1500 TEMP 1000 2000
	Keyword Usage	Optional keyword. By default, this keyword is not used unless it can be determined from the data source.		
H298	Species' formation enthalpy at 298.15 K.			
	Parameters	Optional/Reqd.	Units	Examples
	Enthalpy	Required	kcal/mole	H298 9.32
	Keyword Usage	Optional keyword. By default, this keyword is not used unless it can be determined from the data source.		
NO298	Indicates that the <i>FITDAT</i> program should not try to constrain the species' formation enthalpy at the 298.15 K value. Normally the <i>FITDAT</i> program will attempt to exactly match the temperature fit at the 298.15 K point, but in some cases (for example, the data point is not available) it may be desirable to remove this constraint.			
	Parameters	Optional/Reqd.	Units	Examples
		--	--	NO298
	Keyword Usage	Optional keyword. By default, the fit is constrained to exactly match the input value at 298.15 K.		
S298	Species' formation entropy at 298.15 K.			
	Parameters	Optional/Reqd.	Units	Examples
	Entropy	Required	cal/mole	S298 43.88
	Keyword Usage	Optional keyword. By default, this keyword is not used unless it can be determined from the data source.		
DATA	A table of data will follow, the format and contents of which depends on the data type given with this keyword.			
	Parameters	Optional/Reqd.	Calorie-based Units	Examples

Keyword	Definition			
	Type of data table	Required	--	DATA CHEM DATA JANAF DATA NIST DATA NASA
	Keyword Usage	Optional keyword. By default, the DATA CHEM option is used.		
POLY	A set of polynomial data will follow, the format and contents of which depends on the polynomial type given with this keyword. The CHEM option will display Ansys Chemkin-formatted polynomial records. The SHOM option will display Shomate polynomial records. The NASA option will display NASA-formatted polynomial records.			
	Parameters	Optional/Reqd.	Calorie-based Units	Examples
	Set of polynomial data	Required	--	POLY CHEM POLY SHOM POLY NASA
	Keyword Usage	Optional keyword. By default, the POLY CHEM option is used.		
VIBE	One or more species' vibrational frequency.			
	Parameters	Optional/Reqd.	Units	Examples
	Vibrational frequency	Required	cm ⁻¹	VIBE 999.83
	Keyword Usage	Optional keyword.		
NPTS	Number of points to generate from TMIN to TMAX, when evaluating properties data from POLY or VIBE.			
	Parameters	Optional/Reqd.	Units	Examples
	Number of points	Required	--	NPTS 50
	Keyword Usage	Optional keyword. By default, 100 points are generated.		
DELT	Temperature increment used from TMIN to TMAX, when evaluating properties data from POLY or VIBE.			
	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	Temperature	Required	K	DELT 50
	Keyword Usage	Optional keyword. By default, DELT value depends on the NPTS value.		
END	End of input, and start of the fitting process for the current species.			
	Keyword Usage	Required keyword.		

7.7. FITDAT Examples

This section discusses input files that allow *FITDAT* to provide thermodynamic data fitting coefficients using several different methods. These examples show NIST, Shomate, NASA, and other data formats ([DATA CHEM Input Format \(p. 115\)](#) through [VIBE Input Format \(p. 119\)](#)).

FITDAT is run from the Ansys Chemkin Interface by selecting it under **Utility** on the ribbon or the menu bar (see [FITDAT Utility for Fitting Polynomials to Thermodynamic Data](#) for more information). After running *FITDAT*, users may then launch the Chemkin Post-Processor using the **View > Graphical Post-processor** option. This action will actually result in a warning message and the display of a "Sample Plot", as *FITDAT* does not produce a typical solution file like other Chemkin problem and *FITDAT* results will therefore need to be plotted using the **Import** option in the Chemkin Post-Processor. Select the **File > Import** option in the Post-Processor. This opens a file browser to allow selecting a *species_name.csv* file for plotting of fit results. After the file has been selected, further select the following items from the Select the Import File Format dialog: **Comma** radio button, Skip 2 lines of text (**Skip** slider control), and **Read column titles** check box.

7.7.1. DATA CHEM Input Format

This is an example of the minimum input required to fit default type of data, which is four columns consisting of temperature (K), and species properties C_p (cal/mole-K), S (cal/mole-K), and $H(T) - H(298)$ (kcal/mole). Defaults are PHAS=G, TMIN=300, and TMAX=5000, the first and last positive data points, but keywords may be used to supersede these values.

Figure 7.2: DATA CHEM Input File

```

SPEC OH
ELEM O 1
ELEM H 1
H298 9.32
TEMP 1500
DATA
0300.00 007.165 043.926 000.013
0400.00 007.087 045.974 000.725
:
4900.00 009.232 065.778 038.571
5000.00 009.249 065.965 039.495
END

```

7.7.2. POLY CHEM Input Format

This is an example of the minimum input required to fit data evaluated from an existing Ansys Chemkin -format polynomial; defaults SPEC=OH, ELEM, PHAS=G , TMIN=300, TMAX=5000, and TEMP=1000

are obtained from the polynomial, and H298 by an evaluation of the polynomial, but keywords may be used to supersede these values. This option might be used to generate fits for a different temperature range where the original data are no longer available.

Figure 7.3: POLY CHEM Input File

```
POLY CHEM
OH          1212860    1H    1          G  0300.00    5000.00    1000.00          1
0.02882730E+02 0.10139743E-02 -0.02276877E-05 0.02174683E-09 -0.05126305E-14 2
0.03886888E+05 0.05595712E+02 0.03637266E+02 0.01850910E-02 -0.16761646E-05 3
0.02387202E-07 -0.08431442E-11 0.03606781E+05 0.13588605E+01
END
```

FITDAT evaluates the Ansys Chemkin polynomial as described in [Running *FITDAT* from the User Interface \(p. 109\)](#), to obtain thermodynamic properties for fitting. A table of NPTS temperatures from TMIN to TMAX will be used to evaluate the properties; keywords NPTS or DELT may be used to modify this phase.

7.7.3. DATA NIST Input Format

This is an example of the minimum input required to fit NIST-format data, which is 5 columns consisting of temperature (K), and species properties C_p (cal/mole·K), S (cal/mole·K), $-(G^o - H^o(298.15))/T$ (cal/mole·K) and $H(T) - H(298)$ (kcal/mole). Input data can be obtained from the *NIST Chemistry WebBook*[9] (p. 375),^{p. 124} using the following steps:

1. At the start of the NIST menu (<http://webbook.nist.gov/chemistry/form-ser.html>), choose **calorie-based units** in the toggle under question #3, when selecting the desired units for thermodynamic data.
2. Perform a **Formula Search** (for example, search for OH).
3. Select **View Table** option under the Heat Capacity heading.
4. In the table view, highlight and copy the table text, then paste into a text file.

Defaults are PHAS=G, and TMIN=300, TMAX=6000, the first and last positive data points greater than 298, but keywords may be used to supersede these values.

Figure 7.4: DATA NIST Input File

```
SPEC OH
ELEM O 1
ELEM H 1
H298 9.318131
TEMP 1500.
DATA NIST
300. 7.16 43.95 43.91 0.01
400. 7.09 46.00 44.19 0.73
:
5900. 9.41 67.53 59.42 47.89
6000. 9.43 67.69 59.55 48.83
END
```

7.7.4. POLY SHOM Input Format

This is an example of the minimum input required to convert a Shomate polynomial to Ansys Chemkin format; The Shomate equations are given in Equation 7.1 (p. 117) through Equation 7.3 (p. 117), where $t = \text{Temperature(K)}/1000$. Parameters (A, B, C, D, E, F, G, and $H^\circ f$, 298) can be obtained from the NIST Chemistry WebBook.[9] (p. 375)

1. At the start of the NIST menu(<http://webbook.nist.gov/chemistry/form-ser.html>), choose **calorie-based units** in the toggle under question #3, when selecting the desired units for thermodynamic data.
2. Perform a **Formula Search** (for example, search for OH).
3. Highlight and copy the table of parameters (including the heading row and the rows for the A, B, C, D, E, F, G parameters), then paste these into a text file.

Defaults are PHAS=G, TMIN=298, TMAX=6000, and TEMP=1000 are obtained from the Shomate data, and H298 by an evaluation of the polynomial, but keywords may be used to supersede the defaults.

Figure 7.5: POLY SHOM Input File

```
SPEC OH
ELEM O 1
ELEM H 1
POLY SHOM
Temperature (K) 298. - 1300. 1300. - 6000.
A 7.714551 6.870701
B -2.715801 1.126790
C 3.251781 -0.194724
D -0.919332 0.013085
E -0.000319 -0.656747
F 7.110691 6.313191
G 53.91451 51.17510
END
```

$$C_p = A + Bt + Ct^2 + Dt^3 + \frac{E}{t^2} \quad (7.1)$$

$$H - H(298) = At + \frac{Bt^2}{2} + \frac{Ct^3}{3} + \frac{Et^4}{4} - \frac{E}{t} + F - H(298) \quad (7.2)$$

$$S = A \ln(t) + Bt + \frac{Ct^2}{2} + \frac{Dt^3}{3} - \frac{E}{2t^2} + G \quad (7.3)$$

A table of NPTS temperatures from TMIN to TMAX will be used to evaluate the properties; keywords NPTS or DELT may be used to modify this process.

7.7.5. DATA NASA Input Format

This is an example of the minimum input required to fit NASA-format data, which is at least four columns consisting of temperature (K), and species properties C_p (cal/mole-K), $H(T) - H(298)$ (kcal/mole), and S (cal/mole-K). NASA data can be obtained from the Properties From Coefficients (PFC) [9] (p. 375) program; request **calorie-based units**, and highlight, copy, and paste the resulting table into a text file. Defaults are PHAS=G, TMIN=300, TMAX=6000, the first and last positive data points, and H298 is the column 6 value at T=298.15, but keywords may be used to supersede the defaults.

Figure 7.6: DATA NASA Input File

```

SPEC OH
ELEM O 1
ELEM H 1
DATA NASA
! THERMODYNAMIC FUNCTIONS CALCULATED FROM COEFFICIENTS FOR OH
!      T      Cp      H-H298      S      -(G-H298)/T      H      delta Hf      log K
!      deg-K   cal/mol-K   kcal/mol   cal/mol-K   cal/mol-K   kcal/mol   kcal/mol
!      0        0.        -2.106     0.        INFINITE    6.803     8.853     INFINITE
!      200      7.293    -0.707    41.035    44.572     8.202     8.877     -8.9035
!      298.15   7.143     0.000    43.915    43.915     8.910
!      :
!      :
!      5900     9.620     48.463    67.672    59.458     57.373     6.636     0.3749
!      6000     9.625     49.425    67.834    59.596     58.335     6.573     0.3790
END

```

7.7.6. POLY NASA Input Format

This is an example of the minimum input required to convert a NASA polynomial[10] (p. 375) to Chemkin format. The equations defining polynomials are given in Equation 7.4 (p. 119) through Equation 7.6 (p. 119). NASA polynomial data can be obtained from the Properties From Coefficients (PFC)[11] (p. 375)^{p. 124} and then highlighted, copied, and pasted into a text file. Defaults for SPEC, ELEM, PHAS, TMIN, TMAX, TEMP, and H298 are obtained from the polynomial, but may be superseded by keyword usage.

Figure 7.7: POLY NASA Input File

```

POLY NASA
OH      D0(H-OH): Ruscic,2002. Gurvich,1978 pt1 p110 pt2 p37.
3 g 4/02 0 1.00H 1.00 0.00 0.00 0.00 0 17.00734 37278.206
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8813.106
-1.998858990E+03 9.300136160E+01 3.050854229E+00 1.529529288E-03 -3.157890998E-06
3.315446180E-09 -1.138762683E-12 0.000000000E+00 2.991214235E+03 4.674110790E+00
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8813.106
1.017393379E+06 -2.509957276E+03 5.116547860E+00 1.305299930E-04 -8.284322260E-08
2.006475941E-11 -1.556993656E-15 0.000000000E+00 2.019640206E+04 -1.101282337E+01
6000.000 20000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8813.106
2.847234193E+08 -1.859532612E+05 5.008240900E+01 -5.142374980E-03 2.875536589E-07
-8.228817960E-12 9.567229020E-17 0.000000000E+00 1.468393908E+06 -4.023555580E+02
END

```

Figure 7.8: Format details for POLY NASA Input Files

```

line 1:      OH is species name
line 2:      3 is the number of temperature ranges
              5 sets of elemental composition, that is, 'O 1.00' and 'H 1.00'
              0 in the next field indicates a gas
              17.00734 is the molecular weight
              37278.206 is H298 heat of formation, J/mol
line 3:      200-1000 is the first temperature range,
              7 is the number of Cp/R polynomial coefficients,
              -2,-1,0,1,2,3,4,0 are the T exponents for the coefficients,
              8813.106 is H(298)-H(0), J/mol
line 4:      a1 through a5 for temperatures 200-1000K
line 5:      a6 through a7 for temperatures 200-1000K, a8 (not used),
              integration constants b1, b2
lines 6-end: same as 3-5, for more temperature ranges

```


The resulting non-dimensional thermodynamic properties are

$$\frac{C_p}{R} = a_1 T^{-2} + a_2 T^{-1} + a_3 + a_4 T + a_5 T^2 + a_6 T^3 + a_7 T^4 \quad (7.4)$$

$$\frac{H}{RT} = -a_1 T^{-2} + a_2 T^{-1} \ln(T) + a_3 + \frac{a_4 T}{2} + \frac{a_5 T^2}{3} + \frac{a_6 T^3}{4} + \frac{a_7 T^4}{5} + \frac{b_1}{T} \quad (7.5)$$

$$\frac{S}{R} = \frac{-a_1 T^{-2}}{2} - a_2 T^{-1} + a_3 \ln(T) + a_4 T + \frac{a_5 T^2}{2} + \frac{a_6 T^3}{3} + \frac{a_7 T^4}{4} + b_2 \quad (7.6)$$

A table of NPTS temperatures from TMIN to TMAX will be used to evaluate the properties; keywords NPTS or DELT may be used to modify this process.

7.7.7. DATA JANAF Input Format

This is an example of the minimum input required to fit JANAF-format data, which is at least five columns consisting of temperature (K), and species properties C_p (J/mole-K), S (J/mole-K), G (J/mole-K), and $H(T) - H(298)$ (kJ/mole). Defaults SPEC=OH, PHAS=G, and ELEM are obtained from the CODE line, TMIN=300, TMAX=6000 are the first and last positive data points greater than 298, and $H(298)$ (kJ/mole) is the column 6 value at $T=298.15$, but keywords may be used to supersede the defaults.

Figure 7.9: DATA JANAF Input File

```
DATA JANAF

! Janaf table documentation:
! Col 2-10: Temperature (K)
! Col 11-19: Heat Capacity, Cp (J/K-mole)
! Col 20-29: Entropy, S (J/K-mole)
! Col 30-39: Gibbs Free Energy, G (J/K-mole)
! Col 40-51: Relative Enthalpy, H-H298 (kJ/mole)
! Col 52-62: Enthalpy of Formation, Hf (kJ/mole)
! Col 63-74: Gibbs Energy of Formation, Gf (kJ/mole)
! Col 75-85: log (Equilibrium constant of formation), log(Keq(T))
! Note: some of the above are in KJ and some in J.CODE = 300 H101(g)

CODE = 300 H101(g)

!Hydroxyl (OH)
!
!      0      0.      0.      INFINITE      -9.172      38.390      38.390      INFINITE
25     29.487    106.145    447.063      -8.523      38.411      38.109      -79.625
50     31.487    127.111    282.386      -7.764      38.391      37.805      -39.494
75     32.719    140.171    232.937      -6.957      38.390      37.516
:
:
5900   39.350    282.564    248.604    200.369    27.391    -39.860    0.353
6000   39.423    283.226    249.175    204.308    27.019    -40.997    0.357

!PREVIOUS: June 1977 (1 atm)          CURRENT: June 1977 (1 bar)
END
```

7.7.8. VIBE Input Format

This is an example of the minimum input required to fit vibrational frequency data. Defaults are PHAS=G, TMIN=300, TMAX=6000, and LINR=No (from the fact of more than one VIBE), but keywords may be used to supersede the defaults.

This method is provided for use in cases where little or no information is available in the literature about the molecule of interest. It contains a number of approximations:

1. Translational contributions to the heat capacity are treated classically via the equipartition function. This is generally a good assumption.
2. Rotational contributions to the heat capacity are treated classically via the equipartition function. This is a good assumption for most molecules at higher temperatures.
3. Hindered internal rotors are not explicitly treated, but rather approximated as vibrations. This is a less-good approximation.

In all cases, these approximations are more likely to break down at lower temperatures.

Figure 7.10: VIBE Input File

```
SPEC SIH2
ELEM SI 1
ELEM H 2
H298 58.0
S298 49.4
TEMP 1000
VIBE 999.83
VIBE 2011.69
VIBE 2001.72
END
```

7.7.9. Example *FITDAT* Outputs

Figure 7.11: Example *fitdat.out* file (p. 120) shows the *fitdat.out* file that will be created if the DATA CHEM input file discussed in DATA CHEM Input Format (p. 115) is run through the *FITDAT* utility.

Figure 7.11: Example *fitdat.out* file

```
*****
*                      CHEMKIN Release 4.0                      *
*                      FITDAT Application                        *
*      Thermodynamic properties fitting program.                *
* Copyright 1997-2002 Reaction Design. All Rights Reserved. *
*****
```

	WORKING SPACE PROVIDED	REQUIREMENTS REQUIRED
INTEGER	112	112
REAL	9534	9534

Reading keyword data...

```
Setting SPEC name:      OH
Setting ELEM # 1:      0  1
Setting ELEM # 2:      H  1
Setting H298:          9.320E+00 Kcal/mole
Setting TEMP # 1:      1.000E+03 K
End of keyword input for species OH
```

Species OH Fit:

OH	0	1H	1	G	300.000	5000.000	1000.00	1
	0.29446142E+01	0.91447172E-03	-0.17338418E-06	0.95183610E-11	0.46042672E-15			2

```

0.38598718E+04 0.52419727E+01 0.35069641E+01 0.12114174E-02-0.44383205E-05    3
0.53991545E-08-0.19835349E-11 0.36200845E+04 0.18923732E+01                    4

Reading keyword data...
End of input file...

```

Figure 7.12: Example *fitdat.out* file with more than two temperature ranges (p. 121) shows example output that would result if the input discussed in **DATA CHEM Input Format** (p. 115) is modified to include polynomial coefficients for more than two temperature ranges (for example, adding keyword line: TEMP 2500).

Figure 7.12: Example *fitdat.out* file with more than two temperature ranges

```

*****
*                               CHEMKIN Release 4.0                               *
*                               FITDAT Application                               *
*                               Thermodynamic properties fitting program.          *
* Copyright 1997-2002 Reaction Design. All Rights Reserved. *
*****

      WORKING SPACE REQUIREMENTS
      PROVIDED      REQUIRED
INTEGER          112          112
REAL             9534         9534

Reading keyword data...
Setting SPEC name:          OH
Setting ELEM #  1:          O   1
Setting ELEM #  2:          H   1
Setting H298:              9.320E+00 Kcal/mole
Setting TEMP #  1:          1.000E+03 K
Setting TEMP #  2:          2.500E+03 K
End of keyword input for species OH

Species OH Fit:
OH              O   1H   1          G   300.000  5000.000          1
TEMP  300.000  1000.000  2500.000  5000.000
0.31521126E+01 0.77090695E-03-0.15393767E-06 0.13363294E-10-0.27768811E-15
0.36675921E+04 0.39045946E+01
0.34408417E+01-0.28167277E-03 0.83197801E-06-0.34404565E-09 0.44913015E-13
0.37077941E+04 0.26162167E+01
0.37729215E+01-0.61576963E-03-0.15821000E-06 0.13103019E-08-0.61722943E-12
0.35916670E+04 0.76556823E+00

Reading keyword data...
End of input file...

```

Chapter 8: CHEMKIN Project Input: Keyword Syntax and Rules

In most cases, a Reactor Model input file is written by the Ansys Chemkin Interface before a simulation run based on the Chemkin Project Input. The panel context and "bubble" help within the Interface provide basic guidance for setting up model-specific input parameters. However, in some cases users may want further information about a model parameter usage and in other cases they may want to assemble their own input files outside of the User Interface. For such cases, this chapter together with [Reference Guide to Project Input Keywords \(p. 125\)](#) and [Alphabetical Listing of Project Input Keywords \(p. 139\)](#) contain detailed information about input options for each Reactor Model. This chapter provides an overview of the syntax and rules for such parameter input.

User input information is generally written to a Reactor Model input file in "keyword" format. In this format, each input line starts with an identifying keyword. For some input, only the keyword itself is required, while others require one or more pieces of additional information. Many keywords have default values associated with them. If these default values are appropriate for the user's problem, then these keywords do not need to be included in the input file. In the case of restarts or continuation problems, some of the parameters can be changed from what was used in the previous solution. If these keywords are not included or not changed in the input keyword list for continuations or restarts, then the parameters will retain their former values. In the list of keywords that follow, we indicate whether or not each keyword may be changed on a restart from a previous solution. The order of the keyword input is not important. The general rules governing the syntax of the keyword lines are listed in [Table 8.1: Summary of the Rules for Keywords \(p. 123\)](#).

Note:

Note that you can turn on or off the display of the "Keyword" associated with an Ansys Chemkin Interface input parameter, using the modal option in the Preferences panel.

Table 8.1: Summary of the Rules for Keywords

Rule	Description
1	The first character-string in the line must be a keyword; the length of the character-string depends on keyword descriptions.
2	Any further input associated with the keyword can appear anywhere after the keyword, through column 80. The specific starting column is not important, as long as there is at least one space after the keyword.
3	When more than one piece of information is required, the order in which the information appears is important.
4	When numbers are required as input, they may be stated in integer, floating-point, or "E" format. Ansys Chemkin converts the numbers to the proper type internally. The double precision specification D is not recognized; however, the double precision conversion will be done internally, as necessary.

Rule	Description
5	When species names are required as input, they must appear exactly as they are specified in the <i>Gas-phase Kinetics</i> and <i>Surface Kinetics</i> input files.
6	When more than one piece of information is required, the pieces are delimited by one or more blank spaces.
7	If contradictory or duplicate keywords are input, Ansys Chemkin uses the information that is last read. Under some circumstances, this will result in a warning printed to the output file.
8	A "comment" line is one that has either a period (.), slash (/), or exclamation mark (!) as the first non-blank character. In addition, on any Keyword line, any input that follows an exclamation mark is taken as a comment. All input lines, including comments, are printed to the output.
9	The keyword END must be the last input card. END keywords are required between sets of parameters for continuations.
10	If no parameter is given, then the keyword stands alone on the input line; keywords with parameters are demonstrated with examples.

Chapter 9: Reference Guide to Project Input Keywords

In this chapter, we group the available input reactor project input options (keywords) according to the Reactor Model with which they may be used. Note that many keywords can be used with several different Reactor Models and that there are a few cases where keywords that share the same name may have different meanings for different Reactor Models. General information about keyword syntax and rules is given in [CHEMKIN Project Input: Keyword Syntax and Rules \(p. 123\)](#). A detailed, alphabetical listing of all keywords is given in [Alphabetical Listing of Project Input Keywords \(p. 139\)](#). This chapter is meant to serve as a quick cross-reference to the more detailed information in [Alphabetical Listing of Project Input Keywords \(p. 139\)](#).

9.1. Closed 0-D Reactor Models

9.1.1. Internal Combustion HCCI Engine

The following keywords can be used to build an input file for an IC HCCI Engine Reactor Model:

ADAP (p. 141), ADD (p. 141), AEXT (p. 142), AGGA (p. 145), AGGB (p. 145), AGGD (p. 146), AGGE (p. 146), AGGFD (p. 147), AGGMN (p. 148), AROP (p. 152), ASEN (p. 153), ASTEPS (p. 154), ATLS (p. 157), ATOL (p. 157), AVALUE (p. 159), AVAR (p. 159), BETA (p. 161), CAADV (p. 167), CAATQ (p. 167), CKTRN (p. 169), CLSC (p. 170), CLSM (p. 170), CMPR (p. 171), CNTN (p. 172), CNTT (p. 173), COLR (p. 174), CRLN1 (p. 177), CRLN2 (p. 177), CRRD1 (p. 178), CRRD2 (p. 178), CSVOUTPUT_FILENAME (p. 178), CSVOUTPUT_KOUT (p. 179), CSVOUTPUT_WRITE (p. 180), CYBAR (p. 181), DEG0 (p. 182), DELT (p. 182), DIST (p. 184), DTDEG (p. 186), DTIGN (p. 186), DTSV (p. 188), EGRR (p. 190), END (p. 192), EPSR (p. 197), EPSS (p. 197), EPST (p. 198), EQUI (p. 199), FUEL (p. 211), FVCP (p. 212), GFAC (p. 213), GMHTC (p. 214), GVEL (p. 216), HIMP (p. 216), HTC (p. 219), HTCPRO (p. 219), ICEN (p. 222), ICHF (p. 221), ICHH (p. 221), ICHT (p. 223), ICHW (p. 223), IPSR (p. 228), KLIM (p. 231), LODR (p. 233), LOLR (p. 233), MAXIT (p. 236), MCUT (p. 237), MMASS (p. 239), NADAP (p. 244), NCANG (p. 245), NEWRUN (p. 245), NMOM (p. 247), NNEG (p. 247), NO_SDOUTPUT_WRITE (p. 247), NOCG (p. 248), NO_XMLOUTPUT_WRITE (p. 247), NREV (p. 252), NSOL (p. 252), OPMV (p. 255), OPOC (p. 256), OXID (p. 256), PNDE (p. 261), POLN1 (p. 263), POLN2 (p. 263), PRDL (p. 264), PRES (p. 265), PRNT (p. 266), PROE (p. 268), PSBAR (p. 270), PTM_SECTION_SIZEDEP_A0 (p. 271), PTM_SECTION_SIZEDEP_COLEFF (p. 272), PTM_SECTION_SIZEDEP_DSTAR (p. 272), PTM_SECTION_SIZEDEP_HAMAKER (p. 273), PTM_SECTION_USERBULKROP (p. 275), PTM_SECTIONAL (p. 275), PVFE (p. 276), PVS0 (p. 277), PVSIN (p. 278), PVST (p. 278), QEXP (p. 280), QFUN (p. 280), QLOS (p. 281), QPRO (p. 283), QRGEQ (p. 284), REAC (p. 288), RELAXC (p. 290), RLGAS (p. 292), RLMIX (p. 293), ROP (p. 294), RPM (p. 294), RSTR (p. 295), RTLS (p. 297), RTOL (p. 298), SCLM (p. 302), SCLS (p. 302), SDOUTPUT_WRITE (p. 304), SENT (p. 305), SIZE (p. 308), SOLUTION_TECHNIQUE (p. 310), SSTT (p. 314), STPT (p. 316), SVS0 (p. 318), SVSS (p. 318), SVST (p. 318), TEMP (p. 323), TEXP (p. 325), TIFP (p. 328), TIME (p. 330), TLIM (p. 333), TRAN (p. 336), TRES (p. 338), TRST (p. 339), TSTR (p. 342), TTIM (p. 344), UIGN (p. 346), UREF (p. 347), USET (p. 349), VCPRO (p. 352), VOLC (p. 359), VOLD (p. 359), WENG (p. 363), WOSP1 (p. 364), WOSP2 (p. 365), WOSP3 (p. 365), XMLI (p. 369), XMLOUTPUT_WRITE (p. 369)

9.1.2. Closed Homogeneous Batch Reactor

The following keywords can be used to build an input file for a Closed Homogeneous Reactor Model:

ADAP (p. 141), ADD (p. 141), AEXT (p. 142), AFRA (p. 144), AGGA (p. 145), AGGB (p. 145), AGGD (p. 146), AGGE (p. 146), AGGFD (p. 147), AGGMN (p. 148), AINT (p. 148), AREA (p. 150), AREAQ (p. 151), AROP (p. 152), ASEN (p. 153), ASTEPS (p. 154), ATLS (p. 157), ATOL (p. 157), AVALUE (p. 159), AVAR (p. 159), BETA (p. 161), BLKEQ (p. 162), BULK (p. 164), CLSC (p. 170), CLSM (p. 170), CNTN (p. 172), CNTT (p. 173), COLR (p. 174), CONP (p. 175), CONV (p. 175), COTV (p. 176), CSVOUTPUT_FILENAME (p. 178), CSVOUTPUT_KOUT (p. 179), CSVOUTPUT_WRITE (p. 180), DELT (p. 182), DIST (p. 184), DTIGN (p. 186), DTSV (p. 188), EGRR (p. 190), END (p. 192), ENRG (p. 194), EPSG (p. 196), EPSR (p. 197), EPSS (p. 197), EPST (p. 198), EQUI (p. 199), ETCH (p. 200), FUEL (p. 211), GFAC (p. 213), GMHTC (p. 214), HTC (p. 219), HTRN (p. 220), IPSR (p. 228), IRET (p. 229), ISTP (p. 230), KLIM (p. 231), MAXIT (p. 236), MCUT (p. 237), MMASS (p. 239), NADAP (p. 244), NEWRUN (p. 245), NMOM (p. 247), NNEG (p. 247), NO_SDOUTPUT_WRITE (p. 247), NOCG (p. 248), NO_XMLOUTPUT_WRITE (p. 247), NOCG (p. 248), NSOL (p. 252), OXID (p. 256), PBDEN (p. 257), PNDE (p. 261), PPRO (p. 264), PRES (p. 265), PRNT (p. 266), PROE (p. 268), PTM_SECTION_SIZEDEP_A0 (p. 271), PTM_SECTION_SIZEDEP_COEFF (p. 272), PTM_SECTION_SIZEDEP_DSTAR (p. 272), PTM_SECTION_SIZEDEP_HA-MAKER (p. 273), PTM_SECTION_USERBULKROP (p. 275), PTM_SECTIONAL (p. 275), PVFE (p. 276), QFUN (p. 280), QLOS (p. 281), QPRO (p. 283), QRGEQ (p. 284), QRSEQ (p. 285), REAC (p. 288), RELAXC (p. 290), RLGAS (p. 292), RLMIX (p. 293), ROP (p. 294), RSTR (p. 295), RTLS (p. 297), RTOL (p. 298), SCLM (p. 302), SCLS (p. 302), SCOR (p. 303), SDOUTPUT_WRITE (p. 304), SENG (p. 304), SENT (p. 305), SFAC (p. 306), SIZE (p. 308), SOLUTION_TECHNIQUE (p. 310), SSTT (p. 314), STPT (p. 316), SURF (p. 317), TAMB (p. 320), TEMP (p. 323), TGIV (p. 326), TIFP (p. 328), TIME (p. 330), TLIM (p. 333), TPRO (p. 334), TRAN (p. 336), TRES (p. 338), TRST (p. 339), TSRF (p. 340), TSTR (p. 342), TTIM (p. 344), UIGN (p. 346), USET (p. 349), VOL (p. 359), VPRO (p. 360), VTIM (p. 361), WENG (p. 363), XMLI (p. 369), XMLOUTPUT_WRITE (p. 369)

9.1.3. Closed Partially Stirred Reactor

The following keywords can be used to build an input file for a Closed PaSR Reactor Model:

ADAM (p. 140), ATOL (p. 157), BDF (p. 160), CFL (p. 169), CHEM (p. 169), CLSE (p. 170), CMIX (p. 171), CTOL (p. 180), CURL (p. 181), DASP (p. 182), DT (p. 186), DT0 (p. 186), DTMX (transient) (p. 188), DTSV (p. 188), END (p. 192), EQUI (p. 199), IEM (p. 224), INIT (p. 225), KOUT (p. 232), MAXIT (p. 236), MAXTIME (p. 236), MIX (p. 237), MIXT (p. 238), NCFIT (p. 245), NDPR (p. 245), NNEG (p. 247), NO_SDOUTPUT_WRITE (p. 247), NOCG (p. 248), NO_XMLOUTPUT_WRITE (p. 247), NOJC (p. 249), NPAR (p. 250), PDF (p. 258), PRES (p. 265), QRGEQ (p. 284), QRSEQ (p. 285), RELAXC (p. 290), RLGAS (p. 292), RLMIX (p. 293), RSTR (p. 295), RTOL (p. 298), SCAT (p. 299), SDOUTPUT_WRITE (p. 304), SIZE (p. 308), SSMAXITER (p. 313), TEMP (p. 323), TIME (p. 330), TRES (p. 338), TRMAXITER (p. 338), VOL (p. 359), VPRO (p. 360), WELL (p. 363), XMLOUTPUT_WRITE (p. 369)

9.1.4. Closed Plasma Reactor

The following keywords can be used to build an input file for a Closed Plasma Reactor Model:

ABSL (p. 140), ADAP (p. 141), AEXT (p. 142), AFRA (p. 144), AGGD (p. 146), AGGE (p. 146), AINT (p. 148), AREA (p. 150), AREAQ (p. 151), AROP (p. 152), ASEN (p. 153), ASTEPS (p. 154), ATIM (p. 155), ATLM (p. 156), ATLS (p. 157), ATOL (p. 157), AVALUE (p. 159), AVAR (p. 159), BETA (p. 161), BLKEQ (p. 162), BOHM (p. 78), BPWR (p. 163), BULK (p. 164), CLSC (p. 170), CLSM (p. 170), CNTN (p. 172), CNTT (p. 173), CONP (p. 175), COLR (p. 174), CONV (p. 175), DELT (p. 182), DFAC (p. 183), DIST (p. 184), DTIGN (p. 186), DTSV (p. 188), ELSH (p. 190), END (p. 192), ENGE (p. 193), ENRG (p. 194), EPSG (p. 196), EPSR (p. 197), EPSS (p. 197), EPST (p. 198), ETCH (p. 200), ETMP (p. 201), GFAC (p. 213), GMHTC (p. 214), HTC (p. 219), HTRN (p. 220), IONE (p. 228), IPSR (p. 228), KLIM (p. 231), MAXIT (p. 236), MCUT (p. 237), MMASS (p. 239), NADAP (p. 244),

NEWRUN (p. 245), NMOM (p. 247), NNEG (p. 247), NO_SDOUTPUT_WRITE (p. 247), NO_XMLOUTPUT_WRITE (p. 247), NOCG (p. 248), NSOL (p. 252), PNDE (p. 261), PPRO (p. 264), PRES (p. 265), PRNT (p. 266), PROE (p. 268), PVFE (p. 276), PWRW (p. 279), QFUN (p. 280), QLOS (p. 281), QLSE (p. 282), QPRO (p. 283), REAC (p. 288), RELAXC (p. 290), ROP (p. 294), RSTR (p. 295), RTIM (p. 296), RTLM (p. 297), RTLS (p. 297), RTOL (p. 298), SCLM (p. 302), SCLS (p. 302), SCOR (p. 303), SDOUTPUT_WRITE (p. 304), SENG (p. 304), SENT (p. 305), SFAC (p. 306), SIZE (p. 308), SOLUTION_TECHNIQUE (p. 310), SSTT (p. 314), STPT (p. 316), SURF (p. 317), TAMB (p. 320), TEBND (p. 323), TEMP (p. 323), TGIV (p. 326), TIFP (p. 328), TIME (p. 330), TION (p. 332), TLIM (p. 333), TPRO (p. 334), TRAN (p. 336), TRES (p. 338), TRST (p. 339), TSRF (p. 340), TSTR (p. 342), TTIM (p. 344), USET (p. 349), UIGN (p. 346), VOL (p. 359), VPRO (p. 360), VTIM (p. 361), WENG (p. 363), WPRO (p. 366), XMLI (p. 369), XMLOUTPUT_WRITE (p. 369), XSDF (p. 371), XSEK (p. 371)

9.1.5. Multi-Zone HCCI Engine Simulator

The following keywords can be used to build an input file for a Multi-Zone HCCI Engine Simulator:

ADAP (p. 141), ADD (p. 141), AEXT (p. 142), AGGA (p. 145), AGGB (p. 145), AGGD (p. 146), AGGE (p. 146), AGGFD (p. 147), AGGMN (p. 148), AROP (p. 152), ASEN (p. 153), ASTEPS (p. 154), ASWH (p. 155), ATLS (p. 157), ATOL (p. 157), AVALUE (p. 159), AVAR (p. 159), BETA (p. 161), CAADV (p. 167), CAATQ (p. 167), CKTRN (p. 169), CLSC (p. 170), CLSM (p. 170), CMPR (p. 171), CNTN (p. 172), CNTT (p. 173), COLR (p. 174), CRLN1 (p. 177), CRLN2 (p. 177), CRRD1 (p. 178), CRRD2 (p. 178), CYBAR (p. 181), DEG0 (p. 182), DELT (p. 182), DIST (p. 184), DTDEG (p. 186), DTIGN (p. 186), DTSV (p. 188), END (p. 192), EPSR (p. 197), EPSS (p. 197), EPST (p. 198), EQUI (p. 199), FUEL (p. 211), FVCP (p. 212), GFAC (p. 213), GMHTC (p. 214), GVEL (p. 216), HIMP (p. 216), HTC (p. 219), HTC PRO (p. 219), ICEN (p. 222), ICHF (p. 221), ICHH (p. 221), ICHT (p. 223), ICHW (p. 223), ICHT (p. 223), IPSR (p. 228), KLIM (p. 231), LODR (p. 233), LOLR (p. 233), MAXIT (p. 236), MCUT (p. 237), MMASS (p. 239), MQAFR (p. 241), MZMAS (p. 244), NADAP (p. 244), NCANG (p. 245), NEWRUN (p. 245), NMOM (p. 247), NNEG (p. 247), NO_SDOUTPUT_WRITE (p. 247), NO_XMLOUTPUT_WRITE (p. 247), NOCG (p. 248), NREV (p. 252), NSOL (p. 252), NZONE (p. 254), OPMV (p. 255), OPOC (p. 256), OXID (p. 256), PNDE (p. 261), POLN1 (p. 263), POLN2 (p. 263), PRDL (p. 264), PRES (p. 265), PRNT (p. 266), PROE (p. 268), PSBAR (p. 270), PTM_SECTION_USERBULKROP (p. 275), PTM_SECTIONAL (p. 275), PVFE (p. 276), PVS0 (p. 277), PVSN (p. 278), PVST (p. 278), QEXP (p. 280), QFUN (p. 280), QLOS (p. 281), QPRO (p. 283), QRGEQ (p. 284), RELAXC (p. 290), RLGAS (p. 292), RLMIX (p. 293), ROP (p. 294), RPM (p. 294), RSTR (p. 295), RTLS (p. 297), RTOL (p. 298), SCLM (p. 302), SCLS (p. 302), SCOR (p. 303), SDOUTPUT_WRITE (p. 304), SENT (p. 305), SIZE (p. 308), SOLUTION_TECHNIQUE (p. 310), SSTT (p. 314), STPT (p. 316), TEMP (p. 323), SVS0 (p. 318), SVSS (p. 318), SVST (p. 318), TEXP (p. 325), TIFP (p. 328), TIME (p. 330), TLIM (p. 333), TRAN (p. 336), TRES (p. 338), TRST (p. 339), TSTR (p. 342), TSWH (p. 343), TTIM (p. 344), UIGN (p. 346), UREF (p. 347), USET (p. 349), VCPRO (p. 352), VOL (p. 359), VOLC (p. 359), VOLD (p. 359), WENG (p. 363), WOSP1 (p. 364), WOSP2 (p. 365), WOSP3 (p. 365), XEST (p. 368), XMLI (p. 369), XMLOUTPUT_WRITE (p. 369), ZONEAVG (p. 373)

9.1.6. SI Engine Zonal Simulator

The following keywords can be used to build an input file for an SI Engine Zonal Simulator:

ADAP (p. 141), ADD (p. 141), AEXT (p. 142), AGGA (p. 145), AGGB (p. 145), AGGD (p. 146), AGGE (p. 146), AGGFD (p. 147), AGGMN (p. 148), AROP (p. 152), ASEN (p. 153), ASTEPS (p. 154), ASWH (p. 155), ATLS (p. 157), ATOL (p. 157), AVALUE (p. 159), AVAR (p. 159), BETA (p. 161), CAAC (p. 166), CAADV (p. 167), CAATQ (p. 167), CAEC (p. 167), CASC (p. 168), CKTRN (p. 169), CLSC (p. 170), CLSM (p. 170), CMPR (p. 171), CNTN (p. 172), CNTT (p. 173), COLR (p. 174), CRLN1 (p. 177), CRLN2 (p. 177), CRRD1 (p. 178), CRRD2 (p. 178), CYBAR (p. 181), DEG0 (p. 182), DEGE (p. 182), DELT (p. 182), DIST (p. 184), DTDEG (p. 186), DTIGN (p. 186), DTSV (p. 188), END (p. 192), EPSR (p. 197), EPSS (p. 197), EPST (p. 198), SIZE (p. 308), EQUI (p. 199), FUEL (p. 211), FVCP (p. 212), GFAC (p. 213), GMHTC (p. 214), GVEL (p. 216), HSWC (p. 218), HSWM (p. 219), HSWT (p. 218),

HIMP (p. 216), HTC (p. 219), HTCPRO (p. 219), ICEN (p. 222), ICHF (p. 221), ICHH (p. 221), ICHT (p. 223), ICHW (p. 223), IPSR (p. 228), KLIM (p. 231), LODR (p. 233), LOLR (p. 233), MAXIT (p. 236), MCUT (p. 237), MMASS (p. 239), NADAP (p. 244), NCANG (p. 245), NEWRUN (p. 245), NMOM (p. 247), NNEG (p. 247), NO_SDOUTPUT_WRITE (p. 247), NO_XMLOUTPUT_WRITE (p. 247), NOCG (p. 248), NREV (p. 252), NSOL (p. 252), OPMV (p. 255), OPOC (p. 256), OXID (p. 256), PNDE (p. 261), POLN1 (p. 263), POLN2 (p. 263), PRDL (p. 264), PRES (p. 265), PRNT (p. 266), PROE (p. 268), PSBAR (p. 270), PTM_SECTION_USERBULK-ROP (p. 275), PTM_SECTIONAL (p. 275), PVFE (p. 276), PVS0 (p. 277), PVS1 (p. 278), PVST (p. 278), QEXP (p. 280), QFUN (p. 280), QLOS (p. 281), QPRO (p. 283), QRGEO (p. 284), RELAXC (p. 290), RLGAS (p. 292), RLMIX (p. 293), ROP (p. 294), RPM (p. 294), RSTR (p. 295), RTLS (p. 297), RTOL (p. 298), SCLM (p. 302), SCLS (p. 302), SCOR (p. 303), SDOUTPUT_WRITE (p. 304), SENT (p. 305), SIDR (p. 308), SIKN (p. 308), SIOA (p. 308), SIZE (p. 308), SOLUTION_TECHNIQUE (p. 310), SSTT (p. 314), STPT (p. 316), SVS0 (p. 318), SVSS (p. 318), SVST (p. 318), TEMP (p. 323), TEXP (p. 325), TIFP (p. 328), TIME (p. 330), TLIM (p. 333), TRAN (p. 336), TRES (p. 338), TRST (p. 339), TSTR (p. 342), TTIM (p. 344), UIGN (p. 346), UREF (p. 347), USET (p. 349), VCPRO (p. 352), VOL (p. 359), VOLC (p. 359), VOLD (p. 359), WENG (p. 363), WOSP1 (p. 364), WOSP2 (p. 365), WOSP3 (p. 365), XEST (p. 368), XMLI (p. 369), XMLOUTPUT_WRITE (p. 369), ZONEAVG (p. 373)

9.1.7. Direct Injection Diesel Engine Simulator

The following keywords can be used to build an input file for a Direct Injection Diesel Engine Simulator:

AFRMX (p. 145), ATLRE (p. 156), ATLS (p. 157), AZFAC (p. 160), BMCOE (p. 162), BTMIN (p. 164), CAADV (p. 167), CAIR (p. 167), CRLN1 (p. 177), CRLN2 (p. 177), CRRD1 (p. 178), CRRD2 (p. 178), DIEN (p. 184), DINZL (p. 184), FICA0 (p. 205), FIDUR (p. 206), FIEQM (p. 206), FILFY (p. 206), FIMAS (p. 206), FINJP (p. 206), FINRD (p. 207), FINTL (p. 207), FITMP (p. 207), FLINJ (p. 208), LMLM (p. 233), MVFAC (p. 243), MXITS (p. 243), NO_SDOUTPUT_WRITE (p. 247), NO_XMLOUTPUT_WRITE (p. 247), NZCDC (p. 254), NZDIA (p. 254), NZHOL (p. 254), NZINJ (p. 254), NZLDR (p. 254), NZRDR (p. 255), NZRWL (p. 255), OPMV (p. 255), OPOC (p. 256), POLN1 (p. 263), POLN2 (p. 263), QIAGE (p. 281), SDOUTPUT_WRITE (p. 304), TSFAC (p. 340), TSTAU (p. 341), VCPRO (p. 352), VFFAC (p. 355), VPARI (p. 360), VPMOD (p. 360), XMLOUTPUT_WRITE (p. 369)

9.1.8. Closed Multiphase Reactor

The following keywords can be used to build an input file for a Closed Multiphase Reactor:

AREAM (p. 151), AROP (p. 152), ASEN (p. 153), BULK_MASSFRAC (p. 165), BULK_MOLARITY (p. 165), BULK_MOLEFRAC (p. 166), BULK_SOLVENT (p. 166), EPSS (p. 197), EPST (p. 198), H0 (p. 217), HTCPRO (p. 219), MASS_FRAC (p. 234), MASSTRAN_CEOF (p. 234), MASSTRAN_LEN (p. 235), MASSTRAN_MECHANISM (p. 235), MASSTRAN_TAU (p. 235), MAXIT (p. 236), MOLEFRAC (p. 240), MTDIFF_REFSPEC (p. 241), MTDIFF_SE (p. 241), MTDIFF_TRANINP (p. 242), MTDIFF_USER (p. 242), MTDIFF_WC (p. 242), MTMODEL_FILM (p. 242), MTMODEL_PENET (p. 242), MTMODEL_USER (p. 243), NADAP (p. 244), ROP (p. 294), RTLS (p. 297), STPT (p. 316), USE_TEMPERATURE (p. 348), VFRAC (p. 355)

9.2. Open 0-D Reactor Models

9.2.1. Perfectly Stirred Reactor

The following keywords can be used to build an input file for a PSR Reactor Model:

ABFR (p. 139), ABSL (p. 140), AEXT (p. 142), AFRA (p. 144), AGGA (p. 145), AGGB (p. 145), AGGD (p. 146), AGGE (p. 146), AGGFD (p. 147), AGGMN (p. 148), AINT (p. 148), AREA (p. 150), AREAQ (p. 151), AROP (p. 152),

ASEN (p. 153), ASTEPS (p. 154), ATIM (p. 155), ATLM (p. 156), ATLS (p. 157), ATOL (p. 157), AVALUE (p. 159), AVAR (p. 159), BETA (p. 161), BLKEQ (p. 162), BULK (p. 164), CLSC (p. 170), CLSM (p. 170), CNTN (p. 172), CNNT (p. 173), COLR (p. 174), CPROD (p. 176), DELT (p. 182), DFAC (p. 183), DIST (p. 184), DTIGN (p. 186), DTMN (p. 187), DTMX (steady-state) (p. 187), DTSV (p. 188), EGRR (p. 190), END (p. 192), ENRG (p. 194), EPSG (p. 196), EPSR (p. 197), EPSS (p. 197), EPST (p. 198), EQUI (p. 199), ETCH (p. 200), FLRT (p. 208), FPRO (p. 210), FUEL (p. 211), GFAC (p. 213), GMHTC (p. 214), HTC (p. 219), HTRN (p. 220), INLET (p. 226), IPSR (p. 228), IRET (p. 229), ISTD (p. 230), KLIM (p. 231), MAXIT (p. 236), MAXTIME (p. 236), MCUT (p. 237), MMASS (p. 239), NEWRUN (p. 245), NJAC (p. 246), NO_SDOUTPUT_WRITE (p. 247), NO_XMLOUTPUT_WRITE (p. 247), NMOM (p. 247), NNEG (p. 247), NOCG (p. 248), NOFT (p. 249), NPSR (p. 251), NSOL (p. 252), OXID (p. 256), PBDEN (p. 257), PNDE (p. 261), PNDI (p. 262), PPRO (p. 264), PRES (p. 265), PRNT (p. 266), PROD (p. 267), PROE (p. 268), PROI (p. 269), PSURF (p. 270), PTM_SECTION_SIZEDEP_A0 (p. 271), PTM_SECTION_SIZEDEP_COEFF (p. 272), PTM_SECTION_SIZEDEP_DSTAR (p. 272), PTM_SECTION_SIZEDEP_HAMAKER (p. 273), PTM_SECTION_USERBULKROP (p. 275), PTM_SECTIONAL (p. 275), PVFE (p. 276), PVFI (p. 277), QFUN (p. 280), QLOS (p. 281), QPRO (p. 283), QRGEQ (p. 284), QRSEQ (p. 285), QXCO (p. 319), QXRA (p. 319), REAC (p. 288), RECY (p. 289), RELAXC (p. 290), RELT (p. 291), RLGAS (p. 292), RLMIX (p. 293), ROP (p. 294), RSTR (p. 295), RTIM (p. 296), RTLIM (p. 297), RTLS (p. 297), RTOL (p. 298), SCCM (p. 299), SCCMPRO (p. 300), SCLM (p. 302), SCLS (p. 302), SCOR (p. 303), SDOUTPUT_WRITE (p. 304), SENG (p. 304), SENT (p. 305), SFAC (p. 306), SFLR (p. 307), SIZE (p. 308), SOLUTION_TECHNIQUE (p. 310), SPOS (p. 311), SSMAXITER (p. 313), SSTT (p. 314), STPT (p. 316), STST (p. 317), SURF (p. 317), TAMB (p. 320), TAU (p. 321), TEMP (p. 323), TGIV (p. 326), TIFP (p. 328), TIM1 (p. 328), TIM2 (p. 329), TIME (p. 330), TINL (p. 331), TJAC (p. 333), TLIM (p. 333), TPRO (p. 334), TRAN (p. 336), TRES (p. 338), TRMAXITER (p. 338), TRST (p. 339), TSCCM (p. 339), TSRF (p. 340), TSTR (p. 342), TTIM (p. 344), UFAC (p. 346), UIGN (p. 346), USET (p. 349), USEV (p. 350) (Restart), USEV (p. 350) (XMLI), USRIN (p. 351), VOL (p. 359), VPRO (p. 360), VTIM (p. 361), WENG (p. 363), WPRO (p. 366), XEST (p. 368), XMLI (p. 369), XMLOUTPUT_WRITE (p. 369), XMLS (p. 370)

9.2.2. Plasma Perfectly Stirred Reactor

The following keywords can be used to build an input file for a Plasma PSR Reactor Model:

ABSL (p. 140), ADD (p. 141), AEXT (p. 142), AFRA (p. 144), AGGA (p. 145), AGGB (p. 145), AGGD (p. 146), AGGE (p. 146), AGGFD (p. 147), AGGMN (p. 148), AINT (p. 148), AREA (p. 150), AREAQ (p. 151), AROP (p. 152), ASEN (p. 153), ASTEPS (p. 154), ATIM (p. 155), ATLM (p. 156), ATLS (p. 157), ATOL (p. 157), AVALUE (p. 159), AVAR (p. 159), BETA (p. 161), BLKEQ (p. 162), BOHM (p. 78), BPWR (p. 163), BULK (p. 164), CLSC (p. 170), CLSM (p. 170), CNTN (p. 172), CNNT (p. 173), COLR (p. 174), CPROD (p. 176), DELT (p. 182), DFAC (p. 183), DIST (p. 184), DTIGN (p. 186), DTMN (p. 187), DTMX (steady-state) (p. 187), DTSV (p. 188), EGRR (p. 190), ELSH (p. 190), END (p. 192), ENGE (p. 193), EPSG (p. 196), EPSR (p. 197), EPSS (p. 197), EPST (p. 198), EQUI (p. 199), ETCH (p. 200), ETMP (p. 201), FLRT (p. 208), FPRO (p. 210), FUEL (p. 211), GFAC (p. 213), GMHTC (p. 214), HTC (p. 219), HTRN (p. 220), INLET (p. 226), IONE (p. 228), IPSR (p. 228), IRET (p. 229), ISTD (p. 230), KLIM (p. 231), MAXIT (p. 236), MAXTIME (p. 236), MCUT (p. 237), MMASS (p. 239), NEWRUN (p. 245), NJAC (p. 246), NMOM (p. 247), NNEG (p. 247), NO_SDOUTPUT_WRITE (p. 247), NO_XMLOUTPUT_WRITE (p. 247), NOCG (p. 248), NOFT (p. 249), NPSR (p. 251), NSOL (p. 252), OXID (p. 256), PNDE (p. 261), PNDI (p. 262), PPRO (p. 264), PRES (p. 265), PRNT (p. 266), PROE (p. 268), PROI (p. 269), PSURF (p. 270), PVFE (p. 276), PVFI (p. 277), PWRW (p. 279), QFUN (p. 280), QLSE (p. 282), QPRO (p. 283), QRGEQ (p. 284), QRSEQ (p. 285), QXCO (p. 319), QXRA (p. 319), REAC (p. 288), RECY (p. 289), RELAXC (p. 290), RELT (p. 291), ROP (p. 294), RSTR (p. 295), RTIM (p. 296), RTLIM (p. 297), RTLS (p. 297), RTOL (p. 298), SCCM (p. 299), SCCMPRO (p. 300), SCLM (p. 302), SCLS (p. 302), SCOR (p. 303), SDOUTPUT_WRITE (p. 304), SENG (p. 304), SENT (p. 305), SFAC (p. 306), SFLR (p. 307), SIZE (p. 308), SOLUTION_TECHNIQUE (p. 310), SPOS (p. 311), SSMAXITER (p. 313), SSTT (p. 314), STPT (p. 316), STST (p. 317), SURF (p. 317), TAMB (p. 320), TAU (p. 321), TEBND (p. 323), TEIN (p. 323), TEMP (p. 323), TGIV (p. 326), TIFP (p. 328), TIM1 (p. 328), TIM2 (p. 329), TIME (p. 330), TINL (p. 331), TION (p. 332), TJAC (p. 333), TLIM (p. 333), TPRO (p. 334), TRAN (p. 336),

TRES (p. 338), TRMAXITER (p. 338), TRST (p. 339), TSCCM (p. 339), TSRF (p. 340), TSTR (p. 342), TTIM (p. 344), UFAC (p. 346), UIGN (p. 346), USET (p. 349), USEV (p. 350) (Restart), USEV (p. 350) (XMLI), USRIN (p. 351), VOL (p. 359), VPRO (p. 360), VTIM (p. 361), WENG (p. 363), WPRO (p. 366), XEST (p. 368), XMLI (p. 369), XML-
LOUTPUT_WRITE (p. 369), XMLS (p. 370), XSDF (p. 371), XSEK (p. 371)

9.2.3. Partially Stirred Reactor

The following keywords can be used to build an input file for a PaSR Reactor Model:

ADAM (p. 140), ATOL (p. 157), BDF (p. 160), CFL (p. 169), CHEM (p. 169), CMIX (p. 171), CPROD (p. 176),
CURL (p. 181), DASP (p. 182), DT (p. 186), DT0 (p. 186), DTMX (transient) (p. 188), DTSV (p. 188), END (p. 192),
EQUI (p. 199), FLRT (p. 208), IEM (p. 224), INIT (p. 225), INLET (p. 226), KOUT (p. 232), MAXIT (p. 236), MAX-
TIME (p. 236), MIX (p. 237), MIXT (p. 238), NCFIT (p. 245), NDPR (p. 245), NEWRUN (p. 245), NNEG (p. 247),
NO_SDOUTPUT_WRITE (p. 247), NO_XMLOUTPUT_WRITE (p. 247), NOJC (p. 249), NPAR (p. 250), NPIN (p. 251),
PDF (p. 258), PRES (p. 265), REAC (p. 288), RLGAS (p. 292), RLMIX (p. 293), RELAXC (p. 290), RSTR (p. 295),
RTOL (p. 298), SCAT (p. 299), SDOUTPUT_WRITE (p. 304), SIZE (p. 308), SSMAXITER (p. 313), TAU (p. 321),
TEMP (p. 323), TIME (p. 330), TINL (p. 331), TRES (p. 338), TRMAXITER (p. 338), VOL (p. 359), VPRO (p. 360),
WELL (p. 363), XMLI (p. 369), XMLOUTPUT_WRITE (p. 369), XMLS (p. 370)

9.2.4. Open Multiphase Reactor

The following keywords can be used to build an input file for an Open Multiphase Reactor:

ADAP (p. 141), AREA (p. 150), AREAM (p. 151), AREAQ (p. 151), AROP (p. 152), ASEN (p. 153), ASTEPS (p. 154),
ATLS (p. 157), ATOL (p. 157), AVALUE (p. 159), AVAR (p. 159), BULK_MASSFRAC (p. 165), BULK_MOLAR-
ITY (p. 165), BULK_MOLEFRAC (p. 166), BULK_SOLVENT (p. 166), CSVOUTPUT_FILENAME (p. 178),
CSVOUTPUT_KOUT (p. 179), CSVOUTPUT_WRITE (p. 180), DELT (p. 182), END (p. 192), ENRG (p. 194),
EPSS (p. 197), EPST (p. 198), FLRT (p. 208), FPRO (p. 210), H0 (p. 217), HTC (p. 219), HTCPRO (p. 219), IN-
LT (p. 227), INLTPRO (p. 227), MASS_FRAC (p. 234), MASSTRAN_CEOF (p. 234), MASSTRAN_LEN (p. 235),
MASSTRAN_MECHANISM (p. 235), MASSTRAN_TAU (p. 235), MAXIT (p. 236), MOLEFRAC (p. 240),
MOLFLRT (p. 239), MOLFLRTPRO (p. 239), MTDIFF_REFSPEC (p. 241), MTDIFF_SE (p. 241), MTDIFF_TRAN-
INP (p. 242), MTDIFF_USER (p. 242), MTDIFF_WC (p. 242), MTMODEL_FILM (p. 242), MTMODEL_PEN-
ET (p. 242), MTMODEL_USER (p. 243), NADAP (p. 244), NNEG (p. 247), NO_SDOUTPUT_WRITE (p. 247),
NO_XMLOUTPUT_WRITE (p. 247), PHASE_MASSOUTFLOWRATE (p. 259), PHASE_MOLAROUT-
FLOWRATE (p. 260), PHASE_VOLOWFLOWRATE (p. 260), PHASE_VOLUME (p. 260), PPRO (p. 264),
PRES (p. 265), QLOS (p. 281), QPRO (p. 283), REAC (p. 288), RELAXC (p. 290), ROP (p. 294), RTLS (p. 297),
RTOL (p. 298), SDOUTPUT_WRITE (p. 304), SFAC (p. 306), STPT (p. 316), TAMB (p. 320), TEMP (p. 323),
TGIV (p. 326), TIME (p. 330), TPRO (p. 334), USE_TEMPERATURE (p. 348), VDOT (p. 353), VDOTPRO (p. 353),
VFRAC (p. 355), VOL (p. 358), VPRO (p. 360), XINL (p. 369), XMLOUTPUT_WRITE (p. 369)

9.3. Flow Reactor Models

9.3.1. Plug Flow Reactor

The following keywords can be used to build an input file for a PFR Reactor Model:

ABFR (p. 139), ACHG (p. 140), ADAP (p. 141), ADD (p. 141), ADIA (p. 142), AFLO (p. 143), AFRA (p. 144),
AINT (p. 148), AREA (p. 150), AREAF (p. 151), AREAQ (p. 151), AROP (p. 152), ASEN (p. 153), ASTEPS (p. 154),
ATLM (p. 156), ATLS (p. 157), ATOL (p. 157), AVALUE (p. 159), AVAR (p. 159), BETA (p. 161), BLKEQ (p. 162),
BULK (p. 164), CLSC (p. 170), CLSM (p. 170), CNTN (p. 172), CNTX (p. 173), COLR (p. 174), CPROD (p. 176),

CSVOUTPUT_FILENAME (p. 178), CSVOUTPUT_KOUT (p. 179), CSVOUTPUT_WRITE (p. 180), DIST (p. 184), DPRO (p. 185), DTIGN (p. 186), DX (p. 189), DXMX (p. 189), DXSV (p. 189), EGRR (p. 190), END (p. 192), ENRG (p. 194), EPSG (p. 196), EPSR (p. 197), EPSS (p. 197), EPST (p. 198), EQUI (p. 199), ETCH (p. 200), FLRT (p. 208), FPRO (p. 210), FUEL (p. 211), GFAC (p. 213), GMHTC (p. 214), HTC (p. 219), HTRN (p. 220), IPSR (p. 228), KLIM (p. 231), MCUT (p. 237), MMASS (p. 239), MOMEN (p. 240), NADAP (p. 244), NEWRUN (p. 245), NMOM (p. 247), NNEG (p. 247), NO_SDOUTPUT_WRITE (p. 247), NO_XMLOUTPUT_WRITE (p. 247), NOCG (p. 248), NSOL (p. 252), OXID (p. 256), PBDEN (p. 257), PLUG (p. 261), PNDE (p. 261), PNDI (p. 262), PPRO (p. 264), PRES (p. 265), PRNT (p. 266), PROE (p. 268), PROI (p. 269), PSV (p. 271), PTM_SECTION_NUM (p. 271), PTM_SECTION_SIZEDEP_A0 (p. 271), PTM_SECTION_SIZEDEP_COLEFF (p. 272), PTM_SECTION_SIZEDEP_DSTAR (p. 272), PTM_SECTION_SIZEDEP_HAMAKER (p. 273), PTM_SECTION_SNO (p. 273), PTM_SECTION_SPACING (p. 274), PTM_SECTION_TCOND (p. 274), PTM_SECTION_USERBULKROP (p. 275), PTM_SECTIONAL (p. 275), PVFE (p. 276), PVFI (p. 277), QFUN (p. 280), QLOS (p. 281), QPRO (p. 283), QRGEQ (p. 284), QRSEQ (p. 285), RCHG (p. 287), REAC (p. 288), RLGAS (p. 292), RLMIX (p. 293), ROP (p. 294), RSTR (p. 295), RTIME (p. 296), RTLM (p. 297), RTLS (p. 297), RTOL (p. 298), SCCMPRO (p. 300), SCLM (p. 302), SCLS (p. 302), SCOR (p. 303), SDOUTPUT_WRITE (p. 304), SENG (p. 304), SFAC (p. 306), SIZE (p. 308), SSKIP (p. 313), SSTT (p. 314), SURF (p. 317), TAMB (p. 320), TEMP (p. 323), TGIV (p. 326), TIFP (p. 328), TLIM (p. 333), TPRO (p. 334), TRST (p. 339), TSRF (p. 340), TSTP (p. 342), TSTR (p. 342), UIGN (p. 346), USET (p. 349), USEV (p. 350) (Restart), USEV (p. 350) (XMLI), VDOT (p. 353), VDOTPRO (p. 353), VEL (p. 354), VIS (p. 355), WENG (p. 363), XEND (p. 367), XMLI (p. 369), XMLOUTPUT_WRITE (p. 369), XMLS (p. 370), XRES (p. 371), XSTR (p. 372)

9.3.2. Plasma Plug Flow Reactor

The following keywords can be used to build an input file for a Plasma PFR Reactor Model:

ACHG (p. 140), ADAP (p. 141), ADIA (p. 142), AFLO (p. 143), AFRA (p. 144), AINT (p. 148), AREA (p. 150), AREAF (p. 151), AREAQ (p. 151), AROP (p. 152), ASEN (p. 153), ASTEPS (p. 154), ATLS (p. 157), AVALUE (p. 159), AVAR (p. 159), BETA (p. 161), BLKEQ (p. 162), BOHM (p. 78), BPWR (p. 163), BULK (p. 164), CLSC (p. 170), CLSM (p. 170), CNTN (p. 172), CNTX (p. 173), COLR (p. 174), CPROD (p. 176), DIAM (p. 184), DIST (p. 184), DPRO (p. 185), DTIGN (p. 186), DX (p. 189), DXMX (p. 189), DXSV (p. 189), EGRR (p. 190), ELSH (p. 190), END (p. 192), ENGE (p. 193), ENRG (p. 194), EPSG (p. 196), EPSR (p. 197), EPSS (p. 197), EPST (p. 198), EQUI (p. 199), ETCH (p. 200), ETMP (p. 201), FLRT (p. 208), FPRO (p. 210), FUEL (p. 211), GFAC (p. 213), GMHTC (p. 214), HTC (p. 219), HTRN (p. 220), IONE (p. 228), IPSR (p. 228), KLIM (p. 231), MAXIT (p. 236), MCUT (p. 237), MMASS (p. 239), MOMEN (p. 240), NADAP (p. 244), NEWRUN (p. 245), NMOM (p. 247), NNEG (p. 247), NO_SDOUTPUT_WRITE (p. 247), NO_XMLOUTPUT_WRITE (p. 247), NOCG (p. 248), NSOL (p. 252), OXID (p. 256), PLUG (p. 261), PNDE (p. 261), PNDI (p. 262), PPRO (p. 264), PRES (p. 265), PRNT (p. 266), PROD (p. 267), PROE (p. 268), PROI (p. 269), PSURF (p. 270), PSV (p. 271), PVFE (p. 276), PVFI (p. 277), PWRW (p. 279), QFUN (p. 280), QLOS (p. 281), QLSE (p. 282), QPRO (p. 283), QRGEQ (p. 284), QRSEQ (p. 285), RCHG (p. 287), REAC (p. 288), RELAXC (p. 290), ROP (p. 294), RSTR (p. 295), RTIME (p. 296), RTLS (p. 297), SCCMPRO (p. 300), SCLM (p. 302), SCLS (p. 302), SCOR (p. 303), SDOUTPUT_WRITE (p. 304), SENG (p. 304), SENT (p. 305), SFAC (p. 306), SIZE (p. 308), SOLUTION_TECHNIQUE (p. 310), SSKIP (p. 313), SURF (p. 317), TAMB (p. 320), TEBND (p. 323), TEMP (p. 323), TGIV (p. 326), TIFP (p. 328), TION (p. 332), TLIM (p. 333), TPRO (p. 334), TRST (p. 339), TSRF (p. 340), TSTP (p. 342), TSTR (p. 342), UIGN (p. 346), USET (p. 349), USEV (p. 350) (Restart), USEV (p. 350) (XMLI), VDOT (p. 353), VDOTPRO (p. 353), VELPRO (p. 354), VIS (p. 355), WENG (p. 363), WPRO (p. 366), XEND (p. 367), XMLI (p. 369), XMLOUTPUT_WRITE (p. 369), XMLS (p. 370), XRES (p. 371), XSDF (p. 371), XSEK (p. 371), XSTR (p. 372)

9.3.3. Planar Shear Flow

The following keywords can be used to build an input file for a Planar Shear Flow Reactor Model:

ABFR (p. 139), AFLW (p. 144), AFRA (p. 144), ADIA (p. 142), ATIM (p. 155), ATLM (p. 156), ATOL (p. 157), BETA (p. 161), BULK (p. 164), CLSC (p. 170), CLSM (p. 170), CNTN (p. 172), COLR (p. 174), CPROD (p. 176), DTMN (p. 187), DTMX (steady-state) (p. 187), DX (p. 189), DXMX (p. 189), DXSV (p. 189), END (p. 192), FIXT (p. 207), GASW (p. 212), GFAC (p. 213), GRAV (p. 215), H0 (p. 217), HITE (p. 217), HTRN (p. 220), ICRD (p. 224), IPSR (p. 228), IRET (p. 229), ISTP (p. 230), KNMN (p. 232), MAXIT (p. 236), MAXTIME (p. 236), MCUT (p. 237), MIX (p. 237), MORD (p. 240), MULT (p. 243), NEWRUN (p. 245), NJAC (p. 246), NMOM (p. 247), NO_SDOUTPUT_WRITE (p. 247), NO_XMLOUTPUT_WRITE (p. 247), NOCG (p. 248), NOTP (p. 250), NPTS (p. 251), NSOL (p. 252), PARP (p. 257), PNDE (p. 261), PNDI (p. 262), PRES (p. 265), PRNT (p. 266), PROE (p. 268), PROI (p. 269), PVFE (p. 276), PVFI (p. 277), QLOS (p. 281), QPRO (p. 283), REAC (p. 288), RL-GAS (p. 292), RLMIX (p. 293), RELAXC (p. 290), RSTR (p. 295), RTIM (p. 296), RTLM (p. 297), RTOL (p. 298), SDOUTPUT_WRITE (p. 304), SFAC (p. 306), SIZE (p. 308), SLIP (p. 309), SQRX (p. 311), SSMAXITER (p. 313), SSRX (p. 314), STCH (p. 315), STP0 (p. 316), SURF (p. 317), SYMT (p. 319), TDIF (p. 322), TINF (p. 330), TINL (p. 331), TJAC (p. 333), TPRO (p. 334), TRMAXITER (p. 338), TSPL (p. 340), TSRF (p. 340), TSTR (p. 342), TWAB (p. 345), TWPR (p. 345), TWRE (p. 345), TWST (p. 345), UPROF (p. 347), USET (p. 349), USEV (p. 350), UTRN (p. 351), VCOR (p. 352), VEL (p. 354), VWALL (p. 362), XEND (p. 367), XMLI (p. 369), XMLOUT-PUT_WRITE (p. 369), XMLS (p. 370), XREST (p. 371), XTMP (p. 373)

9.3.4. Cylindrical Shear Flow

The following keywords can be used to build an input file for a Cylindrical Shear Flow Reactor Model:

ABFR (p. 139), ADIA (p. 142), AFRA (p. 144), ATIM (p. 155), ATLM (p. 156), ATOL (p. 157), BETA (p. 161), BULK (p. 164), CLSC (p. 170), CLSM (p. 170), COLR (p. 174), CNTN (p. 172), CPROD (p. 176), DIST (p. 184), DTMN (p. 187), DTMX (steady-state) (p. 187), DX (p. 189), DXMX (p. 189), DXSV (p. 189), END (p. 192), GASW (p. 212), GFAC (p. 213), GRAV (p. 215), H0 (p. 217), HITE (p. 217), HTRN (p. 220), ICRD (p. 224), IPSR (p. 228), IRET (p. 229), ISTP (p. 230), KNMN (p. 232), MAXIT (p. 236), MAXTIME (p. 236), MCUT (p. 237), MIX (p. 237), MORD (p. 240), MULT (p. 243), NEWRUN (p. 245), NJAC (p. 246), NMOM (p. 247)

, NO_SDOUTPUT_WRITE (p. 247), NO_XMLOUTPUT_WRITE (p. 247)

, NOCG (p. 248), NOTP (p. 250), NPTS (p. 251), NSOL (p. 252), PARP (p. 257), PNDE (p. 261), PNDI (p. 262), PRES (p. 265), PRNT (p. 266), PROE (p. 268), PROI (p. 269), PVFE (p. 276), PVFI (p. 277), QLOS (p. 281), QPRO (p. 283), REAC (p. 288), RL-GAS (p. 292), RLMIX (p. 293), RELAXC (p. 290), RSTR (p. 295), RTIM (p. 296), RTLM (p. 297), RTOL (p. 298), SDOUTPUT_WRITE (p. 304), SFAC (p. 306), SIZE (p. 308), SLIP (p. 309), SQRX (p. 311), SSMAXITER (p. 313), SSRX (p. 314), STCH (p. 315), STP0 (p. 316), SURF (p. 317), TDIF (p. 322), TINF (p. 330), TINL (p. 331), TJAC (p. 333), TPRO (p. 334), TRMAXITER (p. 338), TSPL (p. 340), TSRF (p. 340), TSTR (p. 342), TWAB (p. 345), TWPR (p. 345), TWRE (p. 345), TWST (p. 345), UPROF (p. 347), USET (p. 349), USEV (p. 350), UTRN (p. 351), VCOR (p. 352), VEL (p. 354), VWALL (p. 362), XEND (p. 367), XMLI (p. 369), XMLOUTPUT_WRITE (p. 369), XMLS (p. 370), XREST (p. 371), XTMP (p. 373)

9.3.5. Honeycomb Monolith Reactor

The Honeycomb Monolith Reactor Model is a special case of a general plug-flow reactor, where user input parameters describing the honeycomb geometry are used to automatically calculate the available surface area for gas-surface reactions. For details on the calculations performed for the Honeycomb Monolith Reactor Model, see [Honeycomb Monolith Reactor Calculations](#) of the [Chemkin Theory Manual](#).

The following keywords can be used to build an input file for a Honeycomb Monolith Reactor Model:

ACHG (p. 140), ADAP (p. 141), ADIA (p. 142), AEXT (p. 142), AFLO (p. 143), AFRA (p. 144), AINT (p. 148), AREA (p. 150), AREAF (p. 151), AREAQ (p. 151), AROP (p. 152), ASEN (p. 153), ASTEPS (p. 154), ATLS (p. 157), ATOL (p. 157), AVALUE (p. 159), AVAR (p. 159), BETA (p. 161), BLKEQ (p. 162), BULK (p. 164), CLSC (p. 170), CLSM (p. 170), CNTN (p. 172), CNTX (p. 173), COLR (p. 174), CPROD (p. 176), CSVOUTPUT_FILENAME (p. 178), CSVOUTPUT_KOUT (p. 179), CSVOUTPUT_WRITE (p. 180), DIAM (p. 184), DIST (p. 184), DPRO (p. 185), DTIGN (p. 186), DX (p. 189), DXMX (p. 189), DXSV (p. 189), EGRR (p. 190), END (p. 192), ENRG (p. 194), EPSG (p. 196), EPSR (p. 197), EPSS (p. 197), EPST (p. 198), EQUI (p. 199), ETCH (p. 200), FLRT (p. 208), FPRO (p. 210), FUEL (p. 211), GFAC (p. 213), GMHTC (p. 214), HTC (p. 219), HTRN (p. 220), IPSR (p. 228), KLIM (p. 231), MAXIT (p. 236), MCUT (p. 237), MMAX (p. 239), MOMEN (p. 240), NADAP (p. 244), NMOM (p. 247), NNEG (p. 247), NO_SDOUTPUT_WRITE (p. 247), NO_XMLOUTPUT_WRITE (p. 247), NOCG (p. 248), NSOL (p. 252), OXID (p. 256), PLUG (p. 261), PNDE (p. 261), PNDI (p. 262), PPRO (p. 264), PRES (p. 265), PRNT (p. 266), PROE (p. 268), PROI (p. 269), PSURF (p. 270), PSV (p. 271), PVFE (p. 276), PVFI (p. 277), QFUN (p. 280), QLOS (p. 281), QPRO (p. 283), QRGEQ (p. 284), QRSEQ (p. 285), RCHG (p. 287), REAC (p. 288), RLGAS (p. 292), RLMIX (p. 293), RELAXC (p. 290), ROP (p. 294), RSTR (p. 295), RTIM (p. 296), RTIME (p. 296), RTLS (p. 297), RTOL (p. 298), SCCMPRO (p. 300), SCLM (p. 302), SCLS (p. 302), SCOR (p. 303), SDOUTPUT_WRITE (p. 304), SENG (p. 304), SENT (p. 305), SFAC (p. 306), SIZE (p. 308), SOLUTION_TECHNIQUE (p. 310), SSKIP (p. 313), SSTT (p. 314), SURF (p. 317), TAMB (p. 320), TEMP (p. 323), TGIV (p. 326), TIFP (p. 328), TLIM (p. 333), TPRO (p. 334), TRST (p. 339), TSFR (p. 340), TSTP (p. 342), TSTR (p. 342), UIGN (p. 346), USET (p. 349), USEV (p. 350) (Restart), USEV (p. 350) (XMLI), VDOT (p. 353), VDOTPRO (p. 353), VEL (p. 354), VIS (p. 355), WENG (p. 363), XEND (p. 367), XMLI (p. 369), XMLOUTPUT_WRITE (p. 369), XMLS (p. 370), XRES (p. 371), XSTR (p. 372)

9.4. Flame Simulators

9.4.1. Premixed Laminar Burner-stabilized Flame Simulator

The following keywords can be used to build an input file for a Premixed Laminar Burner-stabilized Flame Simulator:

AGGA (p. 145), AGGB (p. 145), AGGD (p. 146), AGGE (p. 146), AGGFD (p. 147), AGGMN (p. 148), APRO (p. 149), ASEN (p. 153), ATIM (p. 155), ATOL (p. 157), BURN (p. 166), CDIF (p. 169), CNTN (p. 172), CPROD (p. 176), CSVOUTPUT_FILENAME (p. 178), CSVOUTPUT_KOUT (p. 179), CSVOUTPUT_WRITE (p. 180), CURV (p. 181), DFAC (p. 183), DIST (p. 184), DTMN (p. 187), DTMX (steady-state) (p. 187), EMPAR (p. 192), END (p. 192), ENRG (p. 194), EPSS (p. 197), FLRT (p. 208), FLTB (p. 209), FLT_PVSPEC (p. 209), FLXB (p. 210), GFAC (p. 213), GRAD (p. 214), GRID (p. 215), HSEN (p. 217), INTM (p. 227), IRET (p. 229), ISTP (p. 230), JJRG (p. 230), KOUT (p. 232), MAXTIME (p. 236), MIX (p. 237), MSFX (p. 241), MULT (p. 243), NADP (p. 244), NJAC (p. 246), NO_SDOUTPUT_WRITE (p. 247), NO_XMLOUTPUT_WRITE (p. 247), NOAGG (p. 248), NOFT (p. 249), NOTP (p. 250) (Reactor), NPTS (p. 251), NSOL (p. 252), NTOT (p. 253), PENG (p. 258), PFLR (p. 259), PPRO (p. 264), PRES (p. 265), PRMN (p. 266), PRNT (p. 266), PROD (p. 267), PSURF (p. 270), PTM_SECTION_NUM (p. 271), PTM_SECTION_SIZEDEP_A0 (p. 271), PTM_SECTION_SIZEDEP_COLEFF (p. 272), PTM_SECTION_SIZEDEP_DSTAR (p. 272), PTM_SECTION_SIZEDEP_HAMAKER (p. 273), PTM_SECTION_SNO (p. 273), PTM_SECTION_SPACING (p. 274), PTM_SECTION_TCOND (p. 274), PTM_SECTION_USERBULKROP (p. 275), PTM_SECTIONAL (p. 275), QFUN (p. 280), RACTV (p. 286), RADGS (p. 287), RADPT (p. 287), REAC (p. 288), RLGAS (p. 292), RLMIX (p. 293), RSTR (p. 295), RTIM (p. 296), RTOL (p. 298), SCLM (p. 302), SCLS (p. 302), SDOUTPUT_WRITE (p. 304), SENT (p. 305), SFLR (p. 307), SFMN (p. 307), SGMAXIT (p. 307), SGTOL (p. 308), SIZE (p. 308), SOLUTION_TECHNIQUE (p. 310), SPOS (p. 311), SSAXITER (p. 313), TBND (p. 321), TDIF (p. 322), TEMP (p. 323), TGIV (p. 326), TIM1 (p. 328), TIM2 (p. 329), TINF (p. 330), TJAC (p. 333), TPRO (p. 334), TPROF (p. 336), TRAN (p. 336), TRCE (p. 337), TRMAXITER (p. 338), TSTR (p. 342), TUNBURNT (p. 344), USE_TPRO_GRID (p. 348), USET (p. 349), USEV (p. 350) (Restart), USEV (p. 350) (XMLI),

UTRN (p. 351), VCOR (p. 352), WDIF (p. 363), WMIX (p. 364), XCEN (p. 367), XEND (p. 367), XIMN (p. 368), XMLI (p. 369), XMLS (p. 370), XMLOUTPUT_WRITE (p. 369), XSTR (p. 372)

9.4.2. Flame Speed Simulator

The following keywords can be used to build an input file for a Flame Speed Simulator:

ASEN (p. 153), ATIM (p. 155), ATOL (p. 157), CDIF (p. 169), CNTN (p. 172), CPROD (p. 176), CSVOUTPUT_FILENAME (p. 178), CSVOUTPUT_KOUT (p. 179), CSVOUTPUT_WRITE (p. 180), CURV (p. 181), DFAC (p. 183), DIST (p. 184), DTMN (p. 187), DTMX (steady-state) (p. 187), EMPAR (p. 192), END (p. 192), ENRG (p. 194), EPSS (p. 197), FLRT (p. 208), FLTB (p. 209), FLT_PVSPEC (p. 209), FLXB (p. 210), FREE (p. 211), GFAC (p. 213), GRAD (p. 214), GRID (p. 215), HSEN (p. 217), INTM (p. 227), IPSR (p. 228), IRET (p. 229), ISTEP (p. 230), JJRG (p. 230), KOUT (p. 232), MAXTIME (p. 236), MIX (p. 237), MSFX (p. 241), MULT (p. 243), NADP (p. 244), NJAC (p. 246), NO_SDOUTPUT_WRITE (p. 247), NO_XMLOUTPUT_WRITE (p. 247), NOAGG (p. 248), NOFT (p. 249), NOTP (p. 250) (Reactor), NPTS (p. 251), NSOL (p. 252), NTOT (p. 253), PENG (p. 258), PFLR (p. 259), PRES (p. 265), PRMN (p. 266), PRNT (p. 266), PROD (p. 267), PSURF (p. 270), PTM_SECTION_NUM (p. 271), PTM_SECTION_SIZEDEP_A0 (p. 271), PTM_SECTION_SIZEDEP_COLEFF (p. 272), PTM_SECTION_SIZEDEP_DSTAR (p. 272), PTM_SECTION_SIZEDEP_HAMAKER (p. 273), PTM_SECTION_SNO (p. 273), PTM_SECTION_SPACING (p. 274), PTM_SECTION_TCOND (p. 274), PTM_SECTION_USERBULKROP (p. 275), PTM_SECTIONAL (p. 275), QFUN (p. 280), RACTV (p. 286), RADGS (p. 287), RADPT (p. 287), REAC (p. 288), RLAS (p. 292), RLMIX (p. 293), RSTR (p. 295), RTIM (p. 296), RTOL (p. 298), SCLM (p. 302), SCLS (p. 302), SDOUTPUT_WRITE (p. 304), SENT (p. 305), SFLR (p. 307), SFMN (p. 307), SGMAXIT (p. 307), SGTOL (p. 308), SIZE (p. 308), SOLUTION_TECHNIQUE (p. 310), SPOS (p. 311), SSMAXITER (p. 313), TDIF (p. 322), TEMP (p. 323), TFIX (p. 326), TIM1 (p. 328), TIM2 (p. 329), TINF (p. 330), TJAC (p. 333), TPRO (p. 334), TPROF (p. 336), TRAN (p. 336), TRCE (p. 337), TRMAXITER (p. 338), TSTR (p. 342), TUNBURNT (p. 344), USET (p. 349), USE_TPRO_GRID (p. 348), USEV (p. 350) (Restart), USEV (p. 350) (XMLI), UTRN (p. 351), VCOR (p. 352), WDIF (p. 363), WMIX (p. 364), XCEN (p. 367), XEND (p. 367), XIMN (p. 368), XMLI (p. 369), XMLOUTPUT_WRITE (p. 369), XMLS (p. 370), XSTR (p. 372)

9.4.3. Opposed-flow Flame Simulator

The following keywords can be used to build an input file for an Opposed-flow Flame Simulator:

AGGA (p. 145), AGGB (p. 145), AGGD (p. 146), AGGE (p. 146), AGGFD (p. 147), AGGMN (p. 148), AINL (p. 148), ASEN (p. 153), ATIM (p. 155), ATOL (p. 157), AXIS (p. 160), CDIF (p. 169), CNTN (p. 172), CPROD (p. 176), CSVOUTPUT_FILENAME (p. 178), CSVOUTPUT_KOUT (p. 179), CSVOUTPUT_WRITE (p. 180), CURV (p. 181), DFAC (p. 183), DIST (p. 184), DTMN (p. 187), DTMX (steady-state) (p. 187), EMPAR (p. 192), END (p. 192), ENRG (p. 194), ENTH_DELTA_IN (p. 196), EPSS (p. 197), FLTB (p. 209), GFAC (p. 213), GRAD (p. 214), GRID (p. 215), HSEN (p. 217), INLET (p. 226), IPSR (p. 228), IRET (p. 229), ISTEP (p. 230), JJRG (p. 230), KOUT (p. 232), MAXTIME (p. 236), MIX (p. 237), MULT (p. 243), NADP (p. 244), NDPR (p. 245), NJAC (p. 246), NOAGG (p. 248), NO_SDOUTPUT_WRITE (p. 247), NO_XMLOUTPUT_WRITE (p. 247), NOFT (p. 249), NOTP (p. 250) (Reactor), NPTS (p. 251), NSOL (p. 252), NTOT (p. 253), PENG (p. 258), PFLR (p. 259), PLAN (p. 261), PLAT (p. 261), PPRO (p. 264), PRES (p. 265), PRNT (p. 266), PROD (p. 267), PSURF (p. 270), PTM_SECTION_NUM (p. 271), PTM_SECTION_SIZEDEP_A0 (p. 271), PTM_SECTION_SIZEDEP_COLEFF (p. 272), PTM_SECTION_SIZEDEP_DSTAR (p. 272), PTM_SECTION_SIZEDEP_HAMAKER (p. 273), PTM_SECTION_SNO (p. 273), PTM_SECTION_SPACING (p. 274), PTM_SECTION_TCOND (p. 274), PTM_SECTION_USERBULKROP (p. 275), PTM_SECTIONAL (p. 275), QFUN (p. 280), RACTV (p. 286), RADGS (p. 287), RADPT (p. 287), REAC (p. 288), RLAS (p. 292), RLMIX (p. 293), RSTR (p. 295), RTIM (p. 296), RTOL (p. 298), SDOUTPUT_WRITE (p. 304), SENT (p. 305), SFLR (p. 307), SFMN (p. 307), SGMAXIT (p. 307), SGTOL (p. 308), SIZE (p. 308), SOLUTION_TECHNIQUE (p. 310), SPOS (p. 311), SSMAXITER (p. 313), TDIF (p. 322), TEMP (p. 323), TGIV (p. 326), TIM1 (p. 328), TIM2 (p. 329), TINF (p. 330), TINL (p. 331), TJAC (p. 333), TMAX (p. 334),

TPRO (p. 334), TRAN (p. 336), TRMAXITER (p. 338), TSRF (p. 340), TSTR (p. 342), UFAC (p. 346), UINL (p. 347), USET (p. 349), UTRN (p. 351), WDIF (p. 363), WMIX (p. 364), XCEN (p. 367), XEND (p. 367), XMLI (p. 369), XMLOUTPUT_WRITE (p. 369), XMLS (p. 370)

9.4.4. Premixed Laminar Burner-stabilized Stagnation Flow Flame Simulator

The following keywords can be used in addition to those listed in [Opposed-flow Flame Simulator](#) (p. 134), [Opposed-flow Flame Simulator](#) (p. 134), to build an input file for a Premixed Laminar Burner-stabilized Stagnation Flow Flame Simulator:

CSVOUTPUT_FILENAME (p. 178), CSVOUTPUT_KOUT (p. 179), CSVOUTPUT_WRITE (p. 180), ENTH_DELTA_IN (p. 196), NO_SDOUTPUT_WRITE (p. 247), NO_XMLOUTPUT_WRITE (p. 247), PTM_SECTION_NUM (p. 271), PTM_SECTION_SIZEDEP_A0 (p. 271), PTM_SECTION_SIZEDEP_COLEFF (p. 272), PTM_SECTION_SIZEDEP_DSTAR (p. 272), PTM_SECTION_SIZEDEP_HAMAKER (p. 273), PTM_SECTION_SNO (p. 273), PTM_SECTION_SPACING (p. 274), PTM_SECTION_TCOND (p. 274), PTM_SECTION_USERBULKROP (p. 275), PTM_SECTIONAL (p. 275), RLGAS (p. 292), RLMIX (p. 293), SCLM (p. 302), SCLS (p. 302), SDOUTPUT_WRITE (p. 304), STAGNATION_FLAME (p. 315), TINL (p. 332), XMLOUTPUT_WRITE (p. 369)

9.4.5. Flame-Extinction Simulator

The following keywords can be used in addition to those listed in [Opposed-flow Flame Simulator](#) (p. 134), [Opposed-flow Flame Simulator](#) (p. 134), to build an input file for a Flame-Extinction Simulator:

ENTH_DELTA_IN (p. 196), EXTINCTION (p. 202), EXT_MAXTFRAC (p. 202), EXT_METHOD (p. 203), EXT_MINTFLAME (p. 203), EXT_MINTFRAC (p. 203), EXT_SAVEINT (p. 204), EXT_STEPS (p. 204), EXT_TSTEP (p. 204), EXT_VFCNTRL (p. 205), NO_SDOUTPUT_WRITE (p. 247), NO_XMLOUTPUT_WRITE (p. 247), RLGAS (p. 292), RLMIX (p. 293), SCLM (p. 302), SCLS (p. 302), SDOUTPUT_WRITE (p. 304), XMLOUTPUT_WRITE (p. 369)

9.4.6. Diffusion Flamelet Generator

ATOL (p. 157), ENDTIMEMAX (p. 193), ENTH_DELTA_IN (p. 196), FLTB (p. 209), IGRIDMETHOD_n (p. 224), INLET (p. 226), MIXFRACBIAS_FUEL (p. 238), MIXFRACBIAS_OXID (p. 238), NO_SDOUTPUT_WRITE (p. 247), NO_XMLOUTPUT_WRITE (p. 247), NP_FUEL (p. 250), NP_OXID (p. 251), NPTS (p. 251), NSTEPS_HIGH (p. 253), NSTEPS_LOW (p. 253), NTOT (p. 253), PRES (p. 265), REAC (p. 288), RTOL (p. 298), SDOUTPUT_WRITE (p. 304), SSDR (p. 312), SSDR_MAX (p. 312), SSDR_MIN (p. 313), TIME (p. 330), TINL (p. 331), TMAX (p. 334), TPRO-FILE_n (p. 336), XMLOUTPUT_WRITE (p. 369)

9.5. CVD Reactors

9.5.1. Stagnation Flow CVD Reactor

The following keywords can be used to build an input file for a Stagnation Flow CVD Reactor Model:

AINL (p. 148), ASEN (p. 153), ATIM (p. 155), ATOL (p. 157), BULK (p. 164), CDCT (p. 168), CHEM (p. 169), CNDT (p. 172), CNDX (p. 172), CNTN (p. 172), COMP (p. 174), COND (p. 175), CPROD (p. 176), CTOL (p. 180), CURV (p. 181), DELT (p. 182), DFAC (p. 183), DIST (p. 184), DT0 (p. 186), DTMN (p. 187), DTMX (steady-state) (p. 187), EMIS (p. 191), EMSG (p. 192), END (p. 192), ENRG (p. 194), EPSS (p. 197), ETCH (p. 200),

FLAM (p. 207), FLRT (p. 208), FLUX (p. 210), FPRO (p. 210), GDOT (p. 212), GFAC (p. 213), GRAD (p. 214), GRID (p. 215), HSEN (p. 217), INIT (p. 225), INJM (p. 225), INJS (p. 225), INJT (p. 225), INJW (p. 226), INJX (p. 226), INLET (p. 226), INTM (p. 227), IPSR (p. 228), IRET (p. 229), ISTEP (p. 230), JJRG (p. 230), LINE (p. 233), LPRT (p. 233), MAXIT (p. 236), MAXTIME (p. 236), MIX (p. 237), MORD (p. 240), MULT (p. 243), NADP (p. 244), NEWRUN (p. 245), NJAC (p. 246), NO_SDOUTPUT_WRITE (p. 247), NO_XMLOUTPUT_WRITE (p. 247), NOCH (p. 249), NOFT (p. 249), NONR (p. 250), NOTP (p. 250), NPTS (p. 251), NSOL (p. 252), NTOT (p. 253), PRES (p. 265), PRNT (p. 266), PROD (p. 267), PWRC (p. 278), QDOT (p. 279), QDTC (p. 279), RADGS (p. 287), RDSK (p. 288), REAC (p. 288), RELAXC (p. 290), REOR (p. 291), RLGAS (p. 292), RLMIX (p. 293), RRAD (p. 295), RSTR (p. 295), RTIM (p. 296), RTOL (p. 298), SCCM (p. 299), SCCMPRO (p. 300), SDOUTPUT_WRITE (p. 304), SENT (p. 305), SFAC (p. 306), SFLR (p. 307), SIZE (p. 308), SPOS (p. 311), SSMAXITER (p. 313), STAG (p. 315), STST (p. 317), SURF (p. 317), TBND (p. 321), TDIF (p. 322), TDSK (p. 323), TEMP (p. 323), TGIV (p. 326), TIM1 (p. 328), TIM2 (p. 329), TIME (p. 330), TINL (p. 331), TJAC (p. 333), TOFF (p. 334), TPRO (p. 334), TRAD (p. 336), TRAN (p. 336), TRCE (p. 337), TRMAXITER (p. 338), TSCCM (p. 339), TSTR (p. 342), TWAL (p. 345), UFAC (p. 346), UINL (p. 347), USET (p. 349), USEV (p. 350) (Restart), USEV (p. 350) (XMLI), UWGT (p. 352), VCOR (p. 352), WMIX (p. 364), WSRC (p. 366), XCEN (p. 367), XEND (p. 367), XMLI (p. 369), XMLOUTPUT_WRITE (p. 369), XMLS (p. 370), XSRC (p. 372), XSTR (p. 372)

9.5.2. Rotating Disk CVD Reactor

The following keywords can be used to build an input file for a Rotating Disk CVD Reactor Model:

AINL (p. 148), ASEN (p. 153), ATIM (p. 155), ATOL (p. 157), BULK (p. 164), CDCT (p. 168), CHEM (p. 169), CNDT (p. 172), CNDX (p. 172), CNTN (p. 172), COMP (p. 174), COND (p. 175), CPROD (p. 176), CTOL (p. 180), CURV (p. 181), DELT (p. 182), DFAC (p. 183), DIST (p. 184), DT0 (p. 186), DTMN (p. 187), DTMX (steady-state) (p. 187), EMIS (p. 191), EMSG (p. 192), END (p. 192), ENRG (p. 194), EPSS (p. 197), ETCH (p. 200), FLAM (p. 207), FLRT (p. 208), FLUX (p. 210), FPRO (p. 210), GDOT (p. 212), GFAC (p. 213), GRAD (p. 214), GRID (p. 215), HSEN (p. 217), INIT (p. 225), INJM (p. 225), INJS (p. 225), INJT (p. 225), INJW (p. 226), INJX (p. 226), INLET (p. 226), INTM (p. 227), IPSR (p. 228), IRET (p. 229), ISTEP (p. 230), JJRG (p. 230), LINE (p. 233), LPRT (p. 233), MAXIT (p. 236), MAXTIME (p. 236), MIX (p. 237), MORD (p. 240), MULT (p. 243), NADP (p. 244), NEWRUN (p. 245), NJAC (p. 246), NO_SDOUTPUT_WRITE (p. 247), NO_XMLOUTPUT_WRITE (p. 247), NOCH (p. 249), NOFT (p. 249), NONR (p. 250), NOTP (p. 250), NPTS (p. 251), NSOL (p. 252), NTOT (p. 253), OINL (p. 255), OMEG (p. 255), PRES (p. 265), PRNT (p. 266), PROD (p. 267), PWRC (p. 278), QDOT (p. 279), QDTC (p. 279), RADGS (p. 287), RDSK (p. 288), REAC (p. 288), RELAXC (p. 290), REOR (p. 291), RLGAS (p. 292), RLMIX (p. 293), RRAD (p. 295), RSTR (p. 295), RTIM (p. 296), RTOL (p. 298), SCCM (p. 299), SCCMPRO (p. 300), SDOUTPUT_WRITE (p. 304), SENT (p. 305), SFAC (p. 306), SFLR (p. 307), SIZE (p. 308), SPOS (p. 311), SSMAXITER (p. 313), STST (p. 317), SURF (p. 317), TBND (p. 321), TDIF (p. 322), TDSK (p. 323), TEMP (p. 323), TGIV (p. 326), TIM1 (p. 328), TIM2 (p. 329), TIME (p. 330), TINL (p. 331), TJAC (p. 333), TOFF (p. 334), TPRO (p. 334), TRAD (p. 336), TRAN (p. 336), TRCE (p. 337), TRMAXITER (p. 338), TSCCM (p. 339), TSTR (p. 342), TWAL (p. 345), UFAC (p. 346), UINL (p. 347), USET (p. 349), USEV (p. 350) (Restart), USEV (p. 350) (XMLI), UWGT (p. 352), VCOR (p. 352), WMIX (p. 364), WSRC (p. 366), XCEN (p. 367), XEND (p. 367), XMLI (p. 369), XMLOUTPUT_WRITE (p. 369), XMLS (p. 370), XSRC (p. 372), XSTR (p. 372)

9.6. Shock Tube Reactors

9.6.1. Normal Incident Shock

The following keywords can be used to build an input file for a Incident Shock Reactor Model:

ATOL (p. 157), CNTN (p. 172), CONC (p. 174), DELT (p. 182), DIA (p. 183), DIST (p. 184), END (p. 192), INIT (p. 225), IPSR (p. 228), ISHK (p. 229), ISKB (p. 230), LGDT (p. 232), NEWRUN (p. 245), NO_SDOUT-

PUT_WRITE (p. 247), NO_XMLOUTPUT_WRITE (p. 247), NSOL (p. 252), P1A (p. 257), P2A (p. 257), RHO1 (p. 291), RHO2 (p. 291), RLGAS (p. 292), RLMIX (p. 293), RTOL (p. 298), SDOUTPUT_WRITE (p. 304), SIZE (p. 308), T1 (p. 319), T2 (p. 319), TIME (p. 330), TSTR (p. 342), TSTR (p. 343), USET (p. 349), VISC (p. 356), VSHK (p. 361), XMLI (p. 369), XMLOUTPUT_WRITE (p. 369), ZNDB, (p. 373) ZNDC (p. 373).

9.6.2. Normal Reflected Shock

The following keywords can be used to build an input file for a Reflected Shock Reactor Model:

ATOL (p. 157), CNTN (p. 172), CONC (p. 174), DELT (p. 182), DIST (p. 184), END (p. 192), INIT (p. 225), IPSR (p. 228), LGDT (p. 232), NEWRUN (p. 245), NO_SDOUTPUT_WRITE (p. 247), NO_XMLOUT-PUT_WRITE (p. 247), NSOL (p. 252), P1A (p. 257), P2A (p. 257), P3A (p. 257), RHO1 (p. 291), RHO2 (p. 291), RHO3 (p. 292), RLGAS (p. 292), RLMIX (p. 293), RSHK (p. 295), RTOL (p. 298), SDOUTPUT_WRITE (p. 304), SIZE (p. 308), T1 (p. 319), T2 (p. 319), T3 (p. 319), TIME (p. 330), TSTR (p. 342), TSTR (p. 343), USET (p. 349), VRS (p. 361), VSHK (p. 361), XMLI (p. 369), XMLOUTPUT_WRITE (p. 369)

9.7. Miscellaneous Reactor Models

9.7.1. Gas Mixer

The following keywords can be used to build an input file for a Gas Mixer Reactor Model:

ABSL (p. 140), ATIM (p. 155), ATOL (p. 157), CNTN (p. 172), CNTT (p. 173), CPROD (p. 176), DELT (p. 182), DFAC (p. 183), DIST (p. 184), DTMN (p. 187), DTMX (steady-state) (p. 187), DTSV (p. 188), END (p. 192), ENRG (p. 194), FLRT (p. 208), FPRO (p. 210), GFAC (p. 213), GMHTC (p. 214), HTC (p. 219), HTRN (p. 220), INLET (p. 226), IPSR (p. 228), IRET (p. 229), ISTP (p. 230), MAXTIME (p. 236), MMASS (p. 239), NEWRUN (p. 245), NJAC (p. 246), NNEG (p. 247), NO_SDOUTPUT_WRITE (p. 247), NO_XMLOUTPUT_WRITE (p. 247), NOFT (p. 249), NPSR (p. 251), NSOL (p. 252), PPRO (p. 264), PRES (p. 265), PRNT (p. 266), QFUN (p. 280), QLOS (p. 281), REAC (p. 288), RELT (p. 291), RTIM (p. 296), RTOL (p. 298), SCCM (p. 299), SCCMPRO (p. 300), SCOR (p. 303), SDOUTPUT_WRITE (p. 304), SFAC (p. 306), SFLR (p. 307), SIZE (p. 308), SPOS (p. 311), SSMAX-ITER (p. 313), STPT (p. 316), STST (p. 317), TAMB (p. 320), TEMP (p. 323), TGIV (p. 326), TIM1 (p. 328), TIM2 (p. 329), TIME (p. 330), TINL (p. 331), TJAC (p. 333), TPRO (p. 334), TRAN (p. 336), TRMAXITER (p. 338), TSCCM (p. 339), TSTR (p. 342), TTIM (p. 344), UFAC (p. 346), USET (p. 349), USEV (p. 350), USRIN (p. 351), VOL (p. 359), VPRO (p. 360), VTIM (p. 361), WENG (p. 363), XMLI (p. 369), XMLOUTPUT_WRITE (p. 369), XMLS (p. 370)

9.7.2. Equilibrium

The following keywords can be used to build an input file for a Equilibrium Reactor Model:

CJ (p. 169), CONX (p. 175), CPROD (p. 176), DIST (p. 184), END (p. 192), ENGY (p. 194), ENTH (p. 196), ENTR (p. 196), FAZE (p. 205), FREE (p. 211), FROZ (p. 211), IPSR (p. 228), NEWRUN (p. 245), NO_SDOUT-PUT_WRITE (p. 247), NO_XMLOUTPUT_WRITE (p. 247), NSOL (p. 252), PEST (p. 258), PH (p. 259), PRES (p. 265), PS (p. 270), PV (p. 276), REAC (p. 288), RLGAS (p. 292), RLMIX (p. 293), SDOUTPUT_WRITE (p. 304), SIZE (p. 308), TEMP (p. 323), TEST (p. 325), TP (p. 334), TS (p. 339), TSTR (p. 342), TV (p. 344), USET (p. 349), VH (p. 355), VOL (p. 359), VS (p. 361), VU (p. 362), XMLI (p. 369), XMLOUTPUT_WRITE (p. 369)

9.7.3. Mechanism Analyzer

The following keywords can be used to build an input file for a Mechanism Analyzer:

ALL (p. 149), CARR (p. 168), DIST (p. 184), END (p. 192), GEN (p. 213), GRXN (p. 215), GTHB (p. 216), IPSR (p. 228), LSCL (p. 234), MAJ (p. 234), NEWRUN (p. 245), NO_SDOUTPUT_WRITE (p. 247), NO_XMLOUT-PUT_WRITE (p. 247), NONE (p. 250), NSOL (p. 252), PFAL (p. 258), PHIA (p. 260), PLOA (p. 261), PNUM (p. 263), PRES (p. 265), SCOV (p. 304), SDOUTPUT_WRITE (p. 304), SIZE (p. 308), SRXN (p. 312), STCK (p. 315), TBTH (p. 322), TBTH (p. 322), TDEL (p. 322), TFAL (p. 325), THIG (p. 327), THRM (p. 327), TLOW (p. 334), TRAN (p. 337), TSTR (p. 342), TSUM (p. 343), USET (p. 349), XBTH (p. 367), XMLI (p. 369), XMLOUT-PUT_WRITE (p. 369)

Chapter 10: Alphabetical Listing of Project Input Keywords

In this chapter we provide detailed information about the meaning and usage of each keyword entry that may be included as part of a Reactor Model input file. [Reference Guide to Project Input Keywords](#) (p. 125) provides a cross-referenced listing that shows which keywords are available for each Reactor Model, while [CHEMKIN Project Input: Keyword Syntax and Rules](#) (p. 123) provides general keyword syntax and rules. The following categorized lists of auxiliary keywords are provided:

- [Table 3.4: Alphabetical Listing of REACTIONS-line Options for Gas-phase Kinetics Data](#) (p. 43)
- [Table 3.7: Alphabetical Listing of Gas-phase Reaction Auxiliary Keywords](#) (p. 47)
- [Table 4.3: Alphabetical Listing of REACTIONS-line Options for Surface Reaction Data](#) (p. 71)
- [Table 4.6: Alphabetical Listing of Surface Reaction Auxiliary Keywords](#) (p. 78)

The alphabetical listing of keywords is distributed over the following sections:

[10.1. Alphabetical Listing of Keywords \[A-E\]](#)

[10.2. Alphabetical Listing of Keywords \[F-O\]](#)

[10.3. Alphabetical Listing of Keywords \[P-S\]](#)

[10.4. Alphabetical Listing of Keywords \[T-Z\]](#)

10.1. Alphabetical Listing of Keywords [A-E]

Table 10.1: Alphabetical Listing of Keywords [A-E]

Keyword	Definition			
AB- FR Solver	This keyword serves as a switch to turn on an empirical active surface area factor when surface reaction rates on the particle surface are calculated. The concept is that not all surface area (or sites) on the particle surface is active. The active surface area during the particle formation phase is found to be a function of total particle mass and gas temperature. The form and the model parameters of this empirical formulation are obtained by fitting predictions to measured data from premixed flames. By default this factor is turned off.			
	Parameters	Optional/Reqd.	Units	Examples
	--	--	--	ABFR
	Keyword Usage	Optional keyword. By default this factor is turned off.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		

Keyword	Definition			
		• Perfectly-stirred Reactor (PSR) • Plug-flow Reactor (PFR)		
ABSL Solver	This keyword is used to override the default value for the absolute perturbation in the solution variable used in the determination of the numerically derived Jacobian.			
	Parameters	Optional/Reqd.	Units	Examples
	Absolute perturbation	Required	--	ABSL 1.E-15
	Keyword Usage	Optional keyword. By default, if the ATOL (p. 157) keyword is given, then the absolute perpetuation is set equal to the ATOL (p. 157) value. ATOL (p. 157) is not specified, then the absolute perturbation is set equal to the square root of the unit round-off error of the machine.		
	Reactor Models	• Closed Plasma Reactor • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR		
ACHG Solver	Maximum absolute change in the surface site fractions (over one time step) for which the preliminary, fictitious transient equations can be considered to have converged to steady state. The convergence test is made against the sum of the ACHG (p. 140) value plus the product of RCHG (p. 287) multiplied by the old site-fraction value. Therefore, if ACHG (p. 140) is set to zero (by default) then only RCHG (p. 287) is used to control the convergence criteria.			
	Parameters	Optional/Reqd.	Units	Examples
	Absolute relative change	Required	--	ACHG 1.0E-7
	Keyword Usage	Optional keyword. By default, only RCHG (p. 287) is used to determine convergence.		
	Reactor Models	• Honeycomb Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		
ADAM Solver	Flag indicating the implicit Adams method of the DVODE solver is used to integrate the equations.			
	Keyword Usage	Optional keyword. By default, the DASPK solver will be used.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR)		

Keyword	Definition			
		• Partially Stirred Reactor (PaSR)		
ADAP Solver	Flag indicating the saving of additional adaptive points for improved resolution of the solution data (for example, for post-processing and plotting) for transient simulations. ADAP is the default. ADAP inserts extra solution points when your solution is changing rapidly (for example, a steep transient or engine ignition occurs). How and when the points are inserted is controlled by the AVALUE (p. 159) , AVAR (p. 159) and ASTEPS (p. 154) keywords. The companion keyword, NADAP (p. 244) , can be used to turn off adaptive time-stepping during continuations, if desired.			
	Keyword Usage	Optional keyword. ADAP is the default.		
	Reactor Models	• Closed Plasma Reactor • Closed Homogeneous Reactor • Honeycomb Reactor • IC HCCI Engine Model • Multi-Zone HCCI Engine Simulator • Plasma Plug Flow Reactor • Multiphase PSR • Plug Flow Reactor • SI Engine Zonal Simulator		
ADD Reactor or Inlet Property	Mole fractions of species that should be added to the inlet or initial composition but excluded from the equivalence-ratio calculation. This keyword is only valid when the equivalence-ratio option is used to specify the inlet or initial composition. These species do not enter into the equivalence ratio computations. One species is entered per line.			
	Parameters	Optional/Reqd.	Units	Examples
	Inlet stream name	Optional (PSRs only) If there is no stream name than the product species applies to the default or all	--	ADD mixture1 AR 0.2

Keyword	Definition			
		defined streams.		
	Species name	Required	--	ADD AR 0.2
	Additive fractions	Required	mole fractions	ADD AR 0.2
	Keyword Usage	Optional keyword. By default, ADD (p. 141) is not used. But either REAC (p. 288) or EQUI (p. 199) / FUEL (p. 211) / OXID (p. 256) / CPROD (p. 176) is required for each inlet stream or to define initial conditions for a closed system.		
	Reactor Models	• Closed Homogeneous Batch Reactor • IC HCCI Engine • Plasma PSR • Plug Flow Reactor • SI Engine Zonal Simulator		
	Notes	• The ADD (p. 141) keywords must be changed as a set, not individually for a restart run. • The ADD (p. 141) keywords must be changed as a set, not individually for a continuation run.		
ADIA Reactor Property	Turns on the adiabatic wall condition for plug-flow or for planar, symmetric, shear-flow models. For planar, non-symmetric shear flow, an adiabatic wall is the default, but for symmetric (planar or cylindrical) shear-flow cases, the ADIA (p. 142) keyword is required for the adiabatic condition.			
	Keyword Usage	Optional keyword. By default, the specified (temperature) condition is used for shear-layer flow. The default behavior for plug-flow depends on the problem type; if the energy equation is being solved, the default is for adiabatic conditions.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Honeycomb Reactor • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		
AEXT	External surface area (for 0-D Homogeneous systems) or surface area per unit length (for Plug Flow Models) used to control heat transfer to the external			

Keyword	Definition			
Reactor Property Profiles	environment. AEXT (p. 142) is usually used to specify area profiles as a function of time (0-D Homogeneous systems) or distance (Plug Flow Models). However, if the AEXT (p. 142) value is only provided at a single point, then the surface area is assumed to be constant as a function of time (for transient 0-D Homogeneous systems) or distance (for Plug Flow Models). See also AREAQ (p. 151) .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Time or Distance, depending on Reactor Model</i>	Required	sec or cm	AEXT 0.0 1.0
	<i>External surface area or surface area per unit length, depending on Reactor Model</i>	Required	cm ² or cm	AEXT 0.0 1.0
	Keyword Usage	Optional keyword. If not specified, the external area is assumed equal to the internal surface area (see AINT (p. 148) or AREA (p. 150)).		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Plasma PSR • SI Engine Zonal Simulator		
AFLO Reactor Property Profiles	Cross-sectional area profile as a function of distance. If only a single AFLO (p. 143) entry is provided, the cross-sectional area is assumed to be a constant at that specified value. See also AREAF (p. 151) and DIAM (p. 184) .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Distance from inlet</i>	Required	cm	AFLO 0.0 1.0
	<i>Cross-sectional area</i>	Required	cm ²	AFLO 0.0 1.0
	Keyword Usage	Optional keyword. If none of DIAM (p. 184) , AFLO (p. 143) , or AREAF (p. 151) keywords are included, then an attempt will be made to use the GEOM user subroutine to determine the flow area.		
	Reactor Models	• Honeycomb Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		

Keyword	Definition			
AFLW Reactor Property	Fraction of the total lower wall surface area that corresponds to a surface material. For example, "AFLW WAFER 0.001" indicates that the material "WAFER" makes up 0.1% of the lower wall surface area. The material name must correspond to a material name declared in the <i>Surface Kinetics</i> input file or an error will occur.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Surface material name</i>	Required	--	AFLW WAFER 0.001
	<i>Fraction of total surface area</i>	Required	--	AFLW WAFER 0.001
	Keyword Usage	Optional keyword. By default, 1.0 is used for all materials in all PSRs.		
	Reactor Models	• Non-symmetric Planar Shear Flow Reactor		
AFRA Reactor Property	Fraction of the total surface area that corresponds to a surface material (see the multiple surface material capability under <i>Surface Kinetics</i>). For example, "AFRA WAFER 0.001" indicates that the material "WAFER" makes up 0.1% of the total reactor surface area. The material name must correspond to a material name declared in the <i>Surface Kinetics</i> input file or an error will occur.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Surface material name</i>	Optional	--	AFRA WAFER 0.001
	<i>Fraction of total surface area</i>	Required	--	AFRA WAFER 0.001
	<i>Reactor number (PSR clusters only)</i>	Optional If no number is given, the keyword is assumed to apply to all reactors in a cluster.	--	AFRA WAFER 0.001 2
	Keyword Usage	Optional keyword. By default, 1.0 is used for all materials in all PSRs.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Honeycomb Reactor		

Keyword	Definition			
		• Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor		
AFRMX Reactor Property/Model	Maximum air entrainment mass flow rate into the spray parcel.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Max air entrainment rate</i>	Required	g/sec	AFRMX 200.0
	Keyword Usage	Optional keyword. Default is 50 g/sec.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
AGGA Reactor Property	The pre-exponential factor of the Arrhenius-like expression for characteristic fusion time.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Material name</i>	Required	--	AGGA SOOT 1.0E10
	<i>Pre-exponential factor</i>	Required	sec	AGGA C(B) 1.0E7
	Keyword Usage	Optional keyword. By default, the pre-exponential factor is 1.0E-30.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Diffusion or Premixed Opposed-flow Flame • IC HCCI Engine • Multi-Zone HCCI Engine Simulator • Perfectly Stirred Reactor (PSR) • Plasma PSR • Premixed Laminar Burner-stabilized Flame • SI Engine Zonal Simulator		
AG-GB Reactor Property	The temperature exponent of the Arrhenius-like expression for characteristic fusion time.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Material name</i>	Optional	--	AGGB SOOT 1.0

Keyword	Definition			
	<i>Temperature exponent</i>	Required		AGGB C(B) 0.5
	Keyword Usage	Optional keyword. By default, the temperature exponent is 0.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Diffusion or Premixed Opposed-flow Flame • IC HCCI Engine • Multi-Zone HCCI Engine Simulator • Perfectly Stirred Reactor (PSR) • Plasma PSR • Premixed Laminar Burner-stabilized Flame • SI Engine Zonal Simulator		
AG-GD	The exponent of the primary particle diameter in the Arrhenius-like expression for characteristic fusion time.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Primary particle name</i>	Optional	--	AGGD C(B) 1.0
	Keyword Usage	Optional keyword. By default, the primary particle diameter is 1.0.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Diffusion or Premixed Opposed-flow Flame • IC HCCI Engine • Multi-Zone HCCI Engine Simulator • Perfectly Stirred Reactor (PSR) • Plasma PSR • Premixed Laminar Burner-stabilized Flame • SI Engine Zonal Simulator		
AGGE	The activation temperature of the Arrhenius-like expression for characteristic fusion time.			

Keyword	Definition			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	AGGE SOOT 0.0
	Activation temperature	Required	K	AGGE C(B) 800
	Keyword Usage	Optional keyword. By default, the activation temperature is 0.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Diffusion or Premixed Opposed-flow Flame • IC HCCI Engine • Multi-Zone HCCI Engine Simulator • Perfectly Stirred Reactor (PSR) • Plasma PSR • Premixed Laminar Burner-stabilized Flame • SI Engine Zonal Simulator		
AGGFD	The fractal dimension of the aggregate.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	AGGFD SOOT 1.0E3.0
	Fractal dimension	Required	--	AGGFD C(B) 1.8
	Keyword Usage	Optional keyword. By default, the fractal dimension is 3.0.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Diffusion or Premixed Opposed-flow Flame • IC HCCI Engine • Multi-Zone HCCI Engine Simulator • Perfectly Stirred Reactor (PSR) • Plasma PSR • Premixed Laminar Burner-stabilized Flame • SI Engine Zonal Simulator		

Keyword	Definition			
AGGMN Reactor Property	The threshold value to include the sintering effect in particle aggregation. For the Moments Method, this indicates the ratio of the collision to the fusion time scale, whereas for the Sectional Method, this indicates the minimum value of the characteristic fusion time.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Material name</i>	Required	--	AGGMN SOOT 1.0E10
	<i>Threshold</i>	Required	-- (Moments)sec (Sectional)	AGGMN SOOT 1.0E-4
	Keyword Usage	Optional keyword. By default, the threshold is 1.0E-3 for the Moments Method and 1.0E-06 for the Sectional Method.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Diffusion or Premixed Opposed-flow Flame • IC HCCI Engine • Multi-Zone HCCI Engine Simulator • Perfectly Stirred Reactor (PSR) • Plasma PSR • Premixed Laminar Burner-stabilized Flame • SI Engine Zonal Simulator		
AINL Inlet Property	The radial velocity spreading rate. At the inlet $x = L$, $v/r = \text{AINL}$.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Radial velocity divided by radius</i>	Required	1/sec	AINL 2.3
	Keyword Usage	Optional keyword. By default, the radial velocity spreading rate is 0.0.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• Supersedes previous AFUE and AOXI keywords.		
AINT	Internal surface area (for 0-D Homogeneous systems) or surface area per unit length (for Plug Flow models) that is considered active for surface chemistry.			

Keyword	Definition			
Reactor Property Profiles	AINT (p. 148) is usually used to specify area profiles as a function of time (0-D Homogeneous systems) or distance (Plug Flow models). However, if the AINT (p. 148) value is only provided at a single point, then the surface area is assumed to be constant as a function of time (for transient 0-D Homogeneous systems) or distance (for Plug Flow models). See also AREA (p. 150).			
	Parameters	Optional/Reqd.	Units	Examples
	Time or distance, depending on Reactor Model	Required	sec or cm	AINT 0.0 1.0
	Internal surface area or area per unit length, depending on Reactor Model	Required	cm2 or cm	AINT 0.0 1.0
	Keyword Usage	Optional keyword. If not specified, the internal surface area is determined based on the hydraulic diameter for a plug-flow, as specified through AFLO (p. 143), AREAF (p. 151), or DIAM (p. 184) keywords. For 0-D Homogenous systems, a value of 0.0 is assumed by default.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Reactor • Perfectly Stirred Reactor (PSR) • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor		
ALL Output	Turns default output on for all of Surftherm's tables.			
	Keyword Usage	Optional keyword. By default, the all output will be printed. See also NONE (p. 250).		
	Reactor Models	• Mechanism Analyzer		
APRO Reactor Property Profiles	Use of the APRO (p. 149) keyword(s) allow the user to specify a piece-wise linear profile as a function of distance for the stream-tube area. The stream-tube area is given relative to the burner area and is therefore dimensionless. Each input provides a pair and the x coordinates must be in ascending order. For example, APRO 0.1 1.2 assigns a relative area of 1.2 at a position 0.1 cm from the burner surface.			
	Parameters	Optional/Reqd.	Units	Examples
	x-coordinates	Required	cm	APRO 0.1 1.2

Keyword	Definition			
	<i>Relative area</i>	Required	dimensionless	APRO 0.1 1.2
	Keyword Usage	Optional keyword. By default, the area ratio is constant at 1.0.		
	Reactor Models	• Premixed Laminar Burner-stabilized Flame		
	Notes	• This keyword can be changed for a restart run.		
AREA	The total internal surface area (for 0-D homogeneous reactors) or surface area per unit length (for plug-flow) in the reactor. The internal surface area represents the area available for surface chemistry. See also AINT (p. 148) .			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Total surface area or surface area per unit length, depending on Reactor Model</i>	Required	cm ² or cm	AREA 200
	<i>Reactor number (PSR clusters only)</i>	Optional If no number is given, the keyword is assumed to apply to all reactors in a cluster.	--	AREA 200 1
	Keyword Usage	Optional keyword. By default, the total surface area is set to 0.0 for 0-D homogeneous reactor models and is determined based on the hydraulic diameter (set using DIAM (p. 184) , AREAF (p. 151) , AFLO (p. 143)) for plug-flow.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Reactor • Perfectly Stirred Reactor (PSR) • Plasma PSR • Plasma Plug Flow Reactor • Multiphase PSR		

Keyword	Definition			
		• Plug Flow Reactor		
AREAF Reactor Property	The total cross-sectional flow area. See also AFLO (p. 143) .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Cross-sectional flow area</i>	Required	cm ²	AREAF 200
	Keyword Usage	Optional keyword. Either DIAM (p. 184) or AREAF (p. 151) must be set, unless the user has implemented the GEOM user subroutine.		
	Reactor Models	• Honeycomb Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		
AREAM Reactor Property	Contact area for mass exchange or reactions between two phases or bulks.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Contact area for mass transfer and reactions</i>	Required	cm ²	AREAM catalyst Gas 50.0
	Keyword Usage	Required for multiphase systems. Two bulk phase names must follow the keyword indicating the bulks in contact. "Gas" indicates the gas phase. Default value of 0 is used for combination of bulks for which the area is not specified.		
	Reactor Models	• Closed Multiphase Reactor • Multiphase PSR		
AREAQ Reactor Property	The total external surface area (for 0-D homogeneous reactors) or surface area per unit length (for plug-flow) in the reactor. The external surface area represents the area available for heat transfer to the external environment. See also AEXT (p. 142) .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Total surface area or surface area per unit length, depending on Reactor Model</i>	Required	cm ² or cm	AREAQ 200
	<i>Reactor number (PSR clusters only)</i>	Optional If no number is given, the keyword	--	AREAQ 200 1

Keyword	Definition			
		is assumed to apply to all reactors in a cluster.		
	Bulk name (multiphase reactors only) Keyword Usage	Optional	--	AREAQ Gas AMBIENT 0.5
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Reactor • Perfectly Stirred Reactor (PSR) • Plasma PSR • Plasma Plug Flow Reactor • Multiphase PSR • Plug Flow Reactor		
AROP Output	Determine the rate-of-production coefficients for all species and print results to the diagnostic output file of the reactor simulation.			
	Keyword Usage	Optional keyword. By default, no rate-of-production values are printed.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Closed Multiphase Reactor • Honeycomb Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR)		

Keyword	Definition			
		• Plasma Plug Flow Reactor • Plasma PSR • Multiphase PSR • Plug Flow Reactor • SI Engine Zonal Simulator		
	Notes	• This keyword can be added but not removed from a continuation run.		
ASEN Output	Calculate the first-order, A-factor sensitivity coefficients (that is, with respect to the gas-phase and surface chemistry rate constants) for species fractions and for other dependent variables in the system. Sensitivity results will be included in the XML Solution File. For 0-D and Plug Flow systems, sensitivity results will also be printed to the diagnostic output file.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>String indicating for which variables sensitivity coefficients will be saved or printed. The string is a space-delimited list containing species names and any one of the following: ALL, AVEL, RVEL, CVEL, FLRT, or TEMP (see Notes)</i>	Optional If no string is given, then ALL is assumed.	--	ASEN H2O ASEN TEMP
	Keyword Usage	Optional keyword. By default, no sensitivity coefficients are computed or printed. See also SENG (p. 304) .		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Closed Multiphase Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor		

Keyword	Definition	
		• Plasma PSR • Multiphase PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • SI Engine Zonal Simulator • Stagnation Flow CVD Reactor
	Notes	• This keyword can be added but not removed from a continuation run. • See also EPSS (p. 197), EPSG (p. 196), EPST (p. 198), SENG (p. 304), and HSEN (p. 217) for other sensitivity options The optional parameter strings are defined as follows: • ALL: all species and all other dependent variables in the solution • AVEL: axial velocity (Plug Flow, Diffusion or Premixed Opposed-flow Flames, Rotating Disk, and Stagnation Flow CVD Reactors only) • CVEL: circumferential velocity (Rotating Disk and Stagnation Flow CVD Reactors only) • RVEL: radial velocity (Diffusion or Premixed Opposed-flow Flames, Rotating Disk, and Stagnation Flow CVD Reactors only) • FLRT: mass flow rate (Premixed Laminar Flame-speed Calculation only) • TEMP: gas temperature
ASTEPS Output	Uses the integrator steps to adaptively insert extra solution data points in addition to those specified by the DTSV (p. 188) option whenever the solver takes the number of integration steps specified by this option. The default is 20, the value used if no argument is provided. The purpose of the ASTEPS (p. 154) keyword is to ensure that during a transient solution, sufficient solution data points are available around the time of a fast transient, for example a rapidly increasing temperature, so that an accurate analysis of the problem is possible (to allow a good plotting resolution).	

Keyword	Definition			
	Parameters	Optional/Reqd.	Units	Examples
	Integration steps	Optional.	--	ASTEPS 20
	Keyword Usage	Optional keyword. By default ASTEPS (p. 154) is set to 20.		
	Reactor Models	• Closed Homogeneous Reactor • Closed Plasma Reactor • Honeycomb Reactor • IC HCCI Engine • Multi-Zone HCCI Engine Simulator • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • SI Engine Zonal Simulator		
	Notes	• For further details, see the description of DTSV (p. 188).		
AS-WH Reactor Property	Crank angle at which the simulation switches from fixed-temperature condition to using energy equation with Woschni correlation as the heat transfer model. By default the energy equation is used starting at zero crank angle.			
	Parameters	Optional/Reqd.	Units	Examples
	Crank angle in degrees.	Required	degree	ASWH 5.0
	Keyword Usage	Optional keyword.		
	Reactor Models	• Multi-Zone HCCI Engine Simulator • SI Engine Zonal Simulator		
ATIM Solver	Absolute tolerance for convergence of Newton iteration as it is used in the pseudo time stepping procedure for steady-state problems employing the <i>Twopnt</i> solver. Since we are not seeking accuracy in a transient solution, this convergence criteria typically does not need to be as stringent as for the Newton iteration on the actual steady-state solution.			
	Parameters	Optional/Reqd.	Units	Examples
	Absolute tolerance	Required	--	ATIM 1.E-6
	Keyword Usage	Optional keyword. By default, the absolute tolerance is 1.E-9. See also RTIM (p. 296) .		

Keyword	Definition			
	Reactor Models	• Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• For a precise definition, see the description of ATOL (p. 157).		
ATLM	ATOL (p. 157) is used for all variables.			
Solver	Parameters	Optional/Reqd.	Units	Examples
	<i>Tolerance</i>	Required	--	ATLM 1.0E-6
	Keyword Usage	ATOL (p. 157) .		
	Reactor Models	• Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Multiphase PSR		
ATLRE	The absolute tolerance to determine the energy fluxes at the droplet surface are balanced. This is one of the convergence criteria for solving the droplet surface temperature. This parameter is associated with the "Solve for Surface T" option of the vaporization model.			
Reactor Property/Model	Parameters	Optional/Reqd.	Units	Examples
	<i>Tolerance</i>	Required	--	ATLRE 1.0E-6
	Keyword Usage	Optional keyword.		

Keyword	Definition			
	Reactor Models	• Direct Injection Diesel Engine Simulator		
ATLS Solver	Absolute tolerance used by the transient DASPK solver, as an indicator of the accuracy desired in the solution for the sensitivity coefficients only. Generally, the sensitivity coefficients need not be solved to a great degree of accuracy, so these tolerances could be lower than the tolerances placed on the physical variables.			
	Parameters	Optional/Reqd.	Units	Examples
	Absolute tolerance	Required	--	ATLS 1.E-3
	Keyword Usage	Optional keyword. The default absolute tolerance is 1.E-5.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator		
ATLTS Reactor Property/Model	The absolute tolerance for the droplet surface temperature. A droplet surface temperature is considered found when the change in the droplet surface temperature of two consecutive iterations is less than the tolerance. This parameter is associated with the "Solve for Surface T" option of the vaporization model.			
	Parameters	Optional/Reqd.	Units	Examples
	Temperature change	Required	K	ATLTS 0.01
	Keyword Usage	Optional keyword. Default is 0.001 K.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
ATOL Solver	Absolute tolerance used by the solvers as an indicator of the accuracy desired in the physical solution. Typically ATOL (p. 157) should be less than the smallest meaningful value of a species mass fraction.			
	Parameters	Optional/Reqd.	Units	Examples
	Absolute tolerance	Required	--	ATOL 1.E-9
	Keyword Usage	Optional keyword. The default values are:		

Keyword	Definition
	CVD, Partially Stirred Reactor (PaSR), Plug Flow Reactor, Shear Flow Reactor: 1.E-8 Open 0-D Reactors run in steady-state mode, Opposed-flow Flame, Premixed Laminar Burner-stabilized Flame, Premixed Laminar Flame-speed Calculation: 1.E-9 Normal Incident Shock, Normal Reflected Shock: 1.E-10 Closed 0-D Reactors and Open 0-D Reactors run in transient mode: 1.E-20 See also RTOL (p. 298).
	Reactor Models • Closed Homogeneous Batch Reactor • Closed Partially Stirred Reactor (PaSR) • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Normal Incident Shock • Normal Reflected Shock • Opposed-flow Flame • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Multiphase PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor

Keyword	Definition			
		• SI Engine Zonal Simulator • Stagnation Flow CVD Reactor		
AVALUE Output	Uses the integrator steps to adaptively insert extra solution data points in addition to those specified by the DTSV (p. 188) option whenever the variable specified by the AVAR (p. 159) keyword moves by $\pm x$ since the last time an extra data point was generated. You must specify a value for AVALUE; there is no default and you must also specify the AVAR (p. 159) keyword. The purpose of the AVALUE keyword is to ensure that during a transient solution, sufficient solution data points are available around the time of a fast transient, for example a rapidly increasing temperature, so that an accurate analysis of the problem is possible (to allow plotting a resolution).			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Integration steps</i>	Required	--	AVALUE 10
	Keyword Usage	Optional keyword. AVAR is required.		
	Reactor Models	• Closed Plasma Reactor • Closed Homogeneous Reactor • Honeycomb Reactor • IC HCCI Engine Model • Multi-Zone HCCI Engine Simulator • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Multiphase PSR • Plug Flow Reactor • SI Engine Zonal Simulator		
	Notes	• See also ASTEPS (p. 154) and AVAR (p. 159) is required when AVALUE is used.		
AV-AR Output	Determines which variable is used for the AVALUE (p. 159) keyword. Parameter <string> should be "temperature" or the name of a particular species to serve as the time-stepping monitor species. There is no default species value. AVAR is required when the AVALUE (p. 159) keyword is used.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>String</i>	Required	--	AVALUE temperature AVALUE CH4

Keyword	Definition			
	Keyword Usage	Optional keyword.		
	Reactor Models	• Closed Plasma Reactor • Closed Homogeneous Reactor • Honeycomb Reactor • IC HCCI Engine Model • Multi-Zone HCCI Engine Simulator • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Multiphase PSR • Plug Flow Reactor • SI Engine Zonal Simulator		
AX-IS Reactor Property	Use a radial, axisymmetric coordinate system.			
	Keyword Usage	Optional keyword. By default, the coordinate system is radially axisymmetric.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame		
AZFAC Reactor Property/Model	The maximum portion of the initial cylinder volume that can be assigned to the spray parcels.			
	Parameters	Optional/Reqd.	Units	Examples
	Maximum total initial parcel volume	Required	--	AZFAC 0.33
	Keyword Usage	Optional keyword. Default is 0.5.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
BDF Solver	Flag indicating the backward differentiation formulas of the DVODE solver is used to integrate the equations.			
	Keyword Usage	Optional keyword. By default, the DASPK solver will be used.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR)		
BDUR Solver	Specifies the value of the "duration of combustion," Dq_c , in the Wiebe function. Dq_c must be greater than 0.			

Keyword	Definition			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Duration of combustion in number of crank angles</i>	Required	degree	BDUR 45.6
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		
BEFF Solver	Specifies the mass fraction of the fresh fuel-air charge being consumed by the premixed flame, that is, the combustion efficiency. The combustion efficiency must be > 0.0 and ≤ 1.0 and is set to 1.0 (complete combustion) by default.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Combustion efficiency</i>	Optional	--	BEFF 0.85
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		
BETA Reactor Property	This is a combined correction factor to the coalescent collision between particles. The van der Waals forces can enhance the collision frequency while non-coalescent collision can reduce the frequency. The default value is 1.0, that is, van der Waals effect is off and collisions are 100% coalescent.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Material name</i>	Required	--	BETA C(B) 0.9
	<i>Enhance factor</i>	Required	--	BETA C(B) 0.9
	Keyword Usage	Optional keyword.		
	Reactor Models	• Closed Homogeneous Batch Reactor		
		• Closed Plasma Reactor		
	• Cylindrical Shear Flow Reactor			
	• Honeycomb Monolith Reactor			
	• IC HCCI Engine			
	• Perfectly Stirred Reactor (PSR)			
	• Planar Shear Flow Reactor			
	• Plasma PSR			
	• Plasma Plug Flow Reactor			
	• Plug Flow Reactor			
	• SI Engine Zonal Simulator			

Keyword	Definition			
BINI Solver	Specifies the value of the "duration of combustion," q_c , in the Wiebe function.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Start of combustion crank angle</i>	Required	degree	BINI -15.3
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		
BLKEQ Reactor Property	Toggle to turn on or off solution of bulk activities for bulk species.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>String "on" or "off" to turn on or off solution of the bulk-species equations</i>	Required	--	BLKEQ ON BLKEQ OFF
	Keyword Usage	Optional keyword. By default, bulk-activity equations are solved when there is more than one bulk species in one or more bulk phases on a material. Otherwise the bulk activities are presumed constant at their initial value.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Reactor • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor		
BM-COE Reactor Property / Model	A multiplier, when set to a value greater than 0, that enables the spray parcels to pass their contents (composition and enthalpy) indirectly to other spray parcels via the air zone for the multi-injection simulations.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Parcel back-mixing coefficient</i>	Required	--	BMCOE 1.0
	Keyword Usage	Optional keyword. Default value = 0.0.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
BLTK Reactor Property	Specifies a boundary-layer thickness. When BLTK (p. 162) is declared, a parabolic velocity profile is specified with a zero velocity at each wall increasing to the velocity specified by VEL (p. 354) at a distance of BLTK (p. 162) from the wall. A flat (constant) velocity profile is used for distances greater than BLTK (p. 162) from			

Keyword	Definition			
	the wall. In addition, if the initial gas temperature differs from the initial surface temperature the application linearly interpolates the gas-phase temperature profile between the wall temperature and the bulk gas temperature over the distance BLTK (p. 162) .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Boundary-layer thickness</i>	Required	cm	BLTK 0.05
	Keyword Usage	Optional keyword. By default, the boundary-layer thickness is set to 0 and a full parabolic velocity is assumed.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
BP-WR Reactor Property	RF bias power at a specified material. The energy that the ions gain in the sheath is estimated as this power divided by the total ion current to that material as calculated in the plasma-reactor model. For example, "BPWR material1 200" specifies an applied bias of 200 W to the material boundary, <i>material1</i> . The ion energy gain calculated from the sheath model results in a reduced effective power deposition to the electrons (unless ELSH (p. 190) is also specified), as described in Homogeneous 0-D Reactor Models of the Chemkin Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Material name</i>	Optional If there is no material name than the multiplier applies to all materials.	--	BPWR material1 200 1
	<i>RF bias power</i>	Required	watts	BPWR 200
	<i>Reactor number (PSR clusters only)</i>	Optional If no number is given, the profile described by the first two values is assumed	--	BPWR material1 200 1

Keyword	Definition			
		to apply to all reactors in a cluster.		
	Keyword Usage	Optional keyword. By default, the RF bias power is set to 0.0.		
	Reactor Models	- Closed Plasma Reactor - Plasma PSR - Plasma Plug Flow Reactor		
BT-MIN	The minimum value of the Spalding heat transfer number to prevent numerical issues at the beginning of liquid vaporization.			
Reactor Property/Model	Parameters	Optional/Reqd.	Units	Examples
	Spalding heat transfer limit	Required	--	BTMIN 0.01
	Keyword Usage	Optional keyword. Default is 0.1		
	Reactor Models	Direct Injection Diesel Engine Simulator		
BULK	The estimated or initial bulk species activities. This is required input for bulk species in bulk phases that are being etched. For example, BULK Ga(d) 1.0 assigns the estimated activity of 1.0 to the Ga(d) bulk phase species.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Bulk species name	Required	--	BULK Ga(d) 1.0
	Bulk activity	Required	--	BULK Ga(d) 1.0
	Keyword Usage	Required keyword. The bulk activity should be specified for bulk species. By default, the initial or estimated bulk species activities are 0.0.		
	Reactor Models	- Closed Homogeneous Batch Reactor - Closed Plasma Reactor - Cylindrical Shear Flow Reactor - Honeycomb Reactor - Perfectly Stirred Reactor (PSR) - Planar Shear Flow Reactor - Plasma Plug Flow Reactor - Plasma PSR - Plug Flow Reactor		

Keyword	Definition			
		- Rotating Disk CVD Reactor - Stagnation Flow CVD Reactor		
	Notes	- The sum of all estimated bulk phase activities for each bulk phase n should equal one. If they do not sum to one, they will be normalized to one, and a warning message will be printed in the diagnostic output. - See also: ETCH (p. 200) keyword. - Formerly ACT keyword for some reactor models in previous Ansys Chemkin versions.		
BULK_MASSFRAC Mass fraction of a species within a bulk phase.				
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>phase name</i>	Required		BULK_MASSFRAC Gas 0.6
	<i>mass fraction of a species within a bulk phase</i>	Required		BULK_MASSFRAC jetFuel 0.4
	Keyword Usage	This keyword is used to specify the composition of the entire reactor. Bulk phase name follows the keyword. "Gas" indicates the gas phase. The composition is normalized to 1 at the start of simulation.		
	Reactor Models	- Closed Multiphase Reactor - Open Multiphase PSR Reactor		
BULK_MOLARITY Molarity of a species within a liquid bulk phase. Used for dilute mixtures.				
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Molarity of a species within a liquid bulk</i>	Optional	--	BULK_MOLARITY nc12h26(l) 1.0
	Keyword Usage	This keyword is used to specify the composition of a dilute liquid bulk. Species name must follow the keyword.		
	Reactor Models	- Closed Multiphase Reactor - Multiphase PSR		

Keyword	Definition			
BULK_MOLEFRAC Reactor Property	Mole fraction of a species within a bulk phase.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Mole fraction of a species within a liquid bulk</i>	Required	--	BULK_MOLEFRAC Gas 0.6 BULK_MOLEFRAC jet-Fuel 0.4
	Keyword Usage	This keyword is used to specify the composition of the entire reactor. Bulk phase name follows the keyword. "Gas" indicates the gas phase. The composition is normalized to 1 at the start of simulation.		
	Reactor Models	• Closed Multiphase Reactor • Multiphase PSR		
BULK_SOLVENT Reactor Property	Solvent specification when molarity is used to specify composition of a liquid bulk phase. Used for dilute mixtures.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Solvent when molarity is used for composition of a liquid bulk</i>	Optional	--	BULK_SOLVENT nc12h26(l)
	Keyword Usage	This keyword specifies the solvent when molarity is used to specify composition of a dilute liquid bulk. Species name must follow the keyword. The BULK_MOLARITY (p. 165) keyword must also be specified when this keyword is used.		
	Reactor Models	• Closed Multiphase Reactor • Multiphase PSR		
BURN Reactor Property	Indicates a burner-stabilized flame problem type, with specified inlet flow rates.			
	Keyword Usage	Required keyword.		
	Reactor Models	• Premixed Laminar Burner-stabilized Flame		
	Notes	• The problem-type can be changed for a restart run. • See also FREE (p. 211) .		
CAAC Output	The crank angle at 50% mass burned and is also referred as the anchoring angle. This is one of the three crank angle parameters required to construct the Wiebe function profile that will pass these three crank angles at their corresponding burned mass fractions. By default, this angle marks when half of the original mass is burned. All three crank angles, CASC (p. 168) , CAAC (p. 166) , and CAEC (p. 167) must be provided.			
	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	<i>Crankangle at 50% mass burned</i>	Required	degree	CAAC 8.1
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		
CAADV	Additional CA shift.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Additional CA shift</i>	Optional	degree	CAADV 1.5
	Keyword Usage	Optional keyword. Optional for use with OPMV (p. 255) or OPOC (p. 256) . Default value = 0.0.		
	Reactor Models	• Direct Injection Diesel Engine Simulator • IC HCCI Engine • Multi-Zone HCCI Engine • SI Engine Zonal Simulator		
CAATQ	Calculates the crank angle for the specified amount of total heat release. The crank angle for 10% and 50% of total heat release will be calculated by default.			
Output	Parameters	Optional/Reqd.	Units	Examples
	<i>Percentage of total heat release</i>	Required	percent	CAATQ 90
	Keyword Usage	Optional keyword.		
	Reactor Models	• IC HCCI Engine • Multi-Zone HCCI Engine Simulator • SI Engine Zonal Simulator		
CAEC	The crank angle at 90% mass burned. This is one of the three crank angle parameters required to construct the Wiebe function profile that will pass these three crank angles at their corresponding burned mass fractions. By default, this angle marks when 90% of the original mass is burned. All three crank angles, CASC (p. 168) , CAAC (p. 166) , and CAEC (p. 167) must be provided.			
Output	Parameters	Optional/Reqd.	Units	Examples
	<i>Crankangle at 90% mass burned</i>	Required	degree	CAEC 23.0
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		
CAIR	Model coefficients for the air entrainment mass flow rate model. There are three parameters required for "before ignition", "after ignition", and "after reaching wall", respectively.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	<i>Coefficient before ignition</i>	Required	--	CAIR 0.9 0.25 1.0
	<i>Coefficient after ignition</i>	Required	--	CAIR 0.9 0.25 1.0
	<i>Coefficient after wall</i>	Required	--	CAIR 0.9 0.25 1.0
	Keyword Usage	Required keyword. Default: before ignition: 1.0, after ignition: 0.58, after hitting wall: 1.2.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
CARR Reactor Property	Specify the named species as the carrier gas. This keyword is used to identify the species in calculating binary diffusion coefficients for tables and for non-dimensionalizations that require a binary diffusion coefficient.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Species name</i>	Optional	--	CARR H2
	<i>Species number</i>	Optional	--	CARR 3
	Keyword Usage	Optional keyword. The default is to use the gas species with the largest mole fraction (from the XBTH (p. 367) input) in the bath-gas composition. If the gas-phase bath-gas composition is not specified, the default is to use the first species in the mechanism.		
	Reactor Models	• Mechanism Analyzer		
CASC Output	The crank angle at 10% mass burned. This is one of the three crank angle parameters required to construct the Wiebe function profile that will pass these three crank angles at their corresponding burned mass fractions. By default, this angle marks when 10% of the original mass is burned. All three crank angles, CASC (p. 168) , CAAC (p. 166) , and CAEC (p. 167) must be provided.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Crankangle at 10% mass burned</i>	Required	degree	CASC -15.4
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		
CD-CT Reactor Property	Include conduction through the substrate in the energy balance. Inclusion of this keyword requires specification of a substrate thickness (CNDX (p. 172)). This value is used only if the disk temperature is being calculated from an energy balance by including keyword RADB (p. 286) . See Equation 15.18 of the Chemkin Theory Manual .			
	Keyword Usage	Optional keyword. By default, conduction through the substrate is not included.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		

Keyword	Definition			
CDIF Solver	Use central differencing on convective terms in the equations.			
	Keyword Usage	Optional keyword. By default, windward differencing is used.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation		
CFL Reactor Property	The Courant-Friedrichs-Lewy (CFL) number for the convective process; this parameter limits the fraction of particles whose properties can be set to the inlet conditions per time step.			
	Parameters	Optional/Reqd.	Units	Examples
	CFL number	Required	--	CFL 1.0
	Keyword Usage	Optional keyword. By default, the CFL (p. 169) number is 0.5.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR)		
CHEM Reactor Property	Specifies that gas-phase chemistry will be included in the calculations.			
	Keyword Usage	Optional keyword. This option is used to reactivate the chemical kinetics if the NOCH (p. 249) option was in effect for the previous calculation for CVD Reactors. For PaSRs, the default is to neglect chemistry and do a mixing calculation only.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR) • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
CJ Problem Type	Chapman-Jouguet detonation. In this case, H, S, V, and T contain the unburned state and TEST (p. 325) gives the burned temperature estimate.			
	Keyword Usage	Optional keyword. The user must include exactly one problem-type keyword		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
CK-TRN Reactor Property	An option to use the Chemkin mixture-averaged transport subroutines to evaluate any transport properties (for example, gas viscosity) needed by the reactor models. This option requires a valid transport linking file from pre-processing of the chemistry set, that is, the chemistry set must include the transport data of all gas species.			
	Keyword Usage	Optional keyword.		
	Reactor Models	• IC HCCI Engine		

Keyword	Definition			
		- Multi-Zone HCCI Engine Simulator - SI Engine Zonal Simulator		
CLSC Reactor Property	Defines a critical particle class under which the oxidation process starts to affect (reduce) the particle number density. This parameter is only used by the particle burnout model and has no effect on particle formation and growth. The default value is the minimum particle class plus the maximum class change due to surface reaction.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	CLSC CARBON 40
	Critical particle class	Required	--	CLSC CARBON 40
	Keyword Usage	Optional keyword. The default value is the minimum particle class plus the maximum class change due to surface reaction.		
	Reactor Models	- Closed Homogeneous Batch Reactor - Closed Plasma Reactor - Cylindrical Shear Flow Reactor - Honeycomb Monolith Reactor - IC HCCI Engine - Perfectly Stirred Reactor (PSR) - Planar Shear Flow Reactor - Plasma PSR - Plasma Plug Flow Reactor - Plug Flow Reactor - SI Engine Zonal Simulator		
CLSE Reactor Property	Flag indicating the reactor is a closed system, that is, mass flow rate is zero.			
	Keyword Usage	Required Keyword.		
	Reactor Models	Closed Partially Stirred Reactor (PaSR)		
CLSM Reactor Property	Defines the smallest particle class that can exist in the system. This parameter is only used by the particle burnout model and has no effect on particle formation and growth. The default value is the smallest inception class defined by the nucleation reactions.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	CLSM CARBON 32

Keyword	Definition			
	<i>Minimum particle class</i>	Required	--	CLSM CARBON 32
	Keyword Usage	Optional keyword.The default value is the smallest inception class defined by the nucleation reactions.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Honeycomb Monolith Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator		
CMIX Reactor Property	The controlling parameter for the modified Curl's and the IEM (p. 224) models for a PaSR.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Time ratio for scalar mixing (Equation 10.1 of the Chemkin Theory Manual)</i>	Required	--	CMIX 1.0
	Keyword Usage	Required keyword, unless WELL (p. 363) keyword is included.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR)		
CM-PR Reactor Property	Engine compression ratio.The compression ratio is defined as the maximum total volume in the cylinder (clearance volume plus swept volume) divided by the clearance volume.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Engine compression ratio</i>	Required	--	CMPR 10
	Keyword Usage	Optional keyword. By default, the ratio is 15.		
	Reactor Models	• IC HCCI Engine		

Keyword	Definition			
		• SI Engine Zonal Simulator		
CNDT Reactor Property	The back-side temperature of the substrate for use in calculation of conduction losses. This value is used only if the disk temperature is being calculated from an energy balance by including keywords RADB (p. 286) and CDCT (p. 168) . See Equation 15.18 of the Chemkin Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Back-side temperature</i>	Required	K	CNDT 350.
	Keyword Usage	Optional keyword. By default, the back-side temperature is 300.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
CNDX Reactor Property	The thickness of the substrate for calculation of conduction losses. This value is used only if the disk temperature is being calculated from an energy balance by including keywords RADB (p. 286) and CDCT (p. 168) . See Equation 15.18 of the Chemkin Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Substrate thickness</i>	Required	cm	CNDX 0.03
	Keyword Usage	Optional keyword. By default, the substrate thickness is 0.0.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
CNTN Reactor Property	Inclusion of this keyword causes Ansys Chemkin to expect keywords for another problem to follow the END (p. 192) keyword. The following problem uses the solution of the previous problem as its initial guess. This capability is very similar to that provided by RSTR (p. 295) . However, in the case of CNTN (p. 172) , several related problems can be solved by one job submission, without having to manipulate the XML Solution File. The solutions resulting from CNTN (p. 172) keywords are written sequentially to one XML Solution File.			
	Keyword Usage	Optional keyword. By default, no continuation is expected.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Honeycomb Reactor • IC HCCI Engine • Non-reactive Gas Mixer		

Keyword	Definition	
		• Normal Incident Shock • Normal Reflected Shock • Opposed-flow Flame Simulator • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor Using Steady-state Solver • SI Engine Zonal Simulator • Stagnation Flow CVD Reactor Using Steady-state Solver
CNTT Reactor Property	This will cause the starting time of the continuation calculation to be equal to the end time of the last solution.	
	Keyword Usage	Optional keyword. By default, the starting time of a continuation is set to zero.
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • SI Engine Zonal Simulator
CNTX Reactor Property	This will cause the starting distance of the continuation calculation to be equal to the end distance of the last solution. This keyword is used for Plug Flow Reactors in place of CNTT (p. 173).	
	Keyword Usage	Optional keyword. By default, the starting distance of a continuation is set to zero.
	Reactor Models	• Honeycomb Reactor

Keyword	Definition			
		• Plasma Plug Flow Reactor • Plug Flow Reactor		
COLR Reactor Property	This flag indicates the collision formulation to be used to calculate the collision rate among particles. Three types of collision formulations are available: free molecular regime (=0), continuum regime (=1), and transition regime (=3). The collision rate in the transition regime is obtained as the harmonic mean of the collision rates of free-molecular regime and continuum regime. By default, formulation for free-molecular collision is used.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	COLR C(B) 1
	Collision regime	Required	--	BETA C(B) 1
	Keyword Usage	Optional keyword. By default, the formulation for the free-molecular regime is used (0).		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Honeycomb Monolith Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator		
COMP Reactor Property	The boundary condition used at the inlet boundary for the gas species equations will be that of a fixed gas composition, as specified by the REAC (p. 288) keywords.			
	Keyword Usage	Optional keyword. By default, a flux balance is solved at the inlet (see keyword FLUX (p. 210)).		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
CONC Output	If this keyword is used, the printed output will appear in molar concentration (mole/cc) rather than mole fraction.			
	Keyword Usage	Optional keyword. By default, mole fractions are printed.		

Keyword	Definition			
	Reactions	• Normal Incident Shock • Normal Reflected Shock		
COND Reactor Property	The thermal conductivity of the substrate in SI units, for use in calculation of conduction losses. This value is used only if the disk temperature is being calculated from an energy balance by including keywords RADB (p. 286) and CDCT (p. 168) . See Equation 15.18 of the Chemkin Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	Thermal conductivity	Required	W/cm K	COND 2.1
	Keyword Usage	Optional keyword. By default, the thermal conductivity is 1.38.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
CONP Problem Type	A transient solution will be obtained with the pressure held constant. The equations solved are those of a constant pressuresystem and the energy equation will be solved.			
	Keyword Usage	Optional keyword. By default, a constant pressure problem is assumed.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor		
CONV Problem Type	A transient solution will be obtained with the volume held constant. The equations solved are those of a constant volume system and the energy equation will be solved. In this case, the pressure is allowed to float.			
	Keyword Usage	Optional keyword. By default, a constant pressure problem is assumed.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor		
CONX Reactor Property	This keyword is used to specify a constant (constrained) mole fraction for a species. For example, CONX H2 0.1 will fix the fraction of hydrogen in the mixture to be 0.1.			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	CONX H20.1
	Mole fraction of the species	Required	mole fraction	CONX H2 0.1
	Keyword Usage	Optional keyword. By default, composition equilibrium is determined for all species.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		

Keyword	Definition			
COTV Problem Type	• A transient solution will be obtained with the • temperature and • volume held • constant at the initial values. In this case, the pressure is allowed to float.			
	Keyword Usage	Optional keyword. By default, a constant pressure is assumed.		
	Reactor Models	• Closed Homogeneous Batch Reactor		
CPROD Inlet or Reactor Property	One of these CPROD (p. 176) inputs must appear for each complete-combustion product species when the equivalence ratio option is used (EQUI (p. 199)) for an inlet stream or for the initial conditions of a closed system.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Inlet stream name (PSRs only)</i>	Optional If there is no stream name than the product species will be used for all defined inlet streams.	--	CPROD mixture1 CO2 CPROD mixture1 H2O
	<i>Species name</i>	Required	--	CPROD H2OCPROD CO2
	Keyword Usage	Required keyword when EQUI (p. 199) option is used for an inlet stream or for the initial conditions in a reactor. The specified group of complete-combustion product species must include all of the elements contained in the fuel and oxidizer species. The products must also be "saturated" species. See the Ansys Chemkin Tutorials Manual for more information.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations • Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame		

Keyword	Definition			
		• Honeycomb Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• The CPROD (p. 176) keywords must be changed as a set, not individually for a restart run. • The CPROD (p. 176) keywords must be changed as a set, not individually for continuation run.		
CRLN1	Specify the intake-side connecting rod length.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Connecting rod length	Required	cm	CRLN1 9.2
	Keyword Usage	Optional keyword. Required for use with OPMV (p. 255) or OPOC (p. 256) .		
	Reactor Models	• Direct Injection Diesel Engine Simulator • IC HCCI Engine • Multi-Zone HCCI Engine • SI Engine Zonal Simulator		
CRLN2	Specify the exhaust-side connecting rod length.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Connecting rod length	Required	cm	CRLN2 8.67

Keyword	Definition			
	Keyword Usage	Optional keyword. Required for use with OPMV (p. 255) or OPOC (p. 256) .		
	Reactor Models	• Direct Injection Diesel Engine Simulator • IC HCCI Engine • Multi-Zone HCCI Engine • SI Engine Zonal Simulator		
CRRD1	Specify the intake-side crank radius.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Crank radius</i>	Required	cm	CRRD1 3.1
	Keyword Usage	Optional keyword. Required for use with OPMV (p. 255) or OPOC (p. 256) .		
	Reactor Models	• Direct Injection Diesel Engine Simulator • IC HCCI Engine • Multi-Zone HCCI Engine • SI Engine Zonal Simulator		
CRRD2	Specify the exhaust-side crank radius.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Crank radius</i>	Required	cm	CRRD2 2.5
	Keyword Usage	Optional keyword. Required fo use with OPMV (p. 255) or OPOC (p. 256) .		
	Reactor Models	• Direct Injection Diesel Engine Simulator • IC HCCI Engine • Multi-Zone HCCI Engine • SI Engine Zonal Simulator		
CSVOUT-PUT_FILE-NAME	Specify CSV output file name.			
Output	Keyword Usage	Optional keyword.		
	Parameters	Optional/Reqd.	Units	Examples
	<i>CSV Output File Name</i>	Optional. It is to be used along with CSVOUTPUT_WRITE . By	--	CSVOUTPUT_FILENAME modelOutput.csv

Keyword	Definition			
		default, the name of the file is Out - put . csv.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Multiphase PSR • Honeycomb Reactor • Internal Combustion Engine		
CSVOUT- PUT_KOUT	Write species mass-fraction to CSV output file.			
Output	Parameters	Optional/Reqd.	Units	Examples
	Species for Mass Fraction	Optional It is to be used along with with CSVOUTPUT_WRITE.	--	CSVOUTPUT_KOUT CH4
	Keyword Usage	Optional keyword. By default, a constant pressure is assumed.		
	Parameters	Optional/Reqd.	Units	Examples
	CSV Output File Name	Optional. It is to be used along with with CSVOUTPUT_WRITE. By default, the name of the file is Out - put . csv.	--	CSVOUTPUT_FILENAME modelOutput.csv
	Reactor Models	• Closed Homogeneous Batch Reactor • Honeycomb Reactor • Internal Combustion Engine • Multiphase PSR • Plug Flow Reactor • Diffusion or Premixed Opposed-flow Flame		

Keyword	Definition			
		• Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Premixed Laminar Burner-stabilized Stagnation Flame		
CSVOUT-PUT_WRITE Output	Write output data to a CSV file.			
	Keyword Usage	Optional keyword. By default, solution data is not written to a CSV file. Note that only a limited data is written to CSV file.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Honeycomb Reactor • Internal Combustion Engine • Plug Flow Reactor • Multiphase PSR • Diffusion or Premixed Opposed-flow Flame • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Premixed Laminar Burner-stabilized Stagnation Flame		
CTOL Reactor Property	Criterion for determining when steady state is reached using a transient solver for Partially Stirred Reactors. The required parameter sets the normalized slope of mean density change in time $(d\bar{p}/dt)$. The default number of time points used to determine the slope is 100; this value can be changed with the keyword NCFIT.			
	Parameters	Optional/Reqd.	Units	Examples
	Normalized slope of mean density	Required	--	CTOL 1.0E-3
	Keyword Usage	Optional keyword. By default, the program does not check for the steady state.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR)		
CTOL Solver	Criterion for determining when steady-state is reached by a transient solver for CVD Reactors. The steady state is reached when the normalized absolute values of all time derivatives are less than CTOL (p. 180).			
	Parameters	Optional/Reqd.	Units	Examples
	Steady-state criterion	Required	--	CTOL 1.0E-2

Keyword	Definition			
	Keyword Usage	Optional keyword. By default, the criterion is 1.0E-4.		
	Reactor Models	- Rotating Disk CVD Reactor - Stagnation Flow CVD Reactor		
CURL	Flag indicating that the modified Curl's model will be used to simulate the molecular mixing within the computational particle.			
Reactor Property	Keyword Usage	Optional keyword. By default, a well mixed model is assumed.		
	Reactor Models	- Closed Partially Stirred Reactor (PaSR) - Partially Stirred Reactor (PaSR)		
CURV	Parameter that controls the degree of mesh adaptation based on the second derivative, or curvature, in the solution. A reasonable value is usually between about 0.1 and 1.0, where no adaptation based on curvature is specified with 1.0.			
Solver	Parameters	Optional/Reqd.	Units	Examples
	<i>Normalized curvature parameter</i>	Required	--	CURV 0.7
	Keyword Usage	Optional keyword. By default, the curvature parameter is set to 0.5.		
	Reactor Models	- Diffusion or Premixed Opposed-flow Flame - Premixed Laminar Burner-stabilized Flame - Premixed Laminar Flame-speed Calculation - Rotating Disk CVD Reactor - Stagnation Flow CVD Reactor		
	Notes	- This keyword can be changed for a restart run. Steady-state 1-D Solution Methods of the Chemkin Theory Manual for more information.		
CY-BAR	The cylinder head area to bore-area ratio.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Ratio of cylinder head area to bore area.</i>	Required	None	CYBAR 1.2
	Keyword Usage	Optional keyword. Default = 1.0.		
	Reactor Models	- IC HCCI Engine - Multi-zone HCCI Engine		

Keyword	Definition			
		• SI Engine Zonal Simulator		
	Notes	• CYBAR should be > 1.0.		
DASP	Flag indicating the DASPK solver is used to integrate the transient equations.			
Solver	Keyword Usage	Optional keyword. By default, the DASPK solver will be used.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR)		
DEGO	The starting crank angle for the transient IC HCCI Engine model, in degrees.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Crank angle	Required	degrees	DEGO 45
	Keyword Usage	Optional keyword. By default, this starting angle is 180 degrees.		
	Reactor Models	• IC HCCI Engine • SI Engine Zonal Simulator		
DE-GE	The ending crank angle for the IC engine simulation. Normally, this is the same as the crank angle at Exhaust Valve Open (EVO).			
Output	Parameters	Optional/Reqd.	Units	Examples
	Crankangle at end of simulation	Required	degree	CAAC 120.5
	Keyword Usage	Optional keyword.		
	Reactor Models	• IC HCCI Engine • Multi-zone HCCI Engine • SI Engine Zonal Simulator		
DELT	The time interval for solution printing to the diagnostic text output file, for the transient solver. Note that the number of time points written to the diagnostic output file is equal to the value given by TIME (p. 330) divided by DELT (p. 182) .			
Solver	Parameters	Optional/Reqd.	Units	Examples
	Time interval	Required	sec	DELT 1.0E-4
	Aurora Usage	Optional keyword. By default, the value of the maximum solver timestep (STPT (p. 316)) is used.		
	Spin Usage	Optional keyword. By default, this is a required keyword for a transient calculation.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor		

Keyword	Definition			
		• IC HCCI Engine • Non-reactive Gas Mixer • Normal Incident Shock • Normal Reflected Shock • Perfectly Stirred Reactor (PSR) • Plasma PSR • Multiphase PSR • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor • SI Engine Zonal Simulator		
	Notes	• Backwards compatible with DT from previous versions.		
DFAC Solver	Factor by which to divide the time step in the steady-state solver, <i>Twopnt's</i> , time stepping procedure when necessary, that is, when the current time step does not converge.			
	Parameters	Optional/Reqd.	Units	Examples
	Division factor	Required	--	DFAC 1.5
	Keyword Usage	Optional keyword. By default, the division factor is set to 2.2.		
	Reactor Models	• Closed Plasma Reactor • Diffusion or Premixed Opposed-flow Flame • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
DIA	Shock-tube diameter, used for boundary layer corrections.			

Keyword	Definition			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Tube diameter</i>	Required	cm	DIA 2.0
	Keyword Usage	Optional keyword. By default, the tube diameter is set to 1.0.		
	Reactor Models	• Normal Incident Shock		
DIAM Reactor Property	Tube diameter or hydraulic diameter, where the diameter is constant along the channel. See also DPRO (p. 185) , AREAF (p. 151) , AFLO (p. 143) and user subroutine GEOM.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Tube diameter</i>	Required	cm	DIAM 5.3
	Keyword Usage	Optional keyword. The user must specify DIAM (p. 184) , DPRO (p. 185) , AREAF (p. 151) , or AFLO (p. 143) , unless the GEOM user routine is to be used.		
	Reactor Models	• Honeycomb Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		
DI-EN Problem Type	Specify that the spray-Combustion Direct Injection Engine Model is used. The Alphabetical Listing of Keywords [F-O] (p. 222) keyword must also be included in the same input file.			
	Keyword Usage	Required keyword.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
DIN-ZL Inlet Property	Define the name of the injector.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Name of injector</i>	Required	--	DINZL modelX
	Keyword Usage	Required keyword.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
DIST XMLI	This keyword is valid with the XMLI (p. 369) option, when the XML Solution File that is used for initialization or restart contains data as a function of axial distance (e.g. from Shear-layer Flow or Plug Flow). In this case, select the values to use in initialization or restart as those corresponding to the distance that is closest to (greater than or equal to) the specified distance.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Axial distance</i>	Required	cm	DIST 5.0
	Keyword Usage	Optional keyword. By default, uses the data from the last axial distance found in the XML Solution File.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations • Closed Homogeneous Batch Reactor		

Keyword	Definition			
	• Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • IC HCCI Engine • Mechanism Analyzer • Non-reactive Gas Mixer • Normal Incident Shock • Normal Reflected Shock • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • SI Engine Zonal Simulator • Stagnation Flow CVD Reactor			
DPRO Reactor Property Profiles	Hydraulic diameter or tube diameter as a function of distance. See also DIAM (p. 184) , AREAF (p. 151) , AFLO (p. 143) , and user subroutine GEOM.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Distance from inlet</i>	Required	cm	DPRO 0.01.0
	<i>Hydraulic diameter</i>	Required	cm	DPRO 0.0 1.0
	Keyword Usage	Optional keyword. The user must enter DIAM (p. 184) , DPRO (p. 185) , AREAF (p. 151) , or AFLO (p. 143) , unless user subroutine GEOM is to be used.		
	Reactor Models	• Honeycomb Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		

Keyword	Definition			
DT Reactor Property	The time step size of the Monte Carlo simulation.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Time step</i>	Required	sec	DT 1.0E-4
	Keyword Usage	Required keyword.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR)		
DT0 Solver	The initial time step size used by the transient solver.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Initial time step size</i>	Required	sec	DT0 1.0E-4
	Keyword Usage	Optional keyword. By default, the initial time step size is set to 1.0E-6.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR) • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• Backwards compatible with H0 (p. 217) keyword.		
DTDEG Solver	The maximum time step in terms of crank angle that may be taken by the DASPK solver for the transient IC HCCI Engine model, in degrees. If DTDEG (p. 186) is specified, then it will overwrite the time step value specified by STPT (p. 316) .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Time step</i>	Required	degrees	DTDEG 30
	Keyword Usage	Optional keyword. By default, this time step is value of STPT (p. 316) .		
	Reactor Models	• IC HCCI Engine • SI Engine Zonal Simulator		
	Notes	• See also: STPT (p. 316) keyword.		
DTIGN Output	Temperature threshold used to determine when ignition has occurred and allow printing of ignition delay times. The ignition temperature will be the initial temperature plus this value. Only applicable when you are solving the energy equation with the transient solver.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Ignition temperature delta</i>	Required	K	DTIGN 200
	Keyword Usage	Optional keyword. See also TLIM (p. 333) .		
	Reactor Models	• Closed Homogeneous Batch Reactor		

Keyword	Definition			
		• Closed Plasma Reactor • Honeycomb Monolith Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator		
DTMN Solver	Minimum time step tolerated in the steady-state solver, <i>Twopnt</i> 's time stepping algorithm before flagging an error condition.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Minimum time step</i>	Required	sec	DTMN 1.E-9
	Keyword Usage	Optional keyword. By default, the minimum time step is 1.E-10.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor • Planar Shear Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation		
DTMX (steady-state) Solver	Maximum time step allowed in <i>Twopnt</i> 's time-stepping algorithm. When this value is reached, the time step size will no longer be increased and time stepping will continue with a fixed time step.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Maximum time step</i>	Required	sec	DTMX 1.E-3
	Keyword Usage	Optional keyword. By default, the maximum time step is 1.E-2.		

Keyword	Definition			
	Reactor Models	• Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
DTMX (transient) Solver	Maximum time step used internally by the solver in transient calculations. DTMX (p. 187) determines the largest time-step the transient solver can take at one time and thereby controls the resolution for interpolation of specified time-profiles.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Maximum time step</i>	Required	sec	DTMX 1.E-3
	Keyword Usage	Optional keyword. By default, the maximum time step is 1.E-4.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR)		
DTSV Output or Solver	Controls the time interval for data to be written to the XML Solution File (e.g., <i>XMLdata.zip</i>). Note that the number of time points written to the XML Solution File is equal to the value given by TIME (p. 330) divided by DTSV (p. 188) .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Time interval for solution saving</i>	Required	sec	DTSV 1.0E-5
	Keyword Usage	Optional keyword. By default, the value of the STPT (p. 316) keyword is used.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR)		

Keyword	Definition			
		• Plasma PSR • Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR) • SI Engine Zonal Simulator		
DX Output or Solver	Distance interval for printing the solution to the diagnostic output file.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Distance interval</i>	Required	cm	DX 0.25.
	Keyword Usage	Optional keyword. By default, the distance interval is the value of the DXMX (p. 189) is used, or XEND (p. 367) divided by 100 if DXMX (p. 189) is not available.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Honeycomb Reactor • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		
DXMX Solver	The maximum distance step that can be used internally by the transient solver. DXMX (p. 189) determines the largest step that the solver can take at one time and thereby controls the resolution for interpolation of specified spatial-profiles. See also DX (p. 189) and DXSV (p. 189) .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Distance interval</i>	Required	cm	DXMX 0.1
	Keyword Usage	Optional keyword. By default, If either DX (p. 189) or DXSV (p. 189) are specified, then DXMX (p. 189) is set to the smallest of these values. If neither DX (p. 189) nor DXSV (p. 189) are specified, then DXMX (p. 189) is set to the value of XEND (p. 367) divided by 100.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Honeycomb Reactor • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		
DXSV Solver	Controls the distance interval for data to be written to the XML Solution File (for example, <i>XMLdata.zip</i>). The number of points written to the XML Solution File is equal to the value given by XEND (p. 367) divided by DXSV (p. 189) .			

Keyword	Definition			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Distance interval</i>	Required	cm	DXSV 0.1
	Keyword Usage	Optional keyword. By default, the value of DXMX (p. 189) is used.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Honeycomb Reactor • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		
EGRR	Specifies the EGR rate for an inlet stream or for the initial conditions in a closed reactor.			
Reactor or Inlet Property	Parameters	Optional/Reqd.	Units	Examples
	<i>EGR ratio</i>	Optional	None	EGRR 0.2
	Keyword Usage	Optional keyword. EGR rate can be used in any reactor model as a feature on input or initial composition panels. EGR specification can be activated when Equivalence ratio option is used to specify inlet or initial composition. Leaving the EGR Rate box empty will use no EGR, but use diluants if specified on the Added Species tab. When EGR Rate is specified, the composition on the Added Species tab is used as the EGR composition. The sum of all the fractions on the Added Species tab should be 1.0 when EGR Rate is specified. If the sum is less than 1, Chemkin will automatically normalize the EGR composition.		
	Reactor Models	• Closed Homogeneous Batch Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Honeycomb Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor		
ELSH	Specified energy loss to ions in the sheath for each ion lost at a specified material. The energy that the ions gain in the sheath is typically assumed to be the sheath voltage, which can be described as a multiplier of kT_e . The value given here is the value of the multiplier. For example, "ELSH material1 5.0" would result in an ion energy gain of $5kT_e$ as it crossed the sheath near the material material1. This			
Reactor Property				

Keyword	Definition			
	energy gain for the ions results in a reduced effective power deposition to the electrons, as described in Plasma Systems of the Chemkin Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Material name</i>	Optional If there is no material name then the multiplier applies to all materials.	--	ELSH material 15.0 1
	<i>Multiplier value</i>	Required	--	ELSH 5.0
	<i>Reactor number (PSR clusters only)</i>	Optional If no number is given, values are assumed to apply to all reactors in a cluster.	--	ELSH material1 5.0 1
	Keyword Usage	Optional keyword. By default, the multiplier is set to 0.0, when no ELSH (p. 190) keyword is included.		
	Reactor Models	• Closed Plasma Reactor • Plasma Plug Flow Reactor • Plasma PSR		
EMIS Reactor Property	The emissivity of the disk. This value is used only if the disk temperature is being calculated from an energy balance by including keyword RADB (p. 286) . See Equation 15.18 of the Chemkin Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Emissivity</i>	Required	--	EMIS 0.9
	Keyword Usage	Optional keyword. By default, the emissivity is 0.85.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		

Keyword	Definition			
EM-PAR Reactor Property	This keyword provides the value of the model parameter C_{part} for computing the overall emissivity of the named particle cloud as given in Equation 13.21 in the Chemkin Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Material name</i>	Required	--	EMPAR soot 700
	<i>Model coefficient</i>	Required	$\text{m}^{-1}\text{K}^{-1}$	EMPAR soot 700
	Keyword Usage	Optional keyword. The default value is 700 ($\text{m}^{-1}\text{K}^{-1}$).		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Burner-stabilized Pre-mixed Flame • Premixed Laminar Flame-speed Calculation		
EMSG Reactor Property Profiles	Approximation of the temperature-dependent emissivity of the gas-mixture, used to calculate a radiation-loss term in the gas energy equation. The radiation is calculated between the gas and the disk (using the gas temperature) and between the gas and the inlet (using the inlet temperature). The EMSG (p. 192) keyword provides temperature, emissivity pairs for the gas mixture.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Temperature</i>	Required	K	EMSG 20000.03
	<i>Emissivity</i>	Required	--	EMSG 2000 0.03
	Keyword Usage	Optional keyword. By default, no gas radiation loss is included in the energy equation.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
END Reactor Property	This keyword signifies the end of the input data for a given reactor description. It must appear after each set of data when continuation jobs are indicated using the CNTN (p. 172) keyword.			
	Keyword Usage	Required keyword.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations • Closed Homogeneous Batch Reactor • Closed Partially Stirred Reactor (PaSR) • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • IC HCCI Engine		

Keyword	Definition			
		• Mechanism Analyzer • Non-reactive Gas Mixer • Normal Incident Shock • Normal Reflected Shock • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Multiphase PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • SI Engine Zonal Simulator • Stagnation Flow CVD Reactor		
EN-D-TIMEMAX Reactor Property	Since the physical time required to reach steady-state normally increases with decreasing values of SSDR, the integration time is increased by the factor SSDR_nominal/currentSSDR for SSDR values smaller than the nominal. The maximum value for the end-time is limited to the value specified by this control.			
	Parameters	Optional/Reqd.	Units	Examples
	Maximum value of end time	Optional	s	ENDTIMEMAX 1.0E+05
	Keyword Usage	Optional keyword. The default value for the Diffusion Flamelet Generator is 1.0E+05		
	Reactor Models	• Diffusion Flamelet Generator		
ENGE Reactor Property	Solve the electron energy equation. The user must still specify a temperature (see ETMP (p. 201)), which provides the initial guess or initial value for the electron temperature.			
	Parameters	Optional/Reqd.	Units	Examples
	Reactor number (PSR clusters only)	Optional	--	ENGE 2

Keyword	Definition			
		If no number is given, values are assumed to apply to all reactors in a cluster.		
	Keyword Usage	Optional keyword. By default, the electron energy equation is not solved.		
	Reactor Models	• Closed Plasma Reactor • Plasma PSR • Plasma Plug Flow Reactor		
	Notes	• ENGE (p. 193) must be specified when electrons are present for all PSRs.		
ENGY	Specifies the starting internal energy for the initial mixture.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Energy	Required	erg/g	ENGY 1.5E9
	Keyword Usage	Optional keyword. The user must specify two state variables and the composition to define the initial mixture.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
EN-RG	Solve the energy equation to determine the gas temperature.			
Problem Type	Parameters	Optional/Reqd.	Units	Examples
	Reactor number (PSR clusters only)	Optional If no number is given, the keyword is assumed to apply to all reactors in a cluster.	--	ENRG 2
	Bulk name	Optional	--	ENRG Gas

Keyword	Definition	
	Keyword Usage	Optional keyword. For the multiphase reactors, the keyword would be effective for the phase name following the keyword. The name of the bulk phase should be used. "Gas" indicates the gas phase. Either TGIV (p. 326) or ENRG (p. 194) must be specified in most cases. For closed homogeneous systems, ICEN (p. 222), CONP (p. 175), CONV (p. 175), or COTV (p. 176) can be specified instead. For Premixed Flamespeed Calculations, ENRG (p. 194) is required.
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Multiphase PSR • Plug Flow Reactor • Premixed Laminar Flame-speed Calculation • Premixed Laminar Burner-stabilized Flame • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor
	Notes	• You must still specify an initial or initial estimate of the gas temperature or temperature profile. See also: TEMP (p. 323) or TPRO (p. 334) keyword. • For steady-state reactor models, this initial temperature is used in solving the intermediate fixed-temperature problem and is an initial guess for the solution of the full problem including the energy equation. • Inclusion of the keywords CONP (p. 175), CONV (p. 175), or ICEN (p. 222), will also indicate that the energy equation should be solved for closed homogeneous systems.

Keyword	Definition			
ENTH	Specifies the starting enthalpy for the initial mixture.			
	Parameters	Optional/Reqd.	Units	Examples
	Enthalpy	Required	erg/g	ENTH 1.5E9
	Keyword Usage	Optional keyword. The user must specify two state variables and the composition to define the initial mixture.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
ENTH_DELTA_IN	Specifies the percentage with respect to the specified inlet enthalpy and is used to compute a new inlet temperature. For example, if the condition specified on the Inlet panel input is {T, Y_CH4} = {300, 1.0} and the input value for the enthalpy delta is -2%, then (a) the new enthalpy is $H_{new} = 0.98 * H(T=300, Y_{CH4}=1)$, and (b) the new inlet temperature is $T_{new} = T(H_{new}, Y_{CH4})$. The typical intended usage is to facilitate flamelet generation at different enthalpy levels. Note that when there is more than one inlet (as in the opposed-flow-based reactor models), the enthalpy change is applied to all inlets the same and, depending on the specified composition, each inlet will have a corresponding temperature.			
	Parameters	Optional/Reqd.	Units	Examples
	Percentage	Required	--	ENTH_DELTA_IN 5.0
	Keyword Usage	Optional keyword.		
	Reactor Models	• Diffusion Flamelet Generator • Extinction of Diffusion or Premixed Opposed-flow Flame • Opposed-flow • Premixed-Burner-Stabilized_Stagnation Flame		
	EN-TR	Specifies the starting entropy for the initial mixture.		
Parameters		Optional/Reqd.	Units	Examples
Entropy		Required	erg/(g · K)	EN-TR 7.0E7
Keyword Usage		Optional keyword. The user must specify two state variables and the composition to define the initial mixture.		
Reactor Models		• Chemical and Phase Equilibrium Calculations		
EPSC	Threshold value for the first-order sensitivity coefficients for the growth rates of all bulk phases with respect to the rate constants. Coefficients below this value are neither printed to the diagnostic output file nor saved in the XML Solution File.			
	Parameters	Optional/Reqd.	Units	Examples
	Threshold value	Required	--	EPSC .01

Keyword	Definition			
	Keyword Usage	Optional keyword. By default, the threshold value for bulk phases is set to 0.001.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Reactor • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor		
	Notes	• This keyword can be added but not removed from a continuation run.		
EPSR Output	Threshold value for the rate-of-production coefficients. Coefficients below this value are neither printed to the diagnostic output file nor saved in the XML Solution File.			
	Parameters	Optional/Reqd.	Units	Examples
	Threshold value	Required	--	EPSR .02
	Keyword Usage	Optional keyword. By default, the threshold value for rate-of-production coefficients is set to 0.01.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • SI Engine Zonal Simulator		
	Notes	• This keyword can be added but not removed from a continuation run.		
EPSS Output	Threshold value for the first-order sensitivity coefficients for the species with respect to the rate constants. Coefficients below this value are neither printed to the diagnostic output file nor saved in the XML Solution File.			

Keyword	Definition			
	Parameters	Optional/Reqd.	Units	Examples
	Threshold value	Required	--	EPSS .01
	Keyword Usage	Optional keyword. By default, the threshold value for species is set to 0.001.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Diffusion or Premixed Opposed-flow Flame • Closed Multiphase Reactor • Honeycomb Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Multiphase PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • SI Engine Zonal Simulator • Stagnation Flow CVD Reactor		
	Notes	• This keyword can be added but not removed from a continuation run.		
EPST Output	Threshold value for the first-order sensitivity coefficients for the gas temperature with respect to the rate constants. Coefficients below this value are neither printed to the diagnostic output file nor saved in the XML Solution File.			
	Parameters	Optional/Reqd.	Units	Examples
	Threshold value	Required	--	EPST .01
	Keyword Usage	Optional keyword. By default, the threshold value for gas temperature is set to 0.001.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor		

Keyword	Definition			
		• Closed Multiphase Reactor • Honeycomb Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Multiphase PSR • Plug Flow Reactor • SI Engine Zonal Simulator		
	Notes	• This keyword can be added but not removed from a continuation run.		
EQRX Solver	Specifies that the products from the premixed flame will be estimated by equilibrium calculation with constant enthalpy and pressure in the 2-zone SI Engine simulation. By default, equilibrium calculation is used to obtain gas product composition from the premixed flame.			
	Parameters	Optional/Reqd.	Units	Examples
	--	Optional	--	EQRX
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		
EQUI Reactor Property	Flag indicating that equilibrium composition will be calculated. The chemical state of the statistical event particles will be determined by the corresponding equilibrium states instead of by time integration of the chemical source terms.			
	Keyword Usage	Optional keyword. By default, chemistry is neglected and a mixing-only calculation is performed. See also CHEM (p. 169) .		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR) • SI Engine Zonal Simulator		
EQUI Reactor or Inlet Property	Specifies the air/fuel equivalence ratio for an inlet stream or for the initial conditions in a closed reactor.			
	Parameters	Optional/Reqd.	Units	Examples
	Inlet stream name (for open systems only)	Optional	--	EQUI mixture1 1.1

Keyword	Definition			
		If there is no stream name than the air/fuel equivalence ratio applies to the default or all defined streams.		
	Air / fuel equivalence ratio	Required	--	EQUI 1.1
	Keyword Usage	Optional keyword. Either REAC (p. 288) or EQUI (p. 199) keywords are required for each inlet stream or to specify the initial conditions of a closed reactor. When EQUI (p. 199) is included, FUEL (p. 211) / OXID (p. 256) / CPROD (p. 176) keywords must also be supplied.		
	Reactor Models	• Closed Homogeneous Batch Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Honeycomb Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor		
ETCH Reactor Property	Inclusion of this keyword indicates that a given bulk phase is expected to be etched instead of grown or deposited. This option changes the form of the equations to be solved for the bulk phase composition, as described in Bulk Species Equations During Etch of the Chemkin Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	Bulk phases	Optional Required if there is more than one bulk phase	--	ETCH BULK1

Keyword	Definition			
	<i>Reactor number (PSR clusters only)</i>	Optional If no number is given, the keyword is assumed to apply to all reactors in a cluster.	--	ETCH BULK1 2
	Keyword Usage	Optional keyword. By default, the names of the unnamed <i>Surface Kinetics</i> bulk phases is: BULK1, BULK2, etc.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Reactor • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• When the keyword ETCH (p. 200) is supplied for a bulk phase, it is required that bulk activities (see BULK (p. 164)) are also included for each bulk-phase species in that phase that is etched.		
ET-MP Reactor Property	The electron temperature in the reactor. This value is used as the initial estimate of the electron temperature for steady-state iteration (when ENGE (p. 193) is included), or as the initial electron temperature value for transient simulations.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Electron temperature</i>	Required	K	ETMP 33000.
	<i>Reactor number (PSR clusters only)</i>	Optional	--	ETMP 33000. 1

Keyword	Definition			
		If no number is given, values are assumed to apply to all reactors in a cluster.		
	Keyword Usage	Optional keyword. By default, the electron temperature is the same as the gas temperature.		
	Reactor Models	• Closed Plasma Reactor • Plasma PSR • Plasma Plug Flow Reactor		
EXT_GET-FLAME-LETS Reactor Property	Compute extinguishing flamelets.			
	Parameters	Optional/Reqd.	Units	Examples
	--	Required when computing the extinguishing flamelets	--	EXT_GETFLAMELETS
	Keyword Usage	Optional.		
	Reactor Models	• Diffusion Flamelet Generator		
EX-TINC-TION Reactor Property	Indicates extinction problem type.			
	Keyword Usage	Required keyword.		
	Reactor Models	• Extinction of Diffusion or Premixed Opposed-flow Flame		
EXT_MAXT FRAC Reactor Property	The fraction multiplying the current T maximum that is used to constrain the flame toward extinction. The extinction simulator finds the location at which T = maximum temperature fraction * (Current maximum temperature — Inlet temperature). Temperature at this location is successively decreased by the user-specified temperature step size until it reaches T = minimum temperature fraction * (Current maximum temperature — Inlet temperature). A new location is then selected using the maximum temperature fraction. This process is repeated until the desired number of steps is reached or until the flame is effectively extinguished.			
	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	<i>Maximum Temperature Fraction</i>	Required	--	EXT_MAXTFRAC 0.8
	Keyword Usage	Required. The default value is 10.8.		
	Reactor Models	• Extinction of Diffusion or Premixed Opposed-flow Flame		
	Notes	• Also see keyword EXT_MINTFRAC (p. 203) .		
EXT_METHOD	Specifies the type of control technique to be used in extinction simulation.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>BOOLEAN</i>	Required	--	EXT_METHOD 0
	Keyword Usage	Optional. By default, the value is 0 which indicates 1-point control. The other possible choice is 1 which indicates 2-point control.		
	Reactor Models	• Extinction of Diffusion or Premixed Opposed-flow Flame		
EXT_MINTFLAME	If the maximum temperature in any solution obtained in the extinction simulation is below this value, the extinction simulator will stop assuming that there is no flame.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Minimum Flame Temperature</i>	Required	K	EXT_MINTFLAME 1500
	Keyword Usage	Optional. The default value is 11500.		
	Reactor Models	• Extinction of Diffusion or Premixed Opposed-flow Flame		
	Notes	• This option is useful to avoid computing solutions beyond extinction point.		
EXT_MINTFRAC	The fraction multiplying the current T maximum that is used to constrain the flame toward extinction. The extinction simulator finds the location at which T = maximum temperature fraction * (Current maximum temperature — Inlet temperature). Temperature at this location is successively decreased by the user-specified temperature step size until it reaches T = minimum temperature fraction * (Current maximum temperature — Inlet temperature). A new location is then selected using the maximum temperature fraction. This process is repeated until the desired number of steps is reached or until the flame is effectively extinguished			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Minimum Temperature Fraction</i>	Required	--	EXT_MINTFRAC 0.2
	Keyword Usage	Required. The default value is 10.2.		

Keyword	Definition			
	Reactor Models	• Extinction of Diffusion or Premixed Opposed-flow Flame		
	Notes	• Also see keyword EXT_MAXTFRAC (p. 202) .		
EXT_NIG- STEPS	Number of (internal) integration steps after which a flamelet file is written when computing extinguishing flamelets.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Number of integration steps</i>	Required when computing the extinguishing flamelets	--	EXT_NIGSTEPS 50
	Keyword Usage	Optional. The default value is 50.		
	Reactor Models	• Diffusion Flamelet Generator		
EXT_SA- VEINT	Frequency of saving solution in extinction simulation.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Saving frequency</i>	Required	--	EXT_SAVEINT 10
	Keyword Usage	Optional. The default value is 10.		
	Reactor Models	• Extinction of Diffusion or Premixed Opposed-flow Flame		
	Notes	• Since extinction problems are numerically intensive, it may be prudent to save solutions frequently. The input value of this keyword indicates the number of solutions are found before an opposed-flow solution is saved in the process of marching towards the extinction point. (A new extinction simulation can be started by using the restart facility.).		
EXT_STEPS	Number of times opposed flow solution is computed in search of the extinction point.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Solution steps</i>	Required	--	EXT_STEPS 100
	Keyword Usage	Optional. The default value is 100.		
	Reactor Models	• Extinction of Diffusion or Premixed Opposed-flow Flame		
EXT_TSTEP	Temperature step by which temperature at control point is decreased in extinction simulator.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Temperature step</i>	Required	K	EXT_TSTEP 5

Keyword	Definition			
	Keyword Usage	Optional. Default value is 5.		
	Reactor Models	Extinction of Diffusion or Premixed Opposed-flow Flame		
EXT_VFCNTRL	Specifies how to constrain nozzle velocities in extinction simulation.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	BOOLEAN	Required	--	EXT_VFCNTRL 1
	Keyword Usage	Required. The default value is 1 which indicates that momentum of the two jets should be balanced. This creates the stagnation plane in the middle. The other option is 0 which indicates that the magnitude of velocity from both nozzles is the same.		
	Reactor Models	Extinction of Diffusion or Premixed Opposed-flow Flame		
	Notes	This option can only be used for 1-point control. For a 2-point control, it is ignored if specified.		

10.2. Alphabetical Listing of Keywords [F-O]

Table 10.2: Alphabetical Listing of Keywords [F-O]

Keyword	Definition	
FAZE	Specifies a fixed-phase constraint on the equilibrium calculation. Species that are originally in a condensed phase (that is, bulk species) will remain in that phase. If not set, the phase constraint has no effect.	
Reactor Property	Keyword Usage	Optional keyword. By default, phase
	Reactor Models	Chemical and Phase Equilibrium
FGM_EXPORT	Write a Flamelet Generated Manifold file.	
Reactor Property	Parameters	Optional/Reqd.
	--	Required when writing an FGM file
	Keyword Usage	Optional.
	Reactor Models	Diffusion Flamelet Generator
FICA0	The start of injection crank angle of the injection.	
Inlet Property	Parameters	Optional/Reqd.
	Injection name	Required
	Crank angle	Required
	Keyword Usage	Required keyword.
	Reactor Models	Direct Injection Diesel Engine Sim

Keyword	Definition	
FIDUR Inlet Property	Duration of injection in number of crank angles of the injection.	
	Parameters	Optional/Reqd.
	<i>Injection name</i>	Required
	<i>Number of crank angle</i>	Required
	Keyword Usage	Required keyword.
	Reactor Models	• Direct Injection Diesel Engine Sim
FIEQM Reactor Property	Specify the eEQMqual-mass spray parcel formation option in the DI engine injection mass rate profile for the injection. By default, the spray parcels might not have the same liquid mass if the injection rate profile is not a user-profile is used), the spray parcels always contain the same liquid mass.	
	Parameters	Optional/Reqd.
	<i>Injection name</i>	Required.
	<i>1</i>	Required.
	Keyword Usage	Optional keyword. Default: OFF, that is, the spray parcels are formed based on the injection mass rate profile.
	Reactor Models	• Direct Injection Diesel Engine Sim
FILFY Inlet Property	Initial liquid fuel component mass fraction of the injection	
	Parameters	Optional/Reqd.
	<i>Injection name</i>	Required
	<i>Liquid component name</i>	Required
	<i>Mass fraction</i>	Required
	Keyword Usage	Required keyword.
	Reactor Models	• Direct Injection Diesel Engine Sim
FIMAS Inlet Property	Total liquid mass of the injection.	
	Parameters	Optional/Reqd.
	<i>Injection name</i>	Required
	<i>Total injection mass</i>	Required
	Keyword Usage	Required keyword.
	Reactor Models	• Direct Injection Diesel Engine Sim
FINJP Inlet Property	A piecewise-linear continuous profile can be used to describe a non-uniform injection rate profile. The profile is defined by a series of data points of normalized crank angle and injection rate pair. The normalized crank angle ranges from 0.0 to 1.0. The injection rate data are in arbitrary units and the direct injection mass is normalized to the total injection mass. By default, a uniform injection rate profile based on the total injection mass is used.	
	Parameters	Optional/Reqd.
	<i>Injection name</i>	Required

Keyword	Definition	
	<i>Crank angle</i>	Required
	<i>Injection rate</i>	Required
	Keyword Usage	Optional keyword.
	Reactor Models	• Direct Injection Diesel Engine Sim
FINRD Inlet Property	Number of divisions (rings) in the radial direction to be applied to the parcels is determined by multiplying the number of divisions in the radial direction by the number of divisions in the axial direction.	
	Parameters	Optional/Reqd.
	<i>Injection name</i>	Required
	<i>Number of divisions</i>	Required
	Keyword Usage	Required keyword.
	Reactor Models	• Direct Injection Diesel Engine Sim
FINTL Inlet Property	Number of divisions in the time/injection direction to be applied to the parcels is determined by multiplying the number of divisions in the radial direction by the number of divisions in the time direction.	
	Parameters	Optional/Reqd.
	<i>Injection name</i>	Required
	<i>Number of divisions</i>	Required
	Keyword Usage	Required keyword.
	Reactor Models	• Direct Injection Diesel Engine Sim
FITMP Inlet Property	Initial liquid temperature of the injection.	
	Parameters	Optional/Reqd.
	<i>Injection name</i>	Required
	<i>Liquid temperature</i>	Required
	Keyword Usage	Required keyword.
	Reactor Models	• Direct Injection Diesel Engine Sim
FIXT Reactor Property	Specifies a fixed-temperature boundary condition on the upper wall (inlet) of the reactor.	
	Parameters	Optional/Reqd.
	<i>Temperature</i>	Optional, if a temperature is not specified, the inlet gas temperature will be used.
	Keyword Usage	Optional keyword. By default, a zero value is used.
	Reactor Models	• Planar Shear Flow Reactor
FLAM Reactor Property	Position and fixed-temperature value for calculating strained, lifted flame on a fixed location of the flame front. The flame front location is specified by the position and fixed-temperature value (inlet gas temperature value) to fix at this position.	
	Parameters	Optional/Reqd.

Keyword	Definition	
	<i>Flame position</i>	Required
	<i>Temperature</i>	Required
	Keyword Usage	Optional keyword. By default, no temperature is specified.
	Reactor Models	- Rotating Disk CVD Reactor - Stagnation Flow CVD Reactor
FLINJ	Assign an injection to an injector.	
Inlet Property	Parameters	Optional/Reqd.
	<i>Injection name</i>	Required
	<i>Injector name</i>	Required
	Keyword Usage	Required keyword.
	Reactor Models	Direct Injection Diesel Engine Simulation
FLRT	The mass flow rate into the reactor for an optionally specified inlet stream (mass flow rate per area) and there is no option for inlet stream name.	
Inlet Property	Parameters	Optional/Reqd.
	<i>Inlet stream name (Not valid for Premixed Laminar Flames)</i>	Optional If there is no stream name then the default stream name applies to the default or to all defined inlet streams.
	<i>Mass flow rate or Mass flux (for Premixed Laminar Flames)</i>	Required
	<i>Keyword Usage</i>	PFRs and Monolith Reactors: Flow Reactors: SCCM (p. 299) SCCMPRO (p. 300) FL (p. 207) none of TAU (p. 321) , FLRT (p. 208) / FPRO (p. 210) then a closed-system is assumed. FL is used for each INLET (p. 226) stream defined. FLRT (p. 208) / FPRO (p. 210) or SCCM (p. 299) defined. Rotating Disk CVD Reactors: RDCVD (p. 227)
	Reactor Models	- Honeycomb Monolith Reactor - Non-reactive Gas Mixer - Partially Stirred Reactor (PaSR) - Perfectly Stirred Reactor (PSR) - Plasma PFR - Plasma PSR - Multiphase PSR

Keyword	Definition	
		• Plug Flow Reactor • Premixed Laminar Burner-stabilized • Premixed Laminar Flame-speed C • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor
FLTB_FGM Reactor Property	Specifies the name of the Flamelet Generation Manifold (FGM) file.	
	Parameters	Optional/Reqd.
	<i>FGM file name</i>	Required when writing an FGM file
	Keyword Usage	Optional.
	Reactor Models	• Diffusion Flamelet Generator
FLT_NPOINTS Reactor Property	Species number of grid points in the progress-variable space.	
	Parameters	Optional/Reqd.
	<i>Number of progress variable points</i>	Required when writing FGM file
	Keyword Usage	Optional. The default value is 50.
	Reactor Models	• Diffusion or Premixed Opposed-fl
FLT_PVSPEC Reactor Property	Species name and its mass-fraction weighting factor to be used in the (for premixed flames).	
	Parameters	Optional/Reqd.
	<i>Species name</i>	Required
	<i>Mass-fraction weighting factor</i>	Required
	Keyword Usage	Required keyword when generating
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor
FLTB Output	Export one-dimensional flamelet tables in the standard flamelet format	
	Parameters	Optional/Reqd.
	<i>Flamelet table filename</i>	Required
	Keyword Usage	Optional keyword. By default, no flamelet FileName_1.FileExt (where FileName_1 is the example given here.) When continuing a flamelet continuation number+1 . For extinction, use "for Saving (EXT_SAVEINT)". Thus, " _n (total steps/EXT_SAVEINT).

Keyword	Definition	
FLUX Reactor Property	Reactor Models	- Opposed-flow Flame Simulator
	This keyword indicates that a flux balance will determine the mass fraction. If FLUX (p. 210) is specified, the REAC (p. 288) keywords are used to determine the inlet gas composition. See Equation 15.3 .	
	Keyword Usage Reactor Models	Optional keyword. By default, a flux balance is used. • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor
FLXB Reactor Property	Use extrapolation to obtain species mass fractions at the outflow (or inlet) mass fraction gradients at the outflow boundary. However, for pollutant species such as CO, NO, and SO ₂ , that their mass fraction profiles have positive gradients at the outflow boundary, use the treatment when mass fraction gradients are not zero at the outflow boundary.	
	Keyword Usage	Optional keyword. By default, zero mass fraction gradients are assumed.
	Reactor Models	• Premixed Laminar Burner-stabilized Reactor • Premixed Laminar Flame-speed Reactor
FPRO Inlet Property Profiles	Used to specify a transient profile or function of mass flow rate vs. time. The FPRO (p. 210) points provided.	
	Parameters	Optional/Reqd.
	<i>Inlet stream name</i>	Optional If there is no stream name then the mass fraction apply to all streams.
	<i>Time</i>	Required
	<i>Flow rate</i>	Required
	Keyword Usage	PFRs and Monolith Reactors: Flow rate is specified. SCCM (p. 299) SCCMFRO (p. 300) FL (p. 210) / none of TAU (p. 321), FLRT (p. 208) / FL (p. 210) then a closed-system is assumed. FL (p. 210) for each INLET (p. 226) stream defined. Reactor Models: FLRT (p. 208) / FPRO (p. 210) inlet stream defined. Rotating Disk CVD Reactor.
	Reactor Models	• Honeycomb Monolith Reactor. • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PFR • Plasma PSR • Multiphase PSR

Keyword	Definition	
		• Plug Flow Reactor (PFR) • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor
FREE Reactor Property	Specifies that the equilibrium species composition will be calculated.	
	Keyword Usage	Optional keyword. By default, the co
	Reactor Models	• Chemical and Phase Equilibrium
FREE Reactor Property	Specifies the problem type, which will be to solve for a freely propaga	
	Keyword Usage	Required keyword.
	Reactor Models	• Premixed Laminar Flame-speed C
	Notes	• The problem-type can be change
FROZ Reactor Property	Specifies that species composition will be frozen or fixed during the e	
	Keyword Usage	Optional keyword. By default, the co
	Reactor Models	• Chemical and Phase Equilibrium
FUEL Inlet or Reactor Property	Defines the fuel mole fraction composition for an inlet stream in an o ratio is specified (EQUI (p. 199)). It must be followed by a species nam for each fuel species, which are used to determine the inlet compositi participate simultaneously as a fuel, oxidizer, or product. The sum of a will be printed and the mole fractions will be normalized so the sum	
	Parameters	Optional/Reqd.
	<i>Inlet stream name (PSRs only)</i>	Optional If there is no stream name than the compassion applies to the default c streams.
	<i>Species name</i>	Required
	<i>Fuel fraction</i>	Required
	Keyword Usage	Required keyword when EQUI (p. 19
	Reactor Models	• Closed Homogeneous Batch Rea • Honeycomb Reactor • IC HCCI Engine • Perfectly Stirred Reactor • Plasma Plug Flow Reactor • Plasma PSR

Keyword	Definition	
		- Plug Flow Reactor - SI Engine Zonal Simulator
	Notes	- The mole fractions are of the fuel - The FUEL (p. 211) keywords must - The FUEL (p. 211) keywords must
FVCP Reactor Property	Specify the piecewise linear profile of the friction velocity coefficient v_{fr} and the mass loss rate. Note that Chemkin requires the friction velocity to be given in cm/s. Users should scale its value to convert the units of the friction velocity to m/s. See Chemkin Theory Manual .	
Parameters		Optional/Reqd.
<i>Crank angle</i>		Required
<i>Friction velocity coefficient</i>		Required
Keyword Usage		Optional keyword.
Reactor Models		- Multi-Zone HCCI Simulator - IC HCCI Engine - SI Engine Zonal Simulator
GASW Reactor Property	Estimated gas-phase mole fractions at the wall boundaries, which may be used to calculate the wall heat flux. The mole fractions should equal one. However, if they do not, a cautionary message will be issued. The actual gas mole fractions at each wall at the initial condition are specified by the GASW (p. 250) keyword (unless the NOTP (p. 250) keyword appears).	
Parameters		Optional/Reqd.
<i>Gas species name</i>		Required
<i>Mole fraction of gas species</i>		Required
Keyword Usage		Optional keyword. By default, value is 1.0.
Reactor Models		- Cylindrical Shear Flow Reactor - Planar Shear Flow Reactor
GDOT Reactor Property	This keyword may be used to specify explicitly the net surface production rate of species i in the <i>Surface Kinetics</i> input file. In order to use this option, the <i>Surface Kinetics</i> input file must be used. The net surface production rate of species i and bulk species must all be zero in the <i>Surface Kinetics</i> input file.	
Parameters		Optional/Reqd.
<i>Species name</i>		Required
<i>Net surface production rate</i>		Required
Keyword Usage		Optional keyword. By default, the net surface production rate is zero.
Reactor Models		Rotating Disk CVD Reactor

Keyword	Definition	
		Stagnation Flow CVD Reactor
GEN Output	Controls the printing of general information about the chemistry set. thermodynamics. The ALL (p. 149) option produces all of the general i is given on the input line, ALL (p. 149) is assumed (the default). The GF	
	Parameters	Optional/Reqd.
	<i>ALL option</i>	Optional
	<i>NONE option</i>	Optional
	Keyword Usage	Optional keyword. By default, the ta
	Reactor Models	Mechanism Analyzer
GFAC Reactor Property	This keyword specifies that the rates of all gas-phase reactions will be useful if convergence difficulties are encountered due to unusually lar with artificially reduced reaction rates, which then can be increased in setting GFAC (p. 213) and SFAC (p. 306) to zero for a perfectly stirred r	
	Parameters	Optional/Reqd.
	<i>Multiplier value</i>	Required
	<i>Reactor number (PSR clusters only)</i>	Optional If no number is given, values are as to all reactors in a cluster.
	Keyword Usage	General: Optional keyword. By defa Non-reactive Mixer: Required
	Reactor Models	- Closed Homogeneous Batch Reactor - Closed Plasma Reactor - Cylindrical Shear Flow Reactor - Diffusion or Premixed Opposed-fl - Honeycomb Reactor - IC HCCI Engine - Non-reactive Gas Mixer - Perfectly Stirred Reactor (PSR) - Planar Shear Flow Reactor - Plasma Plug Flow Reactor - Plasma PSR - Plug Flow Reactor

Keyword	Definition	
		• Premixed Laminar Burner-stabilized • Premixed Laminar Flame-speed C • Rotating Disk CVD Reactor • SI Engine Zonal Simulator • Stagnation Flow CVD Reactor
GMHTC Reactor Property	The reactor wall temperature will be obtained by solving energy conservation between the inner wall surface and the gas mixture inside the reactor. When this option is used, all the external heat fluxes, that is, heat loss and gain, are applied to the wall energy equation instead of the gas phase energy equation included in the wall energy equation.	
	Parameters	Optional/Reqd.
	<i>Material name</i>	Optional. If no material is specified, the same material is used for all materials.
	<i>Heat transfer coefficient</i>	Required
	<i>Reactor number (PSR clusters only)</i>	Optional. If no number is given, the keyword applies to all reactors in a cluster.
	Keyword Usage	Optional keyword. This keyword must not be solved and the reactor wall temperature is specified.
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Monolith Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator
GRAD	Parameter that controls the degree of mesh adaptation based on the gradient, usually between about 0.1 and 1.0, where no adaptation based on gradient	

Keyword	Definition	
Reactor Property	Parameters	Optional/Reqd.
	<i>Gradient of mesh adaptation</i>	Required
	Keyword Usage	Optional keyword. By default, the g
	Reactor Models	• Diffusion or Premixed Opposed-fl • Premixed Laminar Burner-stabiliz • Premixed Laminar Flame-speed C • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor
	Notes	• This keyword can be changed for • Steady-state 1-D Solution Method
GRAV	The value of the acceleration of gravity. The buoyancy term can only be used in the principal flow direction. Thus, GRAV 980 may be used to describe flow that neglects the buoyancy term.	
Reactor Property	Parameters	Optional/Reqd.
	<i>Acceleration of gravity</i>	Required
	Keyword Usage	Optional keyword. By default, the a
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor
GRID	Specifies a point on an initial grid. Up to NTOT (p. 253) of these GRID (p. 215) keywords are a group of coordinate of a mesh point. The GRID (p. 215) keywords are a group of	
Reactor Property Profiles	Parameters	Optional/Reqd.
	<i>mesh point coordinate</i>	Required
	Keyword Usage	Optional keyword. If no GRID (p. 215) is specified, the value of NPTS (p. 251) on the value of NPTS (p. 251) .
	Reactor Models	• Diffusion or Premixed Opposed-fl • Premixed Laminar Burner-stabiliz • Premixed Laminar Flame-speed C • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor
GRXN	Prints out a table of reaction rates and other pertinent information for every gas-phase reaction. The NONE (p. 250) option suppresses certain reactions, they may be optionally specified by their number (g reaction expression (see example input).	
Output		

Keyword	Definition	
	Parameters	Optional/Reqd.
	<i>ALL option</i>	Optional, default is ALL
	<i>NONE option</i>	Optional, default is ALL
	<i>Gas reaction number list</i>	Optional, default is ALL
	<i>Gas reaction expression</i>	Optional, default is ALL
	Keyword Usage	Optional keyword. By default, the ta
	Reactor Models	• Mechanism Analyzer
GTHB Output	Create an extra table of the reaction rates for those reactions that inv by the XBTH (p. 367) keyword) to yield effective reaction rates. The ALL (p. 250) reaction. The NONE (p. 250) option suppresses output for all of the rea be optionally specified by their number (given in the Pre-processor ou input).	
	Parameters	Optional/Reqd.
	<i>ALL option</i>	Optional, default is ALL
	<i>NONE option</i>	Optional, default is ALL
	<i>Gas reaction number list</i>	Optional, default is ALL
	<i>Gas reaction expression</i>	Optional, default is ALL
	Keyword Usage	Optional keyword. By default, the ta
	Reactor Models	• Mechanism Analyzer
GVEL Reactor Property	Activate the Woschni correlation for the average cylinder gas velocity. Internal Combustion Engine Model of the Chemkin Theory Manual .	
	Parameters	Optional/Reqd.
	<i>C₁₁ in the average gas velocity correlation</i>	Required
	<i>C₁₂ parameter in the Woschni correlation</i>	Required
	<i>C₂ parameter in the Woschni correlation</i>	Required
	<i>Ratio of swirl velocity to mean piston speed</i>	Required
	Keyword Usage	Optional keyword. By default, the se
	Reactor Models	• IC HCCI Engine • SI Engine Zonal Simulator
HIMP Reactor Property	Use the Huber correlation to calculate the characteristic gas velocity u	
	Parameters	Optional/Reqd.
	<i>IMEP</i>	Required

Keyword	Definition	
	Keyword Usage	This keyword is optional and works the Woschni gas velocity correlation
	Reactor Models	• IC HCCI Engine • Multi-Zone HCCI Engine • SI Engine Zonal Simulator
HITE Reactor Property	The channel height (for cartesian coordinates), or the reactor radius (for axisymmetry) or the distance from the symmetry line for a symmetric planar channel.	
	Parameters	Optional/Reqd.
	<i>Channel height or radius</i>	Required
	Keyword Usage	Required keyword.
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor
H0 Solver	The initial distance step size used by the transient solver.	
	Parameters	Optional/Reqd.
	<i>Initial time step size</i>	Required
	Keyword Usage	Optional keyword. By default, the initial time step size is 10% of the initial time.
	Reactor Models	• Closed Multiphase Reactor • Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor • Multiphase PSR
HP Problem Type	Constant pressure and enthalpy constraints.	
	Keyword Usage	Optional keyword. Exactly one problem type must be specified.
	Reactor Models	• Chemical and Phase Equilibrium
	Notes	• PH (p. 259) keyword is equivalent to HP.
HSEN Output	Calculate the first-order, heat-of-formation sensitivity coefficients (that is, the partial derivatives of the species fractions and other dependent variables in the system) with respect to the heat-of-formation of the species.	
	Parameters	Optional/Reqd.
	<i>String indicating for which variables sensitivity coefficients will be saved or printed. The string is a space-delimited list containing species names and any one of the following: ALL, AVEL, RVEL, and so on.</i>	Optional If no string is given, then ALL is assumed.

Keyword	Definition	
	<i>CVEL, FLRT, or TEMP (see Notes)</i>	
	Keyword Usage	Optional keyword. By default, no se
	Reactor Models	• Diffusion or Premixed Opposed-fl • Premixed Laminar Burner-stabiliz • Premixed Laminar Flame-speed C • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor
	Notes	• This keyword can be added but r • See also EPSS (p. 197), EPSG (p. 19) The optional parameter strings are • ALL: all species and all other dep • AVEL: axial velocity (Plug Flow, Di Flow CVD Reactors only) • CVEL: circumferential velocity (Ro • RVEL: radial velocity (Diffusion or Reactors only) • FLRT: mass flow rate (Premixed La • TEMP: gas temperature
HSWC Reactor Property	Specifies the crank angle when the entire wall heat loss will be switch , and HSWC (p. 218) are mutually exclusive.	
	Parameters	Optional/Reqd.
	<i>Crank angle</i>	Required
	Keyword Usage	Optional keyword.
	Reactor Models	• SI Engine Zonal Simulator
HSWT Reactor Property	Specifies the burned mass fraction value at which the entire wall heat HSWM (p. 219) , HSWT (p. 218) , and HSWC (p. 218) are mutually exclus	
	Parameters	Optional/Reqd.
	<i>Temperature</i>	Required
	Keyword Usage	Optional keyword.
	Reactor Models	• SI Engine Zonal Simulator

Keyword	Definition	
HSWM Reactor Property	Specifies the burned mass fraction value at which the entire wall heat flux is zero. HSWM (p. 219) , HSWT (p. 218) , and HSWC (p. 218) are mutually exclusive.	
	Parameters	Optional/Reqd.
	<i>Burned mass fraction</i>	Required
	Keyword Usage	Optional keyword.
	Reactor Models	• SI Engine Zonal Simulator
HTC Reactor Property	The overall, per-area, heat-transfer coefficient for convective or conductive heat transfer. The keyword is only relevant when the energy equation is being solved.	
	Parameters	Optional/Reqd.
	<i>Material name</i>	Optional. If no material is specified, the same material is used for all materials.
	<i>Heat transfer coefficient</i>	Required
	<i>Reactor number (PSR clusters only)</i>	Optional. If no number is given, the keyword applies to all reactors in a cluster.
	Keyword Usage	Optional keyword. This keyword must be greater than or equal to zero. See also QLOS (p. 281) and QPSR (p. 281) .
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Monolith Reactor • IC HCCI Engine • Multi-Zone HCCI Engine • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • Plasma Plug Flow Reactor • Multiphase PSR • Plug Flow Reactor • SI Engine Zonal Simulator
HTCPRO Reactor Property Profiles	The profile of the overall heat transfer coefficient for convective or conductive heat transfer at a point in a piecewise-linear profile. The keyword is only relevant when the energy equation is being solved.	
	Parameters	Optional/Reqd.

Keyword	Definition	
	<i>Time or Distance value (depending on Reactor Model)</i>	Required
	<i>Heat transfer coefficient per area</i>	Required
	<i>Reactor number (PSR clusters only)</i>	Optional If no number is given, the profile of the first two values is assumed to apply to a cluster.
	Keyword Usage	Optional keyword. By default, there is no HTRN (p. 220), and QFUN (p. 280).
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Closed Multiphase Reactor • Cylindrical Shear Flow Reactor • Honeycomb Reactor • IC HCCI Engine • Multi-Zone HCCI Engine • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Plasma Plug Flow Reactor • Multiphase PSR • Plug Flow Reactor • SI Engine Zonal Simulator
HTRN Reactor Property	The heat transfer coefficient and ambient temperature for specification of an optionally specified surface material. This keyword is only relevant when used with a reactor model.	
	Parameters	Optional/Reqd.
	<i>Material name (0-D and Plug Flow systems only)</i>	Optional If no material is specified, the same material is used for all materials.
	<i>Heat transfer coefficient</i>	Required

Keyword	Definition	
	<i>Ambient temperature (0-D and Plug Flow systems only)</i>	Required
	<i>Reactor number (PSR clusters only)</i>	Optional If no number is given, the keyword apply to all reactors in a cluster.
	Keyword Usage	Optional keyword. By default, the h
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Honeycomb Reactor • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor
ICHF Inlet Property	Use the wall function heat transfer correlation to compute the wall heat transfer. For more information about this heat transfer correlation, see the Chemkin Theory Manual .	
	Parameters	Optional/Reqd.
	<i>Dimensionless temperature inside turbulent thermal boundary layer</i>	Required.
	<i>Exponent of the viscosity ratio</i>	Required
	<i>Wall temperature</i>	Required
	Keyword Usage	Optional keyword.
	Reactor Models	• Multi-Zone HCCI Simulator • IC HCCI Engine • SI Engine Zonal Simulator
ICHH Reactor Property	Use the Hohenberg formulation to calculate cylinder wall heat transfer.	
	Parameters	Optional/Reqd.

Keyword	Definition	
	<i>parameter_a</i>	Required
	<i>parameter_b</i>	Required
	<i>parameter_c</i>	Required
	<i>parameter_d</i>	Required
	<i>parameter_e</i>	Required
	<i>ambient_temperature</i>	Required
	Keyword Usage	This keyword is optional and works (ICHT, ICHX, ICHW, ICHH, HTC, HTCPR) Default: the Hohenberg heat transfer
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Honeycomb Reactor • IC HCCI Engine • Multi-Zone HCCI Engine • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • SI Engine Zonal Simulator
ICEN Reactor Property	The transient internal combustion (IC) HCCI engine model will be implemented as a function of time, where the function of time is determined by an engine model that provides a pressure and temperature profile for this calculation. This problem type is only allowed for closed systems.	
	Keyword Usage	Optional keyword. By default, a constant volume calculation is performed.
	Reactor Models	• IC HCCI Engine

Keyword	Definition	
	Notes	- See also: CMPR (p. 171), VOLC (p. 171) - SI Engine Zonal Simulator
ICHT Reactor Property	Convective heat transfer correlation for the transient IC HCCI Engine model. $Nu_h = a Re^b Pr^c$. Where Nu_h is the Nusselt number for heat transfer, Re is the Reynolds number, and Pr is the Prandtl number. On the usage of these parameters, see Internal Combustion Engine Model .	
	Parameters	Optional/Reqd.
	The value <i>a</i> in heat transfer correlation	Required
	The value <i>b</i> in heat transfer correlation	Required
	The value <i>c</i> in heat transfer correlation	Required
	Bore diameter	Required
	Wall temperature	Required
	Keyword Usage	Optional keyword. By default, an adiabatic wall condition is used. For more information on the use of the <i>Woschni</i> correlation extensions, see Internal Combustion Engine Model .
	Reactor Models	- IC HCCI Engine - SI Engine Zonal Simulator
ICHW Reactor Property	Use the dimensional <i>Woschni</i> formulation to calculate cylinder wall heat transfer.	
	Parameters	Optional/Reqd.
	<i>parameter_a</i>	Required
	<i>parameter_b</i>	Required
	<i>parameter_c</i>	Required
	<i>ambient_temperature</i>	Required
	Keyword Usage	This keyword is optional and works with the <i>Woschni</i> correlation. It is used in conjunction with <i>ICHX</i> , <i>ICHW</i> , <i>ICHH</i> , <i>HTC</i> , <i>HTCPRO</i> , and <i>HTCZ</i> . The heat transfer coefficient formulation is $h = \frac{q}{T_w - T_g}$.
	Reactor Models	- Closed Homogeneous Batch Reactor - Closed Plasma Reactor - Cylindrical Shear Flow Reactor - Honeycomb Reactor

Keyword	Definition	
		• Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor
ICRD Reactor Model or Reactor Property	Flag to specify coordinate system, which determines the Reactor Model.	
	Parameters	Optional/Reqd.
	<i>Coordinate flag indicating Planar Shear Flow Reactor, with, non-symmetric boundary conditions</i>	Required
	<i>Coordinate flag indicating Planar Shear Flow Reactor, assuming symmetry with respect to the center axis</i>	Required
	<i>Coordinate flag indicating Cylindrical Shear Flow Reactor, using radial coordinates</i>	Required
	Keyword Usage	Required keyword.
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor
	Notes	• Only one-half of the physical domain is the symmetry line
IEM Reactor Property	Flag indicating that the interaction-by-exchange-with-the-mean (IEM) particle.	
	Keyword Usage	Optional keyword. By default, a well-mixed reactor is assumed.
	Reactor Models	• Closed Partially Stirred Reactor (CPaSR) • Partially Stirred Reactor (PaSR)
IGRIDMETHOD_n Reactor Property	Choice for the initial grid profile. Integer n can be 1, 2, or 3 and mean n is the number of grid points in the radial direction. In general, the uniform grid is not very useful and a biased grid should be used for high mixture fraction.	
	Keyword Usage	Required keyword. The default value is 1.
	Reactor Models	• Diffusion Flamelet Generator

Keyword	Definition	
INIT Reactor Property	The initial gas mole fraction of the given species in the reactor for a t species in the problem.	
	Parameters	Optional/Reqd.
	<i>Species name</i>	Required
	<i>Gas fraction</i>	Required
	Keyword Usage	Optional keyword. By default, if no some INIT (p. 225) entries are prese
	Reactor Models	• Closed Partially Stirred Reactor (P • Partially Stirred Reactor (PaSR) • Normal Incident Shock • Normal Reflected Shock • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor
INJM Reactor Property	Total mass flow rate of the injected gas. See Equation 15.5 of the Chem	
	Parameters	Optional/Reqd.
	<i>Mass flow rate</i>	Required
	Keyword Usage	Required keyword when INJS (p. 22
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor
INJS Reactor Property	Injection of gas species at a location along the axis of symmetry can b as a spatially distributed Gaussian source. INJM (p. 225) is the total ma term will be added to Equation 15.5 of the Chemkin Theory Manual . I fractions.	
	Parameters	Optional/Reqd.
	<i>Species name</i>	Required
	<i>Species composition</i>	Required
	Keyword Usage	Optional keyword. By default, there
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor
INJT Reactor Property	Temperature of the injected gas.	
	Parameters	Optional/Reqd.
	<i>Temperature</i>	Required
	Keyword Usage	Optional keyword. By default, no en is not included, this keyword will be

Keyword	Definition	
	Reactor Models	- Rotating Disk CVD Reactor - Stagnation Flow CVD Reactor
INJW	Half-width of the Gaussian gas-injection source. See Equation 15.5 of t	
Reactor Property	Parameters	Optional/Reqd.
	<i>Half-width</i>	Required
	Keyword Usage	Optional keyword. By default, the w
	Reactor Models	- Rotating Disk CVD Reactor - Stagnation Flow CVD Reactor
INJX	Height above the disk which is the center of the Gaussian-shaped inj	
Reactor Property	Parameters	Optional/Reqd.
	<i>Height</i>	Required
	Keyword Usage	Optional keyword. By default, the h
	Reactor Models	- Rotating Disk CVD Reactor - Stagnation Flow CVD Reactor
INLET	Specification of a reactor inlet stream. Specify an optional name for th	
Reactor Property	must also specify the corresponding inlet temperature (TINL (p. 331)), / CPROD (p. 176) / ADD (p. 141)), and flow rate (FLRT (p. 208) or SCCM	
	Parameters	Optional/Reqd.
	<i>Inlet stream name</i>	Required
	<i>Reactor number (PSR clusters only)</i>	Optional If no number is given, values are as to all reactors in a cluster.
	Keyword Usage	Optional keyword. If no streams are in series or that the system is a sing defined).
	Reactor Models	- Diffusion or Premixed Opposed-fl - Non-reactive Gas Mixer - Partially Stirred Reactor (PaSR) - Perfectly Stirred Reactor (PSR) - Plasma PSR - Rotating Disk CVD Reactor - Stagnation Flow CVD Reactor

Keyword	Definition	
	Notes	This keyword can not be changed
INLT Inlet Property	Temperature of the specific phase in the inlet stream.	
	Parameters	Optional/Reqd.
	<i>inlet stream name</i>	Required
	<i>phase name</i>	Required
	<i>temperature of the specific phase</i>	Required
	Keyword Usage	Optional keyword. By default the in
	Reactor Models	Multiphase PSR Reactor
INLTPRO Inlet Property	Temperature profile specified as a function of time of the specific pha	
	Parameters	Optional/Reqd.
	<i>inlet stream name</i>	Required
	<i>phase name</i>	Required
	<i>time value</i>	Required
	<i>temperature of the specific phase</i>	Required
	Keyword Usage	Optional keyword. By default the in
	Reactor Models	Multiphase PSR Reactor
INTM Reactor Property	The estimated peak mole fractions values for "intermediate" species. C desired. It is usually better to estimate values somewhat higher than t gives an estimate fraction of 0.001 for the intermediate HO2. Any give product.	
	Parameters	Optional/Reqd.
	<i>Species name</i>	Required
	<i>Estimated fraction</i>	Required
	Keyword Usage	Optional keyword. By default, the es to a non-zero value on the Reactor
	Reactor Models	- Premixed Laminar Burner-stabiliz - Premixed Laminar Flame-speed C - Rotating Disk CVD Reactor - Stagnation Flow CVD Reactor
	Notes	See Starting Estimates of the Che

Keyword	Definition
IONE Reactor Property	Specified energy loss to ions in the sheath for each ion lost at a specified electron Volts. For example, "IONE material1 30" would result in an ion energy gain for the ions results in a reduced effective power deposited in Electron Energy Equation for Plasma Systems of the Chemkin Theoretical Manual .
	ParametersOptional/Reqd.
	Material nameOptional If there is no material name than the loss applies to all materials.
	Specified energy lossRequired
	Reactor number (PSR clusters only)Optional If no number is given, values are assigned to all reactors in a cluster.
	Keyword Usage Optional keyword. By default, the ion energy loss is applied to all reactors.
	Reactor Models • Closed Plasma Reactor • Plasma Plug Flow Reactor • Plasma PSR
IPSR XMLI	Use this keyword to specify which PSR to use for the initialization (XMLI) that is used for initialization (i.e. on <i>XMLdata.zip</i>).
	ParametersOptional/Reqd.
	PSR numberRequired
	Keyword Usage Optional keyword. By default, the last PSR is used.
	Reactor Models • Chemical and Phase Equilibrium • Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Reactor • Honeycomb Reactor • IC HCCI Engine • Mechanism Analyzer • Non-reactive Gas Mixer • Normal Incident Shock • Normal Reflected Shock • Perfectly Stirred Reactor (PSR)

Keyword	Definition	
		• Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized • Premixed Laminar Flame-speed C • Rotating Disk CVD Reactor • SI Engine Zonal Simulator • Stagnation Flow CVD Reactor
IRET Solver	Number of time steps to be taken in <i>TwoPnt</i> 's pseudo time stepping algorithm	
	Parameters	Optional/Reqd.
	<i>Number of time steps</i>	Required
	Keyword Usage	Optional keyword. By default, the number of time steps is 25. (See Notes below).
	Reactor Models	• Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Premixed Laminar Burner-stabilized • Premixed Laminar Flame-speed C • Plasma PSR • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor
	Notes	• Default value is 25 for PSRs and 5 for other reactor models
ISHK Problem Type	Inclusion of this keyword designates an incident shock problem without a specified shock location	
	Keyword Usage	Required keyword. Either ISHK (p. 295) or RSHK (p. 295) must be specified for this problem type. See also RSHK (p. 295).
	Reactor Models	• Normal Incident Shock

Keyword	Definition	
ISKB Problem Type	Inclusion of this keyword designates an incident shock problem with	
	Keyword Usage	Required keyword. Either ISHK (p. 295) or RSHK (p. 295) must be used to specify the problem type. See also RSHK (p. 295).
	Reactor Models	• Normal Incident Shock
ISTP Solver	Specifies the number of initial pseudo time steps that are taken by the solver before the Newton iteration is attempted. Normally, the Newton iteration will be attempted first, with time steps taken only if the iteration fails. In some circumstances where initial time stepping is desirable. The time step size is specified by the ISTP keyword only applies to the first grid network, not the subsequently refined grid. For more information, please refer to the TRAN (p. 336) option.	
	Parameters	Optional/Reqd.
	<i>Number of initial time steps</i>	Required
	Keyword Usage	Optional keyword. By default, the number of initial time steps is 10.
	Reactor Models	• Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Reactor • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Premixed Laminar Burner-stabilized Reactor • Premixed Laminar Flame-speed Reactor • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor
JJRG Restart	On continuations or restarts, the number of mesh points can be reduced. For problems of continuation problems the number of grid points can grow because of a capability to remove grid points. The old solution is adaptively interpolated. Its effect is carried over to the subsequent continuations, if any. Often a high value, such as the maximum number of grid-points. The reduction of grid-points.	
	Parameters	Optional/Reqd.
	<i>Number of mesh points</i>	Required
	Keyword Usage	Optional keyword. By default, the number of mesh points is 10.
	Reactor Models	• Diffusion or Premixed Opposed-flow Reactor • Premixed Laminar Burner-stabilized Reactor • Premixed Laminar Flame-speed Reactor

Keyword	Definition	
		- Rotating Disk CVD Reactor - Stagnation Flow CVD Reactor
KLIM Output	Calculate the ignition delay as the time when the fraction of the species solving the energy equation with transient solver.	
	Parameters	Optional/Reqd.
	<i>Species name</i>	Required
	Keyword Usage	Optional keyword. See also TIFP (p.
	Reactor Models	- Closed Homogeneous Batch Reactor - Closed Plasma Reactor - Honeycomb Monolith Reactor - IC HCCI Engine - Perfectly Stirred Reactor (PSR) - Plasma PSR - Plasma Plug Flow Reactor - Plug Flow Reactor - SI Engine Zonal Simulator
KMASS Reactor Property	Mass transfer coefficient used to calculate rate of mass exchange between the reactor and the gas phase. The model used to calculate the mass transfer coefficient follows the line with VLE inputs. A separate KMASS is specified for each material which mass transfer model to use. Parameters and units vary depending on the model.	
	Parameters	Optional/Reqd.
	<i>Material name (reactant or product)</i>	Required
	<i>Model</i>	Required The model is specified by using one of the following parameter keywords as the first parameter: CONK: Constant value of mass transfer coefficient. CONDL: Use two-film theory with (i) diffusivity and (ii) length scale. CONDT: Use penetration theory with (i) diffusivity and (ii) time scale.

Keyword	Definition	
	<i>Model parameters</i>	Required For CONK, the mass transfer coefficient is specified by one value. Units are cm/s. For two-film and penetration theories, the first parameter with units of cm/s is the first parameter with units of cm/s. The last parameter is either film thickness or contact time (in s).
	Keyword Usage	Optional keyword. By default, the h
	Reactor Models	• Multiphase Reactor
KNMN	The minimum Knudsen number, above which the wall slip-velocity mo	
Reactor Property	Parameters	Optional/Reqd.
	<i>Minimum Knudsen number</i>	Required
	Keyword Usage	Optional keyword. It is relevant only
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor
KOUT	List of species names whose mass fractions will be printed to the diag	
Output	Parameters	Optional/Reqd.
	<i>List of species names</i>	Required
	Keyword Usage	Optional keyword. By default, none
	Reactor Models	• Diffusion or Premixed Opposed-fl • Closed Partially Stirred Reactor (P • Partially Stirred Reactor (PaSR) • Premixed Laminar Burner-stabiliz • Premixed Laminar Flame-speed C
LGDT	Controls the time interval for data to be written to the XML Solution F	
Solver	Parameters	Optional/Reqd.
	<i>Logarithmic time-step</i>	Required
	Keyword Usage	Optional keyword. If neither DTSV (minus the beginning time, divided
	Reactor Models	• Normal Incident Shock • Normal Reflected Shock

Keyword	Definition	
LINE Reactor Property	An indicator that a linear profile is used for the initial gas species distributions. If the keyword is set, the initial gas species fractions vary linearly from one inlet to the other, with inlet values for the first inlet and the last inlet. If the keyword is not set, the initial gas species fractions vary linearly from the inlet values, specified by keyword REAC (p. 288), to the outlet values.	
	Keyword Usage	Optional keyword. By default, a plate reactor is used for CVD Reactors, the default initial gas species fractions are specified by INIT (p. 225) ; the keyword is ignored for other reactor models.
	Reactor Models	- Rotating Disk CVD Reactor - Stagnation Flow CVD Reactor
LMLM Reactor Property/Model	Minimum amount of liquid mass to activate the vaporization model.	
	Parameters	Optional/Reqd.
	<i>Minimum total liquid mass</i>	Required
	Keyword Usage	Optional keyword. Default is 1.0E-8.
	Reactor Models	Direct Injection Diesel Engine Simulator
LODR Reactor Property	Piston offset to crank radius ratio.	
	Parameters	Optional/Reqd.
	<i>Ratio of piston offset to crank radius.</i>	Required
	Keyword Usage	Optional keyword. Default = 0.0.
	Reactor Models	- IC HCCI Engine - Multi-zone HCCI Engine - SI Engine Zonal Simulator
	Notes	The absolute value of LODR must be less than 1.0. $\text{LODR} < (\text{LOLR} - 1)$.
LOLR Reactor Property	Ratio of the length of the engine connecting rod to the crank radius.	
	Parameters	Optional/Reqd.
	<i>Connection rod to crank radius ratio</i>	Required
	Keyword Usage	Optional keyword. By default, this ratio is 1.0.
	Reactor Models	- IC HCCI Engine - SI Engine Zonal Simulator
LPRT Output	Printing control LPRT (p. 233) turns on extensive printing that provides detailed information that can be informative in understanding the surface reaction behavior.	
	Keyword Usage	Optional keyword. By default, there is no printing.
	Reactor Models	Rotating Disk CVD Reactor

Keyword	Definition										
	Stagnation Flow CVD Reactor										
LSCL Reactor Property	Sets the length scale (cm) for the calculation of gas and surface Damkohler number. <table border="1" data-bbox="751 317 1624 531"> <tr> <td>Parameters</td><td>Optional/Reqd.</td></tr> <tr> <td><i>Length scale</i></td><td>Required</td></tr> <tr> <td>Keyword Usage</td><td>Optional keyword. By default, the length scale is set to 1 cm.</td></tr> <tr> <td>Reactor Models</td><td> Mechanism Analyzer </td></tr> </table>	Parameters	Optional/Reqd.	<i>Length scale</i>	Required	Keyword Usage	Optional keyword. By default, the length scale is set to 1 cm.	Reactor Models	Mechanism Analyzer		
Parameters	Optional/Reqd.										
<i>Length scale</i>	Required										
Keyword Usage	Optional keyword. By default, the length scale is set to 1 cm.										
Reactor Models	Mechanism Analyzer										
LUMPTO Reactor Property	This is an optional approach to species mass conservation closure. In this approach, the mass fraction of each species is set to one minus the sum of all others. <table border="1" data-bbox="751 604 1624 888"> <tr> <td>Parameters</td><td>Optional/Reqd.</td></tr> <tr> <td><i>Species name</i></td><td>Required</td></tr> <tr> <td>Keyword Usage</td><td>Optional keyword.</td></tr> <tr> <td>Reactor Models</td><td> - Cylindrical Shear Flow Reactor - Planar Shear Flow Reactor </td></tr> </table>	Parameters	Optional/Reqd.	<i>Species name</i>	Required	Keyword Usage	Optional keyword.	Reactor Models	- Cylindrical Shear Flow Reactor - Planar Shear Flow Reactor		
Parameters	Optional/Reqd.										
<i>Species name</i>	Required										
Keyword Usage	Optional keyword.										
Reactor Models	- Cylindrical Shear Flow Reactor - Planar Shear Flow Reactor										
MAJ Reactor Property	Sets the "Major Species". This is only used to calculate an effective diffusion coefficient. <table border="1" data-bbox="751 936 1624 1266"> <tr> <td>Parameters</td><td>Optional/Reqd.</td></tr> <tr> <td><i>Species name</i></td><td>Optional</td></tr> <tr> <td><i>Species number</i></td><td>Optional</td></tr> <tr> <td>Keyword Usage</td><td>Optional keyword. The default is to use the first species (the XBTH (p. 367) input) in the bath-gas. The default is to use the second species if the first is not specified.</td></tr> <tr> <td>Reactor Models</td><td> Mechanism Analyzer </td></tr> </table>	Parameters	Optional/Reqd.	<i>Species name</i>	Optional	<i>Species number</i>	Optional	Keyword Usage	Optional keyword. The default is to use the first species (the XBTH (p. 367) input) in the bath-gas. The default is to use the second species if the first is not specified.	Reactor Models	Mechanism Analyzer
Parameters	Optional/Reqd.										
<i>Species name</i>	Optional										
<i>Species number</i>	Optional										
Keyword Usage	Optional keyword. The default is to use the first species (the XBTH (p. 367) input) in the bath-gas. The default is to use the second species if the first is not specified.										
Reactor Models	Mechanism Analyzer										
MASSFRAC Reactor Property	Mass fraction of a bulk phase in the reactor. This specifies the overall composition of the gas, liquid, and solid. <table border="1" data-bbox="751 1339 1624 1759"> <tr> <td>Parameters</td><td>Optional/Reqd.</td></tr> <tr> <td><i>Mass fraction of a bulk phase within the reactor</i></td><td>Required</td></tr> <tr> <td>Keyword Usage</td><td>This keyword is used to specify the mass fraction of a bulk phase. The keyword "Gas" indicates the gas phase. The keyword "Liquid" indicates the liquid phase. The keyword "Solid" indicates the solid phase.</td></tr> <tr> <td>Reactor Models</td><td> - Closed Multiphase Reactor - Multiphase PSR </td></tr> </table>	Parameters	Optional/Reqd.	<i>Mass fraction of a bulk phase within the reactor</i>	Required	Keyword Usage	This keyword is used to specify the mass fraction of a bulk phase. The keyword "Gas" indicates the gas phase. The keyword "Liquid" indicates the liquid phase. The keyword "Solid" indicates the solid phase.	Reactor Models	- Closed Multiphase Reactor - Multiphase PSR		
Parameters	Optional/Reqd.										
<i>Mass fraction of a bulk phase within the reactor</i>	Required										
Keyword Usage	This keyword is used to specify the mass fraction of a bulk phase. The keyword "Gas" indicates the gas phase. The keyword "Liquid" indicates the liquid phase. The keyword "Solid" indicates the solid phase.										
Reactor Models	- Closed Multiphase Reactor - Multiphase PSR										
MASSTRAN_CEOF Reactor Property	User-specified mass transfer coefficient for the bulk phase. The same value is used for all species. <table border="1" data-bbox="751 1833 1624 1879"> <tr> <td>Parameters</td><td>Optional/Reqd.</td></tr> </table>	Parameters	Optional/Reqd.								
Parameters	Optional/Reqd.										

Keyword	Definition	
	<i>Use specified mass transfer coefficient for the bulk phase</i>	Optional
	Keyword Usage	This keyword indicates that the mass transfer coefficient must follow the keyword. .
	Reactor Models	• Closed Multiphase Reactor • Multiphase PSR
MASSTRAN_MECHANISM	Use the mass transfer coefficient from the kinetics input file..	
Reactor Property	Parameters	Optional/Reqd.
	<i>Phase name</i>	Required
	Keyword Usage	This keyword indicates that the mass transfer coefficient must follow the keyword. .
	Reactor Models	• Closed Multiphase Reactor • Multiphase PSR Reactor • Multiphase PSR
MASSTRAN_LEN	Length scale when two-film theory is used to calculate mass transfer coefficient.	
Reactor Property	Parameters	Optional/Reqd.
	<i>Length scale for the given bulk phase</i>	Optional
	Keyword Usage	This keyword indicates use of the mass transfer coefficient. Bulk name must follow the keyword in the mass transfer process. "Gas" is used for gas-liquid bulk phases.
	Reactor Models	• Closed Multiphase Reactor • Multiphase PSR
MASSTRAN_TAU	Time scale when two-film theory is used to calculate mass transfer coefficient.	
Reactor Property	Parameters	Optional/Reqd.
	<i>Time scale for the given bulk phase</i>	Optional
	Keyword Usage	This keyword is used when penetration theory is used for gas-liquid and liquid-liquid bulk phases. Phase name must follow the keyword.
	Reactor Models	• Closed Multiphase Reactor • Multiphase PSR

Keyword	Definition	
MAXIT Solver	Controls the maximum number of iterations the integrator solver can increase this value to give the integrator greater chance to solve your or if the run fails with a "nonlinear solver failed to converge repeatedly"	
	Parameters	Optional/Reqd.
	<i>Iteration number</i>	Required
	Keyword Usage	Optional keyword.
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Partially Stirred Reactor • Closed Plasma Reactor • Closed Multiphase Reactor • Cylindrical Shear Flow Reactor • Honeycomb Reactor • IC HCCI Engine • Multi-Zone HCCI Engine Simulator • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Multiphase PSR • Plug Flow Reactor • Rotating Disk CVD Reactor • SI Engine Zonal Simulator • Stagnation Flow CVD Reactor
MAXTIME Solver	The maximum number times the steady state solver TWOPNT will use for very stiff problems to allow TWOPNT to find a solution by letting it times.	
	Parameters	Optional/Reqd.
	<i>Maximum steady state iterations</i>	Optional
	Keyword Usage	Optional keyword. By default, the m
	Reactor Models	• Cylindrical Shear Flow Reactor

Keyword	Definition	
		• Diffusion or Premixed Opposed-fl • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Premixed Laminar Burner-stabiliz • Premixed Laminar Flame-speed C • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor
	Notes	• SSMAXITER must be ≥ 1.
MCUT Reactor Property	Minimum number of particles required to "switch on" the surface rate [particles/cm ³].	
	Parameters	Optional/Reqd.
	<i>Material name</i>	Required
	<i>Cutoff number density</i>	Required
	Keyword Usage	Optional keyword.
	Reactor Models	• Closed Homogeneous Batch Reac • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Honeycomb Monolith Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator
MIX	Use a mixture-average model for calculating the transport coefficients	

Keyword	Definition	
Reactor Property	Keyword Usage	Optional keyword. By default, mixture
	Reactor Models	• Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-fl • Planar Shear Flow Reactor • Premixed Laminar Burner-stabiliz • Premixed Laminar Flame-speed C • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor
MIX	Flag indicating a mixing-only problem, where chemistry will be ignore	
Reactor Property	Keyword Usage	Optional keyword. This is the default
	Reactor Models	• Closed Partially Stirred Reactor (P • Partially Stirred Reactor (PaSR)
MIXFRACBIAS_FUEL	Bias factor for the grid on the fuel side, that is, between the mixture fr	
Reactor Property	than unity should be given and it means more grid points near the st	
	Parameters	Optional/Reqd.
	<i>Bias factor for grid</i>	Required for corresponding grid c
	Keyword Usage	Required keyword.
	Reactor Models	• Diffusion Flamelet Generator
MIXFRACBIAS_OXID	Bias factor for the grid on the oxidizer side, that is, between the mixtu	
Reactor Property	than unity should be given and it means more grid points near the st	
	Parameters	Optional/Reqd.
	<i>Bias factor for grid</i>	Required for corresponding grid c
	Keyword Usage	Required keyword.
	Reactor Models	• Diffusion Flamelet Generator
MIXT	The characteristic time of the mixing process in the reactor.	
Reactor Property	Parameters	Optional/Reqd.
	<i>Characteristic time</i>	Required
	Reactor Models	• Closed Partially Stirred Reactor (P • Partially Stirred Reactor (PaSR)
MLMT	Specifies the minimum value of gas mass in the zones. By default, the	
Solver	Parameters	Optional/Reqd.
	<i>Value of the b parameter</i>	Optional

Keyword	Definition	
	Keyword Usage	Optional keyword.
	Reactor Models	• SI Engine Zonal Simulator
MMASS MMASS	The reactor wall temperature will be obtained by solving energy conservation at the wall and the heat transfer coefficient between the inner wall surface and the fluid of the reactor wall.	
	Parameters	Optional/Reqd.
	<i>Material name</i>	Optional. If no material is specified, the material of the reactor wall will be used for all materials.
	<i>Thermal mass</i>	Required
	<i>Reactor number (PSR clusters only)</i>	Optional. If no number is given, the number of clusters is assumed to apply to all reactors in the model.
	Keyword Usage	Optional keyword. This keyword must be used if the thermal mass is cal/(cm-K).
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Monolith Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator
MOLFLRT Inlet Property	Molar flow rate of the specific phase in the inlet stream.	
	Parameters	Optional/Reqd.
	<i>inlet stream name</i>	Required
	<i>phase name</i>	Required
	<i>molar flow rate of the specific phase</i>	Required
	Keyword Usage	Optional keyword. By default the inlet flow is specified.
	Reactor Models	• Multiphase PSR Reactor
MOLFLRTPRO	Molar flow rate profile specified as a function of time of the specific phase	

Keyword	Definition	
Inlet Property	Parameters	Optional/Reqd.
	<i>inlet stream name</i>	Required
	<i>phase name</i>	Required
	<i>time value</i>	Required
	<i>molar flow rate of the specific phase</i>	Required
	Keyword Usage	Optional keyword. By default the in
	Reactor Models	• Multiphase PSR Reactor • Multiphase PSR
MOLEFRAC	Mole fraction of a bulk phase in the reactor. This specifies the overall c	
Reactor Property	liquid, and solid.	
	Parameters	Optional/Reqd.
	<i>Mole fraction of a bulk phase within the reactor</i>	Required
	Keyword Usage	Required for multiphase systems. Tw
	Reactor Models	• Closed Multiphase Reactor • Multiphase PSR
MOMEN	Turn on or off solution of the momentum equation for a plug-flow sir	
Reactor Property	Parameters	Optional/Reqd.
	<i>String "ON" or "OFF" to toggle the momentum equation</i>	Required
	Keyword Usage	Optional keyword. By default, the m
	Reactor Models	• Honeycomb Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor
MORD	Maximum order of integration used by the transient solver.	
Solver	Parameters	Optional/Reqd.
	<i>Maximum order of integration</i>	Required

Keyword	Definition	
	Keyword Usage	Optional keyword. By default, the m
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor
MQAFR Reactor Property	The external heat transfer (heat loss) area fraction of each zone.	
	Parameters	Optional/Reqd.
	<i>Area fraction</i>	Required
	<i>Zone number</i>	Required
	Keyword Usage	Optional keyword.
	Reactor Models	• Multi-Zone HCCI Engine Simulator
MSFX Reactor Property	Use a new discretization scheme for convective flux terms. In some cases, this scheme is used across the flame zone. With this new scheme, species mass fluxes are calculated. For species profiles, this new scheme in general incurs more grid points than the old scheme. The major species solutions obtained by these two schemes are subtle.	
	Keyword Usage	Optional keyword. By default, the o
	Reactor Models	• Premixed Laminar Burner-stabiliz
		• Premixed Laminar Flame-speed C
MTDIFF_REFSPEC Reactor Property	Reference species for calculating molecular diffusivity for a liquid phase.	
	Parameters	Optional/Reqd.
	<i>Reference species for diffusivity calculation</i>	Optional
	Keyword Usage	This keyword is used to specify reference species for liquid and gas-liquid systems. The bulk phase
	Reactor Models	• Closed Multiphase Reactor
		• Multiphase PSR
MTDIFF_SE Reactor Property	Using Stokes-Einstein method for calculation of bulk phase diffusivity.	
	Parameters	Optional/Reqd.
	<i>Method for liquid bulk diffusivity calculation</i>	Optional
	Keyword Usage	This keyword is used to specify the method that follows the keyword
		•
	Reactor Models	• Closed Multiphase Reactor

Keyword	Definition	
		Multiphase PSR
MTDIFF_TRANINP Reactor Property	Using Wilke-Chang method for calculation of bulk phase diffusivity. It	
	Parameters	Optional/Reqd.
	<i>Method for gas phase diffusivity calculation</i>	Optional
	Keyword Usage	This keyword is used to specify the
	Reactor Models	- Closed Multiphase Reactor - Multiphase PSR
MTDIFF_USER Reactor Property	User specified diffusivity for the bulk phase.	
	Parameters	Optional/Reqd.
	<i>Use specified diffusivity for the bulk phase</i>	Required
	Keyword Usage	This keyword indicates that diffusiv
	Reactor Models	- Closed Multiphase Reactor - Multiphase PSR
MTDIFF_WC Reactor Property	Using Wilke-Chang method for calculation of bulk phase diffusivity. It	
	Parameters	Optional/Reqd.
	<i>Method for liquid bulk diffusivity calculation</i>	Optional
	Keyword Usage	This keyword is used to specify Will keyword.
	Reactor Models	- Closed Multiphase Reactor - Multiphase PSR
MTMODEL_FILM Reactor Property	For using two-film theory for estimation of mass transfer coefficient b	
	Parameters	Optional/Reqd.
	<i>Model for estimation of mass transfer coefficient between phases</i>	Optional
	Keyword Usage	This keyword indicates use of the t follow the keyword. The same meth process. "Gas" indicates the gas pha
	Reactor Models	- Closed Multiphase Reactor - Multiphase PSR
MTMODEL_PENET Reactor Property	For using penetration theory for estimation of mass transfer coefficient	
	Parameters	Optional/Reqd.

Keyword	Definition	
	<i>Model for estimation of mass transfer coefficient between phases</i>	Optional
	Keyword Usage	This keyword indicates use of the two-phase model to follow the keyword. The same method must be used for the process. "Gas" indicates the gas phase.
	Reactor Models	• Closed Multiphase Reactor • Multiphase PSR
MTMODEL_USER	Use user-specified mass transfer coefficient.	
Reactor Property	Parameters	Optional/Reqd.
	<i>Phase name</i>	Required
	Keyword Usage	This keyword indicates use of user-specified mass transfer coefficient. The same method must be used specifically for the gas phase.
	Reactor Models	• Closed Multiphase Reactor • Multiphase PSR Reactor
MULT	Use full multicomponent model for the transport coefficients and diffusion coefficients.	
Reactor Property	Keyword Usage	Optional keyword. By default, mixture-averaged model is used.
	Reactor Models	• Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Reactor • Planar Shear Flow Reactor • Premixed Laminar Burner-stabilized Reactor • Premixed Laminar Flame-speed Reactor • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor
MVFAC	Artificial scaling factor to modify the vaporization rates.	
Reactor Property/Model	Parameters	Optional/Reqd.
	<i>Scaling factor</i>	Required
	Keyword Usage	Optional keyword. Default is 1.0.
	Reactor Models	• Direct Injection Diesel Engine Simulation
MXITS	The maximum number of iterations allowed to solve for the droplet size using the "T" option of the vaporization model.	
Reactor Property/Model	Parameters	Optional/Reqd.
	<i>Number of iterations</i>	Required

Keyword	Definition	
MZMAS Reactor Property	Keyword Usage	Optional keyword. Default is 50.
	Reactor Models	• Direct Injection Diesel Engine Simulator
	Specifies zone mass fractions. MZM will compute the exact zone volumes to set up the initial zone volumes: An error will be issued if both keywords are specified.	
	Parameters	Optional/Reqd.
	<i>zone mass fraction</i>	Required
	<i>zone number</i>	Required
	Keyword Usage	Optional keyword.
	Reactor Models	• Multi-Zone HCCI Engine Simulator
NADAP Solver	Turns off the saving of adaptive points (see ADAP (p. 141) , which is the default) to save data to file during the simulation run if they have already been turned on with ADAP (p. 141) .	
	Keyword Usage	Optional keyword. By default, ADAP is the default for the command line.
	Reactor Models	• Closed Plasma Reactor • Closed Homogeneous Reactor • Honeycomb Reactor • IC HCCI Engine Model • Multi-Zone HCCI Engine Simulator • Plasma Plug Flow Reactor • Multiphase PSR • Plug Flow Reactor • SI Engine Zonal Simulator
NADP Reactor Property	Number of mesh points that <i>Twopnt</i> can add at one time during each iteration.	
	Parameters	Optional/Reqd.
	<i>Number of mesh points</i>	Required
	Keyword Usage	Optional keyword. By default, no mesh points are added during the <i>Twopnt</i> solver.
	Reactor Models	• Diffusion or Premixed Opposed-flow Reactor • Premixed Laminar Burner-stabilized Reactor • Premixed Laminar Flame-speed Combustor • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor

Keyword	Definition	
	Notes	This keyword can not be changed
NCANG Reactor Property	Run the simulation for 180 degrees of crank angle (0.5 revolution). If the simulation stops at crank angle = 360 (=180+180) degrees (that is, top dead center), the simulation time. The last keyword (of the three) in the input file takes precedence.	
	Parameters	Optional/Reqd.
	<i>number_of_crank_angles</i>	Required
	Keyword Usage	Optional keyword.
	Reactor Models	- IC HCCI Engine - SI Engine Zonal Simulator
NCFIT Reactor Property	Optional number of time points used to determine the slope when using the NCFIT keyword.	
	Parameters	Optional/Reqd.
	<i>Number of time points</i>	Required
	Keyword Usage	Optional keyword. NCFIT is only used with the following reactor models:
		- Closed Partially Stirred Reactor (CPaSR) - Partially Stirred Reactor (PaSR)
NDPR Output or Solver	Frequency of output printing during time integration, given as the number of time points.	
	Parameters	Optional/Reqd.
	<i>Print frequency</i>	Required
	Keyword Usage	Optional keyword. By default, the print frequency is 100.
	Reactor Models	- Closed Partially Stirred Reactor (CPaSR) - Diffusion or Premixed Opposed-flow Reactor (DOPFR) - Partially Stirred Reactor (PaSR)
NEWRUN Reactor Property	Inclusion of this keyword causes Ansys Chemkin to expect keywords for the next simulation. The solution of the previous problem is not used as the initial guess. The solutions resulting from NEWRUN keywords are written sequentially to the output file.	
	Keyword Usage	Optional keyword. By default, no new run is performed.
	Reactor Models	- Chemical and Phase Equilibrium - Closed Homogeneous Batch Reactor - Closed Plasma Reactor - Cylindrical Shear Flow Reactor - Honeycomb Monolith Reactor - IC HCCI Engine

Keyword	Definition	
		• Mechanism Analyzer • Non-reactive Gas Mixer • Normal Incident Shock • Normal Reflected Shock • Partially Stirred Reactor • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • Rotating Disk CVD Reactor Using • SI Engine Zonal Simulator • Stagnation Flow CVD Reactor Using
NINTGSTEPS Reactor Property	The number of internal steps that the solver can take. When the integrator may take many internal time steps. This control acts as a check to avoid action (such as trying a few more steps or declare failure and/or provide	
	Parameters	Optional/Reqd.
	<i>Maximum value of SSDR</i>	Optional
	Keyword Usage	Optional keyword. The default value
	Reactor Models	• Diffusion Flamelet Generator
NJAC Solver	For the steady-state <i>Twopnt</i> solver, specifies the maximum number of a new Jacobian is evaluated. If NJAC=1, then a full Newton method with	
	Parameters	Optional/Reqd.
	<i>Retirement age</i>	Required
	Keyword Usage	Optional keyword. By default, the re
	Reactor Models	• Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-fl • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR

Keyword	Definition	
		• Premixed Laminar Burner-stabilized • Premixed Laminar Flame-speed C • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor
NMOM Reactor Property	Number of moments used in the simulation for tracking particle size o moments of the size distribution function are solved, from the 0 th mo	
	Parameters	Optional/Reqd.
	<i>Number of moments</i>	Required
	Keyword Usage	Optional keyword. Default is the MI
	Reactor Models	• Closed Homogeneous Batch Reac • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Honeycomb Monolith Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator
NO_SDOUTPUT_WRITE Output	Do not write output data to a standard (ascii) print-out file.	
	Keyword Usage	Optional keyword. By default, soluti
	Reactor Models	• All
NO_XMLOUTPUT_WRITE Output	Do not write output data to XML file. Note that the ANSYS CHEMKIN p	
	Keyword Usage	Optional keyword. By default, soluti
	Reactor Models	• All
NNEG Solver	Flag instructing transient solver to try to constrain all components of may help to use this keyword if negative solution components appear	
	Keyword Usage	Optional keyword. By default, the so
	Reactor Models	• Closed Homogeneous Batch Reac

Keyword	Definition	
		• Closed Partially Stirred Reactor (P • Closed Plasma Reactor • Honeycomb Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Plasma PSR • Plasma Plug Flow Reactor • Multiphase PSR • Plug Flow Reactor • SI Engine Zonal Simulator
	Notes	• NNEG (p. 247) can be added to b
NOAGG Reactor Property	Turns off particle aggregation effect. Particle aggregation is included l	
	Parameters	Optional/Reqd.
	<i>Material name</i>	Required
	Keyword Usage	Optional keyword.
	Reactor Models	• Closed Homogeneous Batch Reac • Closed Plasma Reactor • Diffusion or Premixed Opposed-fl • IC HCCI Engine • Multi-Zone HCCI Engine Simulato • Perfectly Stirred Reactor (PSR) • Plasma PSR • Premixed Laminar Burner-stabiliz
NOCG Reactor Property	Exclude coagulation of particles.	
	Keyword Usage	Optional keyword.
	Reactor Models	• Closed Homogeneous Batch Reac

Keyword	Definition	
		• Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Honeycomb Monolith Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator
NOCH Reactor Property	This keyword specifies that the rates of all gas-phase reactions will be input.	
	Keyword Usage	Optional keyword. By default, gas ch
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor
NOFT Solver or Reactor Property	For steady-state cases, when this keyword is specified and an energy c will be skipped. In this case, solution to the energy and species equati	
	Keyword Usage	Optional keyword. By default, the fi
	Reactor Models	• Diffusion or Premixed Opposed-fl • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • Premixed Laminar Burner-stabiliz • Premixed Laminar Flame-speed C • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor
	Notes	• See also, ENRG (p. 194) and ENGE
NOJC Solver	Flag indicating the non-stiff Adams method (no Jacobian) of the DVO	
	Keyword Usage	Optional keyword. By default, the D

Keyword	Definition	
	Reactor Models	• Closed Partially Stirred Reactor (P • Partially Stirred Reactor (PaSR)
NONE Output	Turns default output off for all of <i>Surftherm</i> 's tables. One can use this from only a few features. This keyword will also turn off all previously	
	Keyword Usage	Optional keyword. By default, the A
	Reactor Models	• Mechanism Analyzer
NONR Reactor Property	This keyword specifies that the non-reacting problem will not be solv	
	Keyword Usage	Optional keyword. By default, the n
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor
NOTP Reactor Property	Exclude thermophoresis of particles.	
	Parameters	Optional/Reqd.
	<i>Material name</i>	Required
	Keyword Usage	Optional keyword. By default, therm
	Reactor Models	• Diffusion or Premixed Opposed-fl • Opposed-flow Flame • Premixed Laminar Burner-stabiliz • Premixed Laminar Flame-speed C
NOTP Solver	Do not solve for the initial gas-phase and surface concentrations at th	
	Keyword Usage	Optional keyword. By default, the in
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor
NPAR Reactor Property	The number of statistical events (particles) used by the Monte Carlo p	
	Parameters	Optional/Reqd.
	<i>Number of particles</i>	Required
	Keyword Usage	Required keyword.
	Reactor Models	• Closed Partially Stirred Reactor (P • Partially Stirred Reactor (PaSR)
NP_FUEL Reactor Property	Number of points on the fuel side, that is, between the mixture fractio	
	Parameters	Optional/Reqd.
	<i>Number of grid points</i>	Required for corresponding grid c

Keyword	Definition	
	Keyword Usage	Required keyword.
	Reactor Models	Diffusion Flamelet Generator
NP_OXID Reactor Property	Number of points on the oxidizer side, that is, between the mixture fraction and the oxidizer inlet.	
	Parameters	Optional/Reqd.
	<i>Number of grid points</i>	Required for corresponding grid
	Keyword Usage	Required keyword.
	Reactor Models	Diffusion Flamelet Generator
NPIN Reactor Property	The minimum number of event particles in the reactor whose properties are tracked.	
	Parameters	Optional/Reqd.
	<i>Number of particles</i>	Required
	Keyword Usage	Optional keyword. By default, the number of particles is 1000.
	Reactor Models	Partially Stirred Reactor (PaSR)
NPSR Reactor Property	Number of perfectly stirred reactors (PSRs) or zones in a reactor cluster.	
	Parameters	Optional/Reqd.
	<i>Number of reactors or zones</i>	Required
	Keyword Usage	Optional keyword. By default, the number of reactors is 1.
		- Non-reactive Gas Mixer - Perfectly Stirred Reactor (PSR) - Plasma PSR
NPTS Reactor Property	The number of initial mesh points. The inclusion of NPTS (p. 251) will create a non-uniform mesh in the axial direction for Flames and CVD Reactors, and in the cross-flow direction for CVD Reactors. The inclusion of NPTS (p. 251) will create a non-uniform mesh using the keyword GRID (p. 215) , in which case the number of mesh points is the same as the number of grid points.	
	Parameters	Optional/Reqd.
	<i>Number of mesh points</i>	Required
	Keyword Usage	Optional keyword. By default, the number of mesh points is 1000.
	Reactor Models	- Cylindrical Shear Flow Reactor - Diffusion or Premixed Opposed-flow Reactor - Planar Shear Flow Reactor - Premixed Laminar Burner-stabilized Reactor - Premixed Laminar Flame-speed CVD Reactor - Rotating Disk CVD Reactor - Stagnation Flow CVD Reactor

Keyword	Definition	
NREV Reactor Property	The number of revolutions of the crank used to determine the end time	
	Parameters	Optional/Reqd.
	<i>Number of revolutions</i>	Required
	Keyword Usage	Optional keyword. Either NREV (p. 2)
	Reactor Models	• IC HCCI Engine • SI Engine Zonal Simulator
	Notes	• On a restart, the number of crank
NSOL XMLI	Use this keyword to specify which solution to use for the initialization stored on the XML Solution File that is used for the restart or initialization	
	Parameters	Optional/Reqd.
	<i>Solution used</i>	Required
	Keyword Usage	Optional keyword. By default, the la
	Reactor Models	• Chemical and Phase Equilibrium • Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-fl • Honeycomb Reactor • IC HCCI Engine • Mechanism Analyzer • Non-reactive Gas Mixer • Normal Incident Shock • Normal Reflected Shock • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabiliz • Premixed Laminar Flame-speed C

Keyword	Definition									
		- Rotating Disk CVD Reactor - SI Engine Zonal Simulator - Stagnation Flow CVD Reactor								
NSTEPS_HIGH Reactor Property	Number of steps to be taken to reach the specified maximum value of a subsequent step as $SSDR_{used\ in\ previous\ step} + fixedStepSize$ where $fixedStepSize$ is the specified nominal value. If the specified nominal and maximum values are 1 and 21, respectively, the sequence of SSDR values as {1, 5, 9, 13, 17, 21}. Continuations to the maximum value can be turned off by setting this property to 0. <table><tr><th>Parameters</th><th>Optional/Reqd.</th></tr><tr><td><i>Number of steps to maximum SSDR</i></td><td>Required</td></tr><tr><td>Keyword Usage</td><td>Required keyword.</td></tr><tr><td>Reactor Models</td><td> Diffusion Flamelet Generator </td></tr></table>		Parameters	Optional/Reqd.	<i>Number of steps to maximum SSDR</i>	Required	Keyword Usage	Required keyword.	Reactor Models	Diffusion Flamelet Generator
Parameters	Optional/Reqd.									
<i>Number of steps to maximum SSDR</i>	Required									
Keyword Usage	Required keyword.									
Reactor Models	Diffusion Flamelet Generator									
NSTEPS_LOW Reactor Property	Number of steps to be taken to reach the specified minimum value of a subsequent step as a $constantFactor * SSDR_{Used\ in\ previous\ step}$. That is, $NSTEPS\_LOW = constantFactor * SSDR_{Used\ in\ previous\ step}$. If the specified nominal and minimum values are 1 and 0.001, respectively, the sequence of SSDR values as {1, 0.1, 0.01, 0.001}. Continuations to the minimum value can be turned off by setting this property to 0. <table><tr><th>Parameters</th><th>Optional/Reqd.</th></tr><tr><td><i>Number of steps to maximum SSDR</i></td><td>Required</td></tr><tr><td>Keyword Usage</td><td>Required keyword.</td></tr><tr><td>Reactor Models</td><td> Diffusion Flamelet Generator </td></tr></table>		Parameters	Optional/Reqd.	<i>Number of steps to maximum SSDR</i>	Required	Keyword Usage	Required keyword.	Reactor Models	Diffusion Flamelet Generator
Parameters	Optional/Reqd.									
<i>Number of steps to maximum SSDR</i>	Required									
Keyword Usage	Required keyword.									
Reactor Models	Diffusion Flamelet Generator									
NTOT Reactor Property	Maximum number of grid points allowed during mesh adaptation. <table><tr><th>Parameters</th><th>Optional/Reqd.</th></tr><tr><td><i>Number of grid points</i></td><td>Required</td></tr><tr><td>Keyword Usage</td><td>Optional keyword. The default maximum number of grid points is 100 for Rotating Disk CVD Reactor; 250 for Diffusion Flamelet Generator; 250 for Premixed Laminar Flame-speed CVD Reactor.</td></tr><tr><td>Reactor Models</td><td> - Diffusion or Premixed Opposed-flow Reactor - Premixed Laminar Burner-stabilized Reactor - Premixed Laminar Flame-speed CVD Reactor - Rotating Disk CVD Reactor - Stagnation Flow CVD Reactor </td></tr></table>		Parameters	Optional/Reqd.	<i>Number of grid points</i>	Required	Keyword Usage	Optional keyword. The default maximum number of grid points is 100 for Rotating Disk CVD Reactor; 250 for Diffusion Flamelet Generator; 250 for Premixed Laminar Flame-speed CVD Reactor.	Reactor Models	- Diffusion or Premixed Opposed-flow Reactor - Premixed Laminar Burner-stabilized Reactor - Premixed Laminar Flame-speed CVD Reactor - Rotating Disk CVD Reactor - Stagnation Flow CVD Reactor
Parameters	Optional/Reqd.									
<i>Number of grid points</i>	Required									
Keyword Usage	Optional keyword. The default maximum number of grid points is 100 for Rotating Disk CVD Reactor; 250 for Diffusion Flamelet Generator; 250 for Premixed Laminar Flame-speed CVD Reactor.									
Reactor Models	- Diffusion or Premixed Opposed-flow Reactor - Premixed Laminar Burner-stabilized Reactor - Premixed Laminar Flame-speed CVD Reactor - Rotating Disk CVD Reactor - Stagnation Flow CVD Reactor									

Keyword	Definition	
	Notes	- This keyword can not be changed. - In previous versions, NMAX keyword was used.
NZCDC	Discharge coefficient of the injector.	
Inlet Property	Parameters	Optional/Reqd.
	<i>Injector name</i>	Required
	<i>Discharge coefficient</i>	Required
	Keyword Usage	Required keyword.
	Reactor Models	Direct Injection Diesel Engine Simulation
NZDIA	Diameter of the nozzle hole of the injector.	
Inlet Property	Parameters	Optional/Reqd.
	<i>Injector name</i>	Required
	<i>Diameter</i>	Required
	Keyword Usage	Required keyword.
	Reactor Models	Direct Injection Diesel Engine Simulation
NZHOL	Number of nozzle holes in the injector.	
Inlet Property	Parameters	Optional/Reqd.
	<i>Injector name</i>	Required
	<i>Number of holes</i>	Required
	Keyword Usage	Required keyword.
	Reactor Models	Direct Injection Diesel Engine Simulation
NZINJ	Number of injections from the injector.	
Inlet Property	Parameters	Optional/Reqd.
	<i>Injector name</i>	Required
	<i>Number of injections</i>	Required
	Keyword Usage	Required keyword.
	Reactor Models	Direct Injection Diesel Engine Simulation
NZLDR	Nozzle hole length to diameter ratio of the injector.	
Inlet Property	Parameters	Optional/Reqd.
	<i>Injector name</i>	Required
	<i>Length to diameter ratio</i>	Required
	Keyword Usage	Required keyword.
	Reactor Models	Direct Injection Diesel Engine Simulation
NZONE	Specifies the number of zones to be used in the multi-zone simulation. The default value is 1 (= single zone model). The multi-zone simulation will be issued. The default value is 1 (= single zone model). The multi-zone simulation will be issued.	

Keyword	Definition	
Reactor Property	Parameters	Optional/Reqd.
	<i>Number of zones</i>	Required
	Keyword Usage	Optional keyword.
	Reactor Models	• Multi-Zone HCCI Engine Simulator
NZRDR	Ratio of the radius of the inside rounded corner to the nozzle diameter.	
Inlet Property	Parameters	Optional/Reqd.
	<i>Injector name</i>	Required
	<i>Corner radius to diameter ratio</i>	Required
	Keyword Usage	Required keyword.
	Reactor Models	• Direct Injection Diesel Engine Simulator
NZRWL	The characteristic distance from the nozzle to the cylinder wall or the distance from the nozzle to the wall. If this value, the wall-impingement submodel will be activated. The wall-impingement submodel assumes all liquid mass will rebound back into the spray parcel. The model assumes all liquid mass will rebound back into the spray parcel.	
Inlet Property	Parameters	Optional/Reqd.
	<i>Injector name</i>	Required
	<i>Nozzle distance</i>	Required
	Keyword Usage	Optional keyword. Default is 1.0E6.
	Reactor Models	• Direct Injection Diesel Engine Simulator
OINL	The inlet-gas spin rate. At the inlet $x=L$, $v/r = \text{OINL}$.	
Reactor Property	Parameters	Optional/Reqd.
	<i>Inlet-gas spin rate</i>	Required
	Keyword Usage	Optional keyword. By default, the inlet-gas spin rate is zero.
	Reactor Models	• Rotating Disk CVD Reactor
OMEG	The disk rotation rate; also specifies the Rotating Disk CVD Reactor model.	
Problem Type and Reactor Property	Parameters	Optional/Reqd.
	<i>Disk rotation rate</i>	Required
	Keyword Usage	Required keyword. See also STAG (p. 255) .
	Reactor Models	• Rotating Disk CVD Reactor
OPMV	Specify the conventional opposed-piston movement.	
Reactor Property	Keyword Usage	Optional keyword (required to turn on the opposed-piston movement).
	Reactor Models	• Direct Injection Diesel Engine Simulator
		• IC HCCI Engine
		• Multi-Zone HCCI Engine

Keyword	Definition	
		• SI Engine Zonal Simulator
OPOC Reactor Property	Specify the opposed-piston opposed cylinder movement.	
	Keyword Usage	Optional keyword (required to turn
	Reactor Models	• Direct Injection Diesel Engine Sim • IC HCCI Engine • Multi-Zone HCCI Engine • SI Engine Zonal Simulator
OXID Inlet or Reactor Property	Defines the oxidizer mole fraction composition for an inlet stream in a equivalence ratio is specified (EQUI (p. 199)). It must be followed by a must appear for each oxidizer species, which are used to determine th Any given species can participate simultaneously as a fuel, oxidizer, or does not, a warning message will be printed and the mole fractions w	
	Parameters	Optional/Reqd.
	<i>Inlet stream name (PSRs only)</i>	Optional If there is no stream name than the fraction composition applies to the defined streams.
	<i>Species name</i>	Required
	<i>Fuel fraction</i>	Required
	Keyword Usage	Required keyword when EQUI (p. 19
	Reactor Models	• Closed Homogeneous Batch Reactor • Honeycomb Reactor • IC HCCI Engine • Perfectly Stirred Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • SI Engine Zonal Simulator
	Notes	• The mole fractions are of the oxid • The OXID (p. 256) keywords must • The OXID (p. 256) keywords must

10.3. Alphabetical Listing of Keywords [P-S]

Table 10.3: Alphabetical Listing of Keywords [P-S]

Keyword	Definition			
P1A Reactor Property	Pressure before the incident shock.			
	Parameters	Optional/Reqd.	Units	Examples
	Pressure	Required	atm	P1A 1.0
	Keyword Usage	Optional Keyword. The shock velocity and any two of temperature, pressure, or density must be specified for conditions before the incident shock. See also T1 (p. 319) and RHO1 (p. 291) .		
	Reactor Models	• Normal Incident Shock • Normal Reflected Shock		
P2A Reactor Property	Pressure after the incident shock.			
	Parameters	Optional/Reqd.	Units	Examples
	Pressure	Required	atm	P2A 2.3
	Keyword Usage	Optional Keyword. Any two of temperature, pressure, or density must be specified for conditions after the incident shock. See also T2 (p. 319) and RHO2 (p. 291) .		
	Reactor Models	• Normal Incident Shock • Normal Reflected Shock		
P3A Reactor Property	Pressure after the reflected shock, given as p_5 in the equations.			
	Parameters	Optional/Reqd.	Units	Examples
	Pressure	Required	atm	P3A 2.3
	Keyword Usage	Optional Keyword. Any two of temperature, pressure, or density must be specified for conditions before the reflected shock. See also T3 (p. 319) and RHO3 (p. 292) .		
	Reactor Models	• Normal Reflected Shock		
PARP Output	Partial-pressures of the gas-phase species will be used in the diagnostic output file.			
	Keyword Usage	Optional keyword. By default, mass fractions are printed, not partial pressures.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
PB-DEN	This keyword resets all bulk species densities defined in the surface mechanism to the value given by this keyword.			

Keyword	Definition			
Output	Parameters	Optional/Reqd.	Units	Examples
	<i>material_name</i>	Required	None	PBDEN ligA 2.15
	<i>bulk_density</i>	Required	g/cm ³	PBDEN ligA 2.15
	Keyword Usage	Optional keyword.		
	Reactor Models	• Closed Homogeneous Reactor • Perfectly Stirred Reactor (PSR) • Plug Flow Reactor (PFR)		
PDF Output	Request the probability distribution of a scalar to be output to a <i>pdf.plt</i> file. Any number of PDF (p. 258) entries is allowed.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Scalar (temperature or species name)</i>	Required	--	PDF T
	Keyword Usage	Optional keyword. By default, no PDF (p. 258) is printed.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR)		
PENG Reactor Property	Include the energy conservation equation for particles.			
	Keyword Usage	Optional keyword.		
	Reactor Models	• Opposed-flow Flame • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation		
PEST Reactor Property	Specifies an estimate of the equilibrium pressure.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Pressure</i>	Required	atm	PEST 1.1
	Keyword Usage	Optional keyword. May help convergence to the equilibrium pressure, or assure an appropriate equilibrium pressure is calculated when a second, trivial solution exists.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
PFAL Output	Analyze the pressure fall-off of a gas phase reaction, that is, creates a table of reaction rates versus total gas pressure at a constant temperature. The ALL (p. 149) option is the default and produces tables for every gas-phase reaction. The NONE (p. 250) option suppresses output for all of the reactions. If reaction information is desired for only certain reactions, they may be optionally specified by their number (given in the Pre-processor output) or by typing an exact duplicate of the reaction expression (see example input).			
	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	<i>ALL option</i>	Optional, default is ALL	--	PFAL ALL
	<i>NONE option</i>	Optional, default is ALL	--	PFAL NONE
	<i>Gas reaction number list</i>	Optional, default is ALL	--	PFAL 2 5
	<i>Gas reaction expression</i>	Optional, default is ALL	--	PFAL 2CH3(+M)<=>C2H6(+M)
	Keyword Usage	Optional keyword. By default, the table output is determined by the ALL (p. 149) or NONE (p. 250) keyword.		
	Reactor Models	• Mechanism Analyzer		
PFLR	Set the minimum bounds of the particle moments to a slightly negative number to allow the solver more room to search for a solution.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Minimum bound</i>	Required	--	PFLR -1.0d-06
	Keyword Usage	Optional keyword.		
	Reactor Models	• Opposed-flow Flame • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation		
	PH	Constant pressure and enthalpy constraints.		
Problem Type	Keyword Usage	Optional keyword. Exactly one problem type keyword must be included.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
	Notes	HP keyword is equivalent.		
	PHASE_MASSOUTFLOWRATE	Specified mass outflow rate of the phase.		
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>phase name</i>	Required		PHASE_MASSOUTFLOWRATE urea 0.0
	<i>mass outflow rate of the phase</i>	Required	g/sec	PHASE_MASSOUTFLOWRATE urea 0.0

Keyword	Definition			
	Keyword Usage	Optional keyword. Bulk name must follow the keyword. "Gas" is not valid for the keyword.		
	Reactor Models	• Multiphase PSR		
PHASE_MOLAROUTFLOWRATE	Specified molar outflow rate of the phase.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>phase name</i>	Required		PHASE_MOLAROUTFLOWRATE urea 0.0
	<i>molar outflow rate of the phase</i>	Required	mole/sec	PHASE_MOLAROUTFLOWRATE urea 0.0
	Keyword Usage	Optional keyword. Bulk name must follow the keyword. "Gas" is not valid for the keyword.		
	Reactor Models	• Multiphase PSR		
PHASE_VOLOUTFLOWRATE	Specified volumetric outflow rate of the phase.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>phase name</i>	Required		PHASE_VOLOUTFLOWRATE urea 0.0
	<i>volumetric outflow rate of the phase</i>	Required	cm ³ /sec	PHASE_VOLOUTFLOWRATE urea 0.0
	Keyword Usage	Optional keyword. Bulk name must follow the keyword. "Gas" is not valid for the keyword.		
	Reactor Models	• Multiphase PSR Reactor		
PHASE_VOLUME	Specified volume of the phase.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>phase name</i>	Required		PHASE_VOLUME urea 10.0
	<i>volume of the phase</i>	Required	cm ³	PHASE_VOLUME urea 10.0
	Keyword Usage	Optional keyword. Bulk name must follow the keyword. "Gas" is not valid for the keyword.		
	Reactor Models	• Multiphase PSR		
PHIA	Set the upper limit of the pressure range (in atmospheres) in tables where the gas pressure is varied.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Pressure</i>	Required	atm	PHIA 2.
	Keyword Usage	Optional keyword. By default, the pressure is 1.315789 atm (1000 Torr).		
	Reactor Models	• Mechanism Analyzer		

Keyword	Definition			
	Notes	• In previous versions, keyword PHIG was used with units of Torr		
PLAN Reactor Property	Use a planar coordinate system, which is appropriate for a Tsuji burner configuration.			
	Keyword Usage	Optional keyword. By default, the coordinate system is radial and axisymmetric.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame		
PLAT Reactor Property	Use a plateau profile to set up initial solution estimates, rather than a linear profile.			
	Keyword Usage	Optional keyword. By default, the plateau profile is used.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame		
PLOA Reactor Property	Set the lower limit of the pressure range (in atmospheres) in tables where the gas pressure is varied.			
	Parameters	Optional/Reqd.	Units	Examples
	Pressure	Required	atm	PLOA 1.0
	Keyword Usage	Optional keyword. By default, the pressure is 0.001315789 atm (1 Torr)		
	Reactor Models	• Mechanism Analyzer		
	Notes	• In previous versions, keyword PLOW was used with units of Torr		
PLUG Reactor Property	Indicates that plug-flow equations will be solved and that the Reactor Model will be one of the family of Plug Flow Reactors.			
	Keyword Usage	Required keyword.		
	Reactor Models	• Honeycomb Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		
PNDE Reactor Property	Assigns the initial (or estimate for steady-state calculations) number density of the particle consisting of the designated bulk species. The default value is 0. The reactor number is optional. When no reactor number is given, the same initial number density will apply to all reactors in the network. If neither PVFE (p. 276) nor PROE (p. 268) is given, the initial/estimate values of the moments are computed as $M_0 = \text{PNDE}$ $M_i = (\Delta C_{\text{nuc1}}) \times M_{i-1} \quad 1 < i \leq \text{NMOM}$			

Keyword	Definition			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	PNDE CARBON 1.0E10 4
	Number density	Required	particles/cm ³	PNDE CARBON 1.0E10 4
	Reactor number	Optional	--	PNDE CARBON 1.0E10 4
	Keyword Usage	Optional keyword. The default value is value for the number density is 0.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Honeycomb Monolith Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator		
PNDI	Assigns the number density of the particle consisting of the designated material name to the named inlet stream. The default value is 0. The stream name is optional if there is only one inlet.			
Inlet Property	Parameters	Optional/Reqd.	Units	Examples
	Stream name	Optional if only one inlet.	--	PNDI exhaust CARBON 1.0E12
	Material name	Required	--	PNDI exhaust CARBON 1.0E12
	Mass density	Required	particles/cm ³	PNDI exhaust CARBON 1.0E12
	Keyword Usage	Optional keyword. The default value for the mass density is 0.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Honeycomb Monolith Reactor		

Keyword	Definition			
		• Perfectly-stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Plasma Plug Flow Reactor • Plug-flow Reactor (PFR)		
PNUM Reactor Property	Set the total number of pressure entries in tables where the gas pressure is varied. The default is 10. Note that the changes in the pressure are determined on a logarithmic scale.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Number of pressures</i>	Required	--	PNUM 10
	Keyword Usage	Optional keyword. By default, the number of pressures is 10.		
	Reactor Models	• Mechanism Analyzer		
POLN1 Reactor Property	Specify intake-side piston pin offset distance (optional).			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Offset distance</i>	Required	cm	POLN1 0.5
	Keyword Usage	Optional keyword. Optional for use with OPMV (p. 255) or OPOC (p. 256) . Default value = 0.0.		
	Reactor Models	• Direct Injection Diesel Engine Simulator • IC HCCI Engine • Multi-Zone HCCI Engine • SI Engine Zonal Simulator		
POLN2 Reactor Property	Specify exhaust-side piston pin offset distance (optional).			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Offset distance</i>	Required	cm	POLN2 1.1
	Keyword Usage	Optional keyword. Optional for use with OPMV (p. 255) or OPOC (p. 256) . Default value = 0.0.		
	Reactor Models	• Direct Injection Diesel Engine Simulator • IC HCCI Engine • Multi-Zone HCCI Engine • SI Engine Zonal Simulator		

Keyword	Definition			
Reactor Property Profiles	PPRO Reactor pressure profile specified as a function of time for transient 0-D homogeneous systems or as a function of distance for Plug Flow Reactors.			
	Parameters	Optional/Reqd.	Units	Examples
	Time or Distance value, depending on Reactor Model	Required	sec or cm	PPRO 1.0E-4 1.0
	Pressure	Required	atm	PPRO 1.0E-4 1.0
	Reactor number (PSR clusters only)	Optional If no number is given, the profile described by the first two values is assumed to apply to all reactors in a cluster.	--	PPRO 1.0E-4 1.0
	Keyword Usage	Optional keyword. By default, no profile is provided.		
	Reactor Models	- Closed Homogeneous Batch Reactor - Closed Plasma Reactor - Diffusion or Premixed Opposed-flow Flame - Honeycomb Reactor - Non-reactive Gas Mixer - Perfectly Stirred Reactor (PSR) - Plasma Plug Flow Reactor - Plasma PSR - Multiphase PSR - Plug Flow Reactor		
Reactor Property	PRDL The Prandlt number used in the generalized heat transfer correlation.			
	Parameters	Optional/Reqd.	Units	Examples
	Prandlt number	Required	--	PRDL 0.77

Keyword	Definition			
	Keyword Usage	Optional keyword. By default, the value is 0.7.		
	Reactor Models	• IC HCCI Engine • SI Engine Zonal Simulator		
PRES Reactor Property	The reactor pressure in atmospheres. Depending on the Reactor Model and problem type, the pressure specified can serve as the pressure constraint (for constant-pressure problems), as an initial guess for pressure (for steady-state problems where pressure is a variable), or as the initial reactor pressure (for transient cases where pressure is a variable). For the Mechanism Analyzer, this is the bath-gas pressure.			
	Parameters	Optional/Reqd.	Units	Examples
	Reactor pressure	Required	atm	PRES 1.0
	Reactor number (PSR clusters only)	Optional If no number is given, the keyword is assumed to apply to all reactors in a cluster.	--	PRES 1.0 1
	Keyword Usage	Required keyword in most cases. Optional keyword only for Mechanism Analyzer, where the default is 1 atm.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations • Closed Homogeneous Batch Reactor • Closed Partially Stirred Reactor (PaSR) • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • IC HCCI Engine • Mechanism Analyzer • Non-reactive Gas Mixer		

Keyword	Definition			
	- Partially Stirred Reactor (PaSR) - Perfectly Stirred Reactor (PSR) - Planar Shear Flow Reactor - Plasma Plug Flow Reactor - Plasma PSR - Multiphase PSR - Plug Flow Reactor - Premixed Laminar Burner-stabilized Flame - Premixed Laminar Flame-speed Calculation - Rotating Disk CVD Reactor - SI Engine Zonal Simulator - Stagnation Flow CVD Reactor			
	Notes	- In previous version, PRMT was an alternate keyword that allowed pressure input in millitorr units, for 0-D homogeneous and plug-flow systems only. - In previous versions, this was PBTH for the Mechanism Analyzer.		
PRMN Reactor Property	Minimum mole fraction value applied to the estimated values of the flame products, when the (default) equilibrium is used to determine product estimates. Ignored in the case that PROD2 (p. 267) keywords are present.			
	Parameters	Optional/Reqd.	Units	Examples
	Product fraction	Required	mole fractions	PRMN 1.0E-10
	Keyword Usage	Optional keyword. By default, the flame product fraction is set to 0.		
	Reactor Models	- Premixed Laminar Burner-stabilized Flame - Premixed Laminar Flame-speed Calculation		
PRNT Output	Printing control. "PRNT 0" provides printed output for only the solution (plus sensitivity coefficients and rates-of-production coefficients, when requested). "PRNT 1" provides an additional summary of the iteration path from the solver. "PRNT 2" includes printing at every stage of the <i>Twopnt</i> solver's Newton iteration and time stepping procedure. More printing is sometimes helpful when diagnosing problems and trying to adjust the input parameters to optimize convergence. However, since the increased printing requires more function evaluations to show			

Keyword	Definition			
	how the solution is progressing, the computer time increases with increased printing.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Print control number</i>	Required	--	PRNT 1
	Keyword Usage	Optional keyword. By default, the print control is set to 1.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • SI Engine Zonal Simulator • Stagnation Flow CVD Reactor		
PROD	Estimated values of the gas-phase mole fractions at the far end of the domain (that is, the deposition surface for CVD reactors or the burned state at XEND (p. 367) for Premixed Laminar Flames) or in the middle of the flame (for Opposed-flow Flames). The sum of the product mole fractions should equal to 1.0; if they do not, then a warning message will be printed to the diagnostic output file and the mole fractions will be normalized so that they do sum to one.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Species name</i>	Required	--	PROD H2O 0.5
	<i>Mole fraction</i>	Required	--	PROD H2O 0.5

Keyword	Definition																			
	Keyword Usage	Optional keyword. If PROD2 (p. 267) keywords are not provided, then an equilibrium calculation will be used to determine the estimated product composition (see also PRMN (p. 266)).																		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor																		
	Notes	• Any given species may simultaneously be included as a reactant (REAC (p. 288)), intermediate (INTM (p. 227)), and product (PROD2 (p. 267)). • The PROD2 (p. 267) keywords must be changed as a set, not individually for a restart run. • The PROD2 (p. 267) keywords must be changed as a set, not individually for continuation run.																		
PROE Reactor Property	Assigns the initial (or estimate for steady-state calculations) number density of the particle consisting of the designated material name. The default value is 0. The reactor number is optional. When no reactor number is given, the same initial particle mass density will apply to all reactors in the network. The PROE (p. 268) keyword must be used in conjunction with the PNDE (p. 261) keyword and is mutually exclusive to keyword PVFE (p. 276). When both PNDE and PROE are given, the moments are calculated as $M_0 = \text{PNDE}$ $M_1 = \frac{\text{PROE}}{m_0}$ $M_i = (\Delta C_{\text{nuc1}}) \times M_{i-1} \quad 1 < i \leq \text{NMOM}$ where m_0 is the mass of a material name molecule and ρ_B is the mass density of the bulk material. <table><tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr><tr><td><i>Material name</i></td><td>Required</td><td>--</td><td>PROE CARBON 1.0E-10 1</td></tr><tr><td><i>Mass density</i></td><td>Required</td><td>gm/cm³</td><td>PROE CARBON 1.0E-10 1</td></tr><tr><td><i>Reactor number</i></td><td>Optional</td><td>--</td><td>PROE CARBON 1.0E-10 1</td></tr></table>				Parameters	Optional/Reqd.	Units	Examples	<i>Material name</i>	Required	--	PROE CARBON 1.0E-10 1	<i>Mass density</i>	Required	gm/cm ³	PROE CARBON 1.0E-10 1	<i>Reactor number</i>	Optional	--	PROE CARBON 1.0E-10 1
Parameters	Optional/Reqd.	Units	Examples																	
<i>Material name</i>	Required	--	PROE CARBON 1.0E-10 1																	
<i>Mass density</i>	Required	gm/cm ³	PROE CARBON 1.0E-10 1																	
<i>Reactor number</i>	Optional	--	PROE CARBON 1.0E-10 1																	

Keyword	Definition			
	Keyword Usage	Optional keyword. The default value for the mass density is 0. PNDE (p. 261) keyword required. Cannot be used with PVFE (p. 276).		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Honeycomb Monolith Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator		
PROI Inlet Property	Assigns the mass density of the particle consisting of the designated material name to the named inlet stream. The default value is 0. The stream name is optional if there is only one inlet. The PROI keyword must be used in conjunction with the PNDI (p. 262) keyword and is mutually exclusive to keyword PVFI (p. 277).			
	Parameters	Optional/Reqd.	Units	Examples
	Stream name	Optional if there is only one inlet.	--	PROI EGR CARBON 1.0E-10
	Material name	Required	--	PROI EGR CARBON 1.0E-10
	Number density	Required	gm/cm ³	PROI EGR CARBON 1.0E-10
	Keyword Usage	Optional keyword. Must be used with PNDI (p. 262). Cannot be used with PVFI (p. 277). The default value for the number density is 0.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Honeycomb Monolith Reactor • Perfectly-stirred Reactor (PSR) • Planar Shear Flow Reactor		

Keyword	Definition			
		• Plasma PSR • Plasma Plug Flow Reactor • Plug-flow Reactor (PFR)		
PS Problem Type	Constant pressure and entropy constraints.			
	Keyword Usage	Optional keyword. Exactly one problem-type keyword must be included.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
	Notes	• SP (p. 310) keyword.is equivalent.		
PS-BAR Reactor Property	The piston head area to bore area ratio.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Ratio of piston head area to bore area.</i>	Required	None	PSBAR 1.1
	Keyword Usage	Optional keyword. Default = 1.0.		
	Reactor Models	• IC HCCI Engine • Multi-zone HCCI Engine • SI Engine Zonal Simulator		
	Notes	PSBAR should be > 1.0.		
PSURF Inlet Property	Initial surface coverage on particles by the surface site species in the inlet flow.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Stream name</i>	Optional if there is only one inlet.	--	PSURF inlet1 C(S) 0.1
	<i>Surface species name</i>	Required	--	PSURF inlet1 C(S) 0.1
	<i>Surface coverage</i>	Required	--	PSURF inlet1 C(S) 0.1
	Keyword Usage	Optional keyword		
	Reactor Models	• Honeycomb Reactor • Opposed-flow Flame • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR		

Keyword	Definition			
		• Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation		
PSV Solver	Pseudo-velocity for use in modifying the surface species equations for improved convergence. This pseudo-convection term is incorporated into the surface site fraction equations in order to convert algebraic equations to differential equations. The value of the PSV (p. 271) should be small enough such that it has no effect on the solution results, but large enough to affect the convergence behavior. If not supplied, then the unmodified equations are used. The modified equations are sometimes helpful in reaching steady-state conditions for problems with stiff surface chemistry (e.g. catalytic combustion), but should not be used if no convergence problems are encountered. A recommended value to try for PSV (p. 271) would be about 1/10th of the inlet velocity, but the simulation should be repeated with smaller or larger values to make sure that it has no effect on the solution.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Pseudo-velocity</i>	Required	cm/sec	PSV 10 .
	Keyword Usage	Optional keyword. By default, the value is set to 10* ATOL (p. 157).		
	Reactor Models	• Honeycomb Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		
PTM_SECTION_NUM	The number of sections to use for the specified material.			
	Parameters	Optional/Reqd.	Units	Examples
Reactor Property	<i>Material name</i>	Required	--	PTM_SECTION_NUM SOOT 30
	<i>Number of sections</i>	Required	--	PTM_SECTION_NUM SOOT 30
	Keyword Usage	Required when the Sectional Model is used.		
	Reactor Models	• Opposed-flow Flame • Plug Flow Reactor • Premixed Laminar Burner Stabilized Flame • Premixed Laminar Burner Stabilized Stagnation Flame • Premixed Laminar Flame Speed Calculator		
PTM_SECTION_SIZE	Tanh function constant that is used to blend lower and upper bounds of collision efficiency.			

Keyword	Definition			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	None	PTM_SECTION_SIZEDEP_A0 SOOT 5
	A0	Required	None	PTM_SECTION_SIZEDEP_A0 SOOT 5
	Keyword Usage	Optional keyword. Default size is 7.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Internal Combustion Engine • Perfectly Stirred Reactor (PSR) • Diffusion or Premixed Opposed Flow Flame • Plug Flow Reactor • Premixed Laminar Burner Stabilized Flame • Premixed Laminar Burner Stabilized Stagnation Flame • Premixed Laminar Flame Speed Calculator		
PTM_SECTION_SIZEDEP_COLEFF	Use size-dependent collision efficiency for particles .			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	None	PTM_SECTION_SIZEDEP_COLEFF SOOT
	Keyword Usage	Optional keyword. Not used by default.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Internal Combustion Engine • Perfectly Stirred Reactor (PSR) • Diffusion or Premixed Opposed Flow Flame • Plug Flow Reactor • Premixed Laminar Burner Stabilized Flame • Premixed Laminar Burner Stabilized Stagnation Flame • Premixed Laminar Flame Speed Calculator		
PTM_SECTION_SIZEDEP_DSTAR	Limit diameter for size-dependent collision efficiency.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	None	PTM_SECTION_SIZEDEP_DSTAR SOOT 13-06

Keyword	Definition			
	Diameter	Required	None	PTM_SECTION_SIZEDEP_DSTAR SOOT 13-06
	Keyword Usage	Optional keyword. No default value is given and must be specified by user when using size-dependent collision efficiency. For soot simulation, the value generally ranges from 10 to 20 nm.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Internal Combustion Engine • Perfectly Stirred Reactor (PSR) • Diffusion or Premixed Opposed Flow Flame • Plug Flow Reactor • Premixed Laminar Burner Stabilized Flame • Premixed Laminar Burner Stabilized Stagnation Flame • Premixed Laminar Flame Speed Calculator		
PTM_SECTION_SIZEDEP_HAMAKER	Hamaker constant for computing potential well depth when using size-dependent collision efficiency for particles.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	None	PTM_SECTION_SIZEDEP_HAMAKER SOOT 5e-13
	Diameter	Required	None	PTM_SECTION_SIZEDEP_HAMAKER SOOT 5e-13
	Keyword Usage	Optional keyword. Default value is 7e-13 erg.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Internal Combustion Engine • Perfectly Stirred Reactor (PSR) • Diffusion or Premixed Opposed Flow Flame • Plug Flow Reactor • Premixed Laminar Burner Stabilized Flame • Premixed Laminar Burner Stabilized Stagnation Flame • Premixed Laminar Flame Speed Calculator		
PTM_SECTION_SNO	Number of "atoms" in the smallest section for the specified material. When etching reactions are present, the number of sectional atoms parameter needs to be unity. When only growth is present, the user can give some higher value to avoid			

Keyword	Definition			
Reactor Property	calculations for smaller particles that will never be present. However, this value must not be greater than the number of atoms in the smallest nucleating particle.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	PTM_SECTION_SNO SOOT 1
	Number of sectional "atoms"	Required	--	PTM_SECTION_SNO SOOT 1
	Keyword Usage	Required when the Sectional Model is used.		
	Reactor Models	• Opposed-flow Flame • Plug Flow Reactor • Premixed Laminar Burner Stabilized Flame • Premixed Laminar Burner Stabilized Stagnation Flame • Premixed Laminar Flame Speed Calculator		
PTM_SECTION_SPACING	Geometric spacing factor to be used for sections.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	PTM_SECTION_SPACING CARBON 2.0
	Geometric spacing factor	Required	--	PTM_SECTION_SPACING CARBON 2.0
	Keyword Usage	Required when the Sectional Model is used.		
	Reactor Models	• Opposed-flow Flame • Plug Flow Reactor • Premixed Laminar Burner Stabilized Flame • Premixed Laminar Burner Stabilized Stagnation Flame • Premixed Laminar Flame Speed Calculator		
PTM_SECTION_TCOND	Thermal conductivity of particle material. This is a required input when any of the flame models are using the Sectional Model with thermophoresis.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	PTM_SECTION_TCOND CARBON 2.0E+05
	Thermal conductivity of "material"	Required	erg/s-cm-K	PTM_SECTION_TCOND CARBON 2.0E+05
	Keyword Usage	Required when the Sectional Model with thermophoresis is used.		
	Reactor Models	• Opposed-flow Flame		

Keyword	Definition			
		• Plug Flow Reactor • Premixed Laminar Burner Stabilized Flame • Premixed Laminar Burner Stabilized Stagnation Flame • Premixed Laminar Flame Speed Calculator		
PTM_SECTION_USERBULKROP	User-specified enhancement factor for the growth/etching reactions on particles. This can be used only with the sectional method. Note that the user-routines library must be compiled and linked; see the Chemkin Application Programming Interface Manual for details.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	None	PTM_SECTION_USERBULKROP CARBON
	Keyword Usage	Optional keyword. Not used by default.		
	Reactor Models	• Closed Homogeneous Batch Reactor • IC HCCI Engine • Multi-Zone HCCI Engine Simulator • SI Engine Zonal Simulator • Perfectly Stirred Reactor (PSR) • Plug Flow Reactor • Opposed-flow Flame • Premixed Laminar Burner Stabilized Flame • Premixed Laminar Burner Stabilized Stagnation Flame • Premixed Laminar Flame Speed Calculator		
PTM_SECTIONAL	Signals that sectional model is to be used. This is a required keyword when the Sectional Model is used.			
	Keyword Usage	Required when the Sectional Model is used.		
	Reactor Models	• Closed Homogeneous Batch Reactor • IC HCCI Engine • Multi-Zone HCCI Engine Simulator • SI Engine Zonal Simulator • Perfectly Stirred Reactor (PSR) • Opposed-flow Flame		

Keyword	Definition			
		• Plug Flow Reactor • Premixed Laminar Burner Stabilized Flame • Premixed Laminar Burner Stabilized Stagnation Flame • Premixed Laminar Flame Speed Calculator		
PV Problem Type	Constant pressure and volume constraints.			
	Keyword Usage	Optional keyword. Exactly one problem-type keyword must be included.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
	Notes	• VP keyword is equivalent.		
PVFE Reactor Property	Assigns the initial (or estimate for steady state calculations) number density of the particle consisting of the designated material name. The default value is 0. The reactor number is optional. When no reactor number is given, the same initial particle volume fraction will apply to all reactors in the network. The PVFE keyword must be used in conjunction with the PNDE (p. 261) keyword and is mutually exclusive to keyword PROE (p. 268) . When both PNDE and PVFE are given, the moments are calculated as			
	$M_0 = \text{PNDE}$			
	$M_1 = \frac{\rho_B \times \text{PVFE}}{m_0}$			
	$M_i = (\Delta C_{\text{nuc1}}) \times M_{i-1} \quad 1 < i \leq \text{NMOM}$			
	where m_0 is the mass of a material name molecule and ρ_B is the mass density of the bulk material.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	PVFE CARBON 1.0E-10 4
	Volume fraction	Required	cm ³ /cm ³	PVFE CARBON 1.0E-10 4
	Reactor number	Optional	--	PVFE CARBON 1.0E-10 4
	Keyword Usage	Optional keyword. The default value is value for the volume fraction is 0. PNDE (p. 261) keyword required.		
Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Honeycomb Monolith Reactor			

Keyword	Definition			
		• IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator		
PVFI Inlet Property	Assigns the volume fraction of the particle consisting of the designated material name to the named inlet stream. The default value is 0. The stream name is optional if there is only one inlet. The PVFI keyword must be used in conjunction with the PNDI (p. 262) keyword and is mutually exclusive to keyword PROI (p. 269) .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Stream name</i>	Optional if there is only one inlet.	--	PVFI inlet1 CARBON 1.0E--9
	<i>Material name</i>	Required	--	PVFI inlet1 CARBON 1.0E-9
	<i>Number density</i>	Required	cm ³ /cm ³	PVFI inlet1 CARBON 1.0E-9
	Keyword Usage	Optional keyword. Must be used with PNDI (p. 262) . Cannot be used with PROI (p. 269) . The default value for the number density is 0.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Honeycomb Monolith Reactor • Perfectly-stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Plasma Plug Flow Reactor • Plug-flow Reactor (PFR)		
PVSO Reactor Property	Specify the reference gas viscosity at the reference temperature of the power-law for viscosity.			
	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	<i>Reference gas viscosity at reference temperature</i>	Required.	g/cm-s	PVS0 1.716E-4
	Keyword Usage	Optional.		
	Reactor Models	- Multi-Zone HCCI Simulator - IC HCCI Engine - SI Engine Zonal Simulator		
PVSN	Specify the exponent of the temperature ratio term of the power-law for viscosity.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Exponent of temperature ratio term</i>	Required.	--	PVSN 0.5
	Keyword Usage	Optional.		
	Reactor Models	- Multi-Zone HCCI Simulator - IC HCCI Engine - SI Engine Zonal Simulator		
PVST	Specify the reference temperature of the power-law for viscosity.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Reference temperature</i>	Required.	K	PVST 273.15
	Keyword Usage	Optional.		
	Reactor Models	- Multi-Zone HCCI Simulator - IC HCCI Engine - SI Engine Zonal Simulator		
PWRC	The power being supplied to heat the deposition surface or disk. This value is used only if the disk temperature is being calculated from an energy balance by including keyword RADB (p. 286) . See Equation 15.18 of the Chemkin Theory Manual .			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Power</i>	Required	cal/(cm ² . sec)	PWRC 15.E7
	Keyword Usage	Optional keyword. By default, the power is 0.0.		
	Reactor Models	Rotating Disk CVD Reactor		

Keyword	Definition			
		• Stagnation Flow CVD Reactor		
PWRW Reactor Property	Total power deposition to the plasma.			
	Parameters	Optional/Reqd.	Units	Examples
	Total power deposition	Required	Watts	PWRW 1000.
	Reactor number (PSR clusters only)	Optional If no number is given, the value is assumed to apply to all reactors in a cluster.	--	PWRW 1000. 1
	Keyword Usage	Required keyword.		
	Reactor Models	• Closed Plasma Reactor • Plasma Plug Flow Reactor • Plasma PSR		
QDOT Reactor Property	The power being supplied to heat the gas as a spatially distributed Gaussian heat source. QDOT (p. 279) is the total power, that is, the spatial integral of the heat source function. See Equation 15.14 of the Chemkin Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	Power	Required	erg/(cm ² . sec)	QDOT 1.0E7
	Keyword Usage	Optional keyword. By default, the power is 0.0.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
QDTC Reactor Property	The power being supplied to heat the gas as a spatially distributed Gaussian heat source. QDTC (p. 279) is the total power, that is, the spatial integral of the heat source function. See Equation 15.14 of the Chemkin Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	Power	Required	cal/(cm ² . sec)	QDTC 1.0E7

Keyword	Definition			
	Keyword Usage	Optional keyword. By default, the power is 0.0.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
QEXP Reactor Property	Specifies the gas chemistry heat release rate that defines the start of the expansion period. This keyword will take effect only when the gas heat release equation is solved (activated by keyword: QRGEQ (p. 284)).			
	Parameters	Optional/Reqd.	Units	Examples
	heat_release_rate	Required	cal/sec	QEXP 0.5
	Keyword Usage	Optional keyword. Default is 0.1 cal/sec.		
	Reactor Models	• Multi-Zone HCCI Simulator • IC HCCI Engine • SI Engine Zonal Simulator		
QFUN Reactor Property User Subroutine	Reactor heat loss will be given as a specified function of time (for 0-D homogeneous reactors) or as a function of distance (for Plug Flow Reactors), through a user-programmed subroutine. FUNCTION PSQFUN (LENIQ, LENRQ, IQFUN, RQFUN) must be provided to specify the heat loss and linked to the application program. See the Application Programming Interface Manual for details on how to work with user subroutines.			
	Keyword Usage	Optional keyword. By default, the value there is no heat loss from the reactor. The units returned from the user subroutine must be in erg/sec. See also QPRO (p. 283) .		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame		

Keyword	Definition			
		- Premixed Laminar Flame-speed Calculation - SI Engine Zonal Simulator		
	Notes	- See also QPRO (p. 283) as an alternate way to specify heat-loss as a function of time. - Keywords QFUN (p. 280), QLOS (p. 281) and QPRO (p. 283) are mutually exclusive.		
QIAGE	The time delay to turn on the droplet temperature equation at the beginning of liquid vaporization to prevent possible convergence issues at the start of injection. When the Droplet Surface T = Core T option is selected, a very large time delay can force the droplet temperature to be constant, that is, equal to the initial liquid temperature, throughout the simulation.			
Reactor Property/Model	Parameters	Optional/Reqd.	Units	Examples
	Time	Required	seconds	QIAGE 1.0E-3
	Keyword Usage	Optional keyword. Default is 0.0 sec.		
	Reactor Models	Direct Injection Diesel Engine Simulator		
QLOS	The heat loss or heat flux from the reactor to the external environment at an optionally specified surface material. The units are for a total heat loss for 0-D homogeneous reactors, or for heat flux per area for all channel-flow reactors (Plug Flow Reactor, Honeycomb Reactor, Plasma Plug Flow Reactor, and Shear Flow Reactors). This option is only relevant when the energy equation is being solved.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Material name (for 0-D homogeneous and plug-flow reactors only)	Optional If no material is specified, the value will be used for all materials.	--	QLOS material1 50
	Bulk name (multiphase reactors only)	Optional	--	QLOS Gas AMBIENT 0.5
	Heat loss or Heat flux (depending on Reactor Model)	Required	cal/sec or cal/cm2-s	QLOS 50
	Reactor number (PSR clusters only)	Optional If no number	--	QLOS material1 50 1

Keyword	Definition			
		is given, the keyword is assumed to apply to all reactors in a cluster.		
	Keyword Usage	Optional keyword. By default, there is no heat loss from the reactor. See also QPRO (p. 283) , HTRN (p. 220) , and QFUN (p. 280) . For the multiphase reactors, the keyword is effective for the phase name following the keyword. The name of the bulk phase should be used. "Gas" indicates the gas phase.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Honeycomb Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Multiphase PSR • Plug Flow Reactor • Perfectly Stirred Reactor (PSR) • SI Engine Zonal Simulator		
QLSE	This is an additional energy loss term for the electrons that may be introduced to account for inelastic collisional losses that are not already included explicitly in the <i>Gas-phase Kinetics</i> reaction mechanism. Energy loss values are specified here as a function of electron temperature and are given per ionization event to be consistent with the work of Lee, et al. [12] (p. 375) For example, "QLSE 34800. 100." would represent an electron energy loss of 100 eV/ionization event for an electron temperature of 34800 K (3.0 eV).			
Reactor Property Profiles	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	Energy loss	Required	eV	QLSE 34800. 100.
	Electron temperature	Required	K	QLSE 34800. 100.
	Keyword Usage	Optional keyword. By default, the additional energy loss term is 0.0.		
	Reactor Models	• Closed Plasma Reactor • Plasma Plug Flow Reactor • Plasma PSR		
QPRO Reactor Property Profiles	The heat loss profile or heat flux profile from the reactor to the external environment at an optionally specified surface material, given as a piece-wise linear function of time or distance. Each QPRO (p. 283) entry represents a point in a piecewise-linear profile. The units are for a total heat loss vs. time for 0-D homogeneous reactors, or for heat flux per area vs. distance for all channel-flow reactors (Plug Flow Reactor, Honeycomb Reactor, Plasma Plug Flow Reactor, and Shear Flow Reactors). This option is only relevant when the energy equation is being solved.			
	Parameters	Optional/Reqd.	Units	Examples
	Time or Distance value (depending on Reactor Model)	Required	sec or cm	QPRO 1.0E-4 10.0
	Heat loss or Heat flux (depending on Reactor Model)	Required	cal/sec or cal/cm2-sec	QPRO 1.0E-4 10.0
	Reactor number (PSR clusters only)	Optional If no number is given, the profile described by the first two values is assumed to apply to all reactors in a cluster.	--	QPRO 1.0E-4 10.0 1
	Keyword Usage	Optional keyword. By default, there is no heat loss from the reactor. See also QLOS (p. 281) , HTRN (p. 220) , and QFUN (p. 280) .		
	Reactor Models	• Closed Homogeneous Batch Reactor		

Keyword	Definition			
		• Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Honeycomb Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Plasma Plug Flow Reactor • Multiphase PSR • Plug Flow Reactor • SI Engine Zonal Simulator		
QRGEQ Output	Solve a separate equation that integrates the heat release due to gas-phase reactions to obtain a more accurate heat-release profile. If this option is not checked, only local heat release rates will be reported at each saved or printed time steps. Only applicable when you are solving the energy equation with transient solver.			
	Parameters	Optional/Reqd.	Units	Examples
	Keyword Usage	Optional keyword. By default, the heat release integration equation is not solved.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Monolith Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator		

Keyword	Definition			
QRSEQ Output	Solve a separate equation that integrates the heat release due to surface reactions to obtain a more accurate heat-release profile. If this option is not checked, only local heat release rates will be reported at each saved or printed time steps. Only applicable when you are solving the energy equation with transient solver.			
	Parameters	Optional/Reqd.	Units	Examples
	Keyword Usage	Optional keyword. By default, the heat release integration equation is not solved.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Monolith Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor		
QXCO Recycling	This keyword defines the heat-transfer coefficient and the heat-transfer surface area for thermal conductive/convective heat flux between the two specified reactors in a reactor cluster. The direction of the heat flux will come from the higher-temperature reactor to the lower-temperature reactor. This keyword is only relevant when the ENRG (p. 194) keyword is used and when there are multiple reactors in a cluster.			
	Parameters	Optional/Reqd.	Units	Examples
	Reactor Number	Required	--	QXCO 3 6 1.0E-3 1000.
	Reactor Number	Required	--	QXCO 3 6 1.0E-3 1000.
	Heat-transfer coefficient	Required	cal/(cm ² · sec · K)	QXCO 3 6 1.0E-3 1000.
	Heat-transfer surface area	Required	cm ²	QXCO 3 6 1.0E-3 1000.
	Keyword Usage	Optional keyword. By default, there is no heat exchange between reactors.		
	Reactor Models	• Perfectly Stirred Reactor (PSR) • Plasma PSR		
	Notes	• The order of the two reactor numbers that define the heat connection is not important.		

Keyword	Definition			
		This parameter is used in conjunction with the external surface area (AREAQ (p. 151) or AEXT (p. 142)).		
QXRA Recycling	This keyword defines the thermal emissivity/absorptivity and the heat-transfer surface area for thermal radiative flux between the two specified reactors in a reactor cluster. The direction of the heat flux will come from the higher-temperature reactor to the lower-temperature reactor. This keyword is only relevant when the ENRG (p. 194) keyword is used and when there are more than one reactor in a cluster.			
	Parameters	Optional/Reqd.	Units	Examples
	Reactor Number	Required	--	QXRA 2 3 0.1 1000.
	Reactor Number	Required	--	QXRA 2 3 0.1 1000.
	Emissivity/absorptivity	Required	--	QXRA 2 3 0.1 1000.
	Heat-transfer surface area	Required	cm ²	QXRA 2 3 0.1 1000 .
	Keyword Usage	Optional keyword. By default, there is no heat exchange between reactors. Note that the order of the two reactor numbers that define the heat connection is un-important.		
	Reactor Models	- Perfectly Stirred Reactor (PSR) - Plasma PSR		
	Notes	- The order of the two reactor numbers that define the heat connection is not important. - This parameter is used in conjunction with the external surface area (AREAQ (p. 151) or AEXT (p. 142)).		
RACTV Reactor Property	By default, when the gas-phase thermal radiation calculation is on, contributions from all major radiating species (such as CO ₂ , H ₂ O, CO, and CH ₄) will not be included. A major radiating species is a species of which the absorption coefficient is available to the application. This keyword allows the user to include the contribution of a major species in the radiation heat loss calculation.			
	Parameters	Optional/Reqd.	Units	Examples
	Species symbol	Required	--	RACTV CO
	Keyword Usage	Optional keyword.		
	Reactor Models	- Diffusion or Premixed Opposed-flow Flame - Burner-stabilized Pre-mixed Flame - Premixed Laminar Flame-speed Calculation		
RADB	Use an energy balance to determine the disk or susceptor (deposition surface) temperature. If RADB (p. 286) is specified, TDSK (p. 323) is used as the initial guess for the susceptor temperature.			

Keyword	Definition			
Reactor Property	Keyword Usage	Optional keyword. By default, the susceptor temperature is fixed as TDSK (p. 323) .		
	Reactor Models	- Rotating Disk CVD Reactor - Stagnation Flow CVD Reactor		
RADGS Reactor Property	Turns on the radiation heat loss term in the gas energy equation. The optional model number indicates which thermal radiation model will be employed to calculate the radiation intensity.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Reactor number</i>	Required	--	RADGS 0
	Keyword Usage	Currently, the optically-thin limit model is the only model implemented and hence is the default model. The model number for the optically-thin limit model is 0.		
	Reactor Models	- Diffusion or Premixed Opposed-flow Flame - Burner-stabilized Pre-mixed Flame - Premixed Laminar Flame-speed Calculation		
RADPT Reactor Property	Allows radiative heat loss contribution from particulates associated with the named material to be included independently.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Material Name</i>	Required	--	RADPT CO
	Reactor Models	- Diffusion or Premixed Opposed-flow Flame - Burner-stabilized Pre-mixed Flame - Premixed Laminar Flame-speed Calculation		
RCHG Solver	Maximum relative change in the surface site fractions (over one time step) for which the initial fictitious transient equations that establish the initial surface site fractions can be considered to have converged to steady state.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Maximum relative change</i>	Required	--	RCHG 1.0E-3
	Keyword Usage	Optional keyword. By default, the maximum relative change is set to 1.0E-6.		
	Reactor Models	- Honeycomb Reactor - Plasma Plug Flow Reactor - Plug Flow Reactor		

Keyword	Definition			
RDSK Reactor Property	Ratio of the substrate radius to the separation distance between it and the upper radiating disk. This is used in calculating a surface radiation balance. RRAD (p. 295) is used only if the disk temperature is being calculated by including keyword RADB (p. 286) . See Equation 15.18 of the Chemkin Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Ratio of substrate</i>	Required	--	RDSK 3.0
	Keyword Usage	Optional keyword. This is keyword is required only when RRAD (p. 295) and RADB (p. 286) are included.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
REAC Inlet or Reactor Property	Mole fraction of the reagent gases entering the reactor for an inlet stream or for the initial conditions in a closed system. For example, REAC fuel1 C2H2 0.5, would indicate that acetylene has a mole fraction of 0.5 in the inlet stream named fuel1. The sum of all the reactant mole fractions should equal to one. However, if they do not the fractions will be normalized so that they do sum to one, and a warning message will be printed to the output file.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Inlet stream name (for PSRs and CVD Reactors only)</i>	Optional If there is no stream name than the reactant and mole fraction apply to all streams.	--	REAC fuel1 C2H2 0.5
	<i>Species name</i>	Required	--	REAC C2H2 0.5
	<i>Reactant fraction</i>	Required	mole fractions	REAC C2H2 0.5
	Keyword Usage	Required keyword, except in cases where an equivalence ratio option is used (EQUI (p. 199)).		
	Reactor Models	• Chemical and Phase Equilibrium Calculations • Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame		

Keyword	Definition			
		• Honeycomb Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Multiphase PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• The REAC (p. 288) keywords must be changed as a set, not individually for a restart run. • The REAC (p. 288) keywords must be changed as a set, not individually for continuation run.		
RECY Recycling	For a cluster of reactors (NPSR > 1), specifies recycling or routing of a mass flow from one reactor to another and the fractional flow associated with this stream.			
	Parameters	Optional/Reqd.	Units	Examples
	Reactor Number, from which the flow originates	Required	--	RECY 2 1 0.3
	Reactor Number, to which the flow is transferred	Required	--	RECY 2 1 0.3
	Percent that will be recycled from Reactor 2 back into Reactor 1	Required	--	RECY 2 1 0.3
	Keyword Usage	Optional keyword. By default all flow out of a reactor in will flow into the next reactor in the series (e.g. RECY 1 2 1.0 and RECY 2 3 1.0 for a three-reactor system). If		

Keyword	Definition	
		recycle loops are defined, then the effective "recycling" from the upstream into the downstream reactor will be one minus the sum of the recycle streams out of the upstream reactor into other reactors.
	Reactor Models	• Perfectly Stirred Reactor (PSR) • Plasma PSR
RE-LAXC Solver	Controls the convergence method used for transient runs. When applied, it uses a relaxed scheme whereby the integrator solver tries harder to achieve a solution at each time, but occasionally may result in increased time to solve your problem or numerical instabilities. Therefore, you should use this only if your transient run fails with a "nonlinear solver failed to converge repeatedly" message or you believe your problem is very stiff, highly nonlinear or discontinuous.	
	Keyword Usage	Optional keyword.
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Partially Stirred Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Honeycomb Reactor • IC HCCI Engine • Multi-Zone HCCI Engine Simulator • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Multiphase PSR • Plug Flow Reactor • Rotating Disk CVD Reactor • SI Engine Zonal Simulator • Stagnation Flow CVD Reactor

Keyword	Definition			
RELT Solver	This keyword is used to override the default value for the relative perturbation in the solution variable used in the determination of the numerically derived Jacobian.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Relative perturbation</i>	Required	--	RELT 1.E-15
	Keyword Usage	Optional keyword. By default, the relative perturbation is set equal to the square root of the unit round-off error of the machine.		
	Reactor Models	• Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR		
RE-OR Reactor Property	The option may be used when the TRCE (p. 337) option is in effect. Using TRCE (p. 337) , the conservation equation for the last species in the gas-phase and each surface and bulk phase is not solved: the last species concentration (mass fraction or site fraction) is chosen so that the fractions sum to one. The REOR (p. 291) option causes TRCE (p. 337) to choose dynamically and locally (at each mesh point and in each phase) the species of largest concentration and not solve its conservation equation.			
	Keyword Usage	Optional keyword. By default, the last species in each phase is chosen.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
RHO1 Reactor Property	Mass density before the incident shock.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Mass density</i>	Required	gm/cm ₃	RHO1 1.E-4
	Keyword Usage	Optional keyword. The shock velocity and any two of temperature, pressure, or density must be specified for conditions before the incident shock. See also T1 (p. 319) and P1A (p. 257) .		
	Reactor Models	• Normal Incident Shock • Normal Reflected Shock		
RHO2 Reactor Property	Mass density after the incident shock.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Mass density</i>	Required	g/cm ₃	RHO2 1.E-4

Keyword	Definition			
	Keyword Usage	Optional keyword. Any two of temperature, pressure, or density must be specified for conditions after the incident shock. See also T2 (p. 319) and P2A (p. 257) .		
	Reactor Models	• Normal Incident Shock • Normal Reflected Shock		
RHO3	Mass density after the reflected shock.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Mass density	Required	g/cm ³	RHO3 1.E-4
	Keyword Usage	Optional keyword. Any two of temperature, pressure, or density must be specified for conditions after the reflected shock. See also T3 (p. 319) and P3A (p. 257) .		
	Reactor Models	• Normal Reflected Shock		
RL-GAS	This optional keyword is used to turn the real gas model on or off. Setting the option value to 1 will activate the real gas model if the gas reaction mechanism contains the real gas data. A value of 0 = turn OFF the real gas model and 1= turn ON the model.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Enabled	Required	g/cm ³	RLGAS 1
	Keyword Usage	Optional keyword. By default, the real gas model is turned OFF.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Partially Stirred Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Flame-Extinction Simulator • Honeycomb Reactor • IC HCCI Engine • Multi-Zone HCCI Engine Simulator • Normal Incident Shock • Normal Reflected Shock • Partially Stirred Reactor (PaSR)		

Keyword	Definition			
		• Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plug Flow Reactor • Rotating Disk CVD Reactor • SI Engine Zonal Simulator • Stagnation Flow CVD Reactor		
RL-MIX Reactor Property	This optional keyword will activate the selected real gas mixing rule if the real gas model is turned on (by RLGAS). A value of 0 = use the Van der Waals mixing rule and 1 = use the pseudocritical method (see Real Gas Data (p. 41)).			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Method</i>	Required	None	RLMIX 0
	Keyword Usage	Optional keyword. By default, the van der Waals method will be applied.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Partially Stirred Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Flame-Extinction Simulator • Honeycomb Reactor • IC HCCI Engine • Multi-Zone HCCI Engine Simulator • Normal Incident Shock • Normal Reflected Shock • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plug Flow Reactor • Rotating Disk CVD Reactor • SI Engine Zonal Simulator • Stagnation Flow CVD Reactor		

Keyword	Definition			
ROP Output	Inclusion of this keyword causes the rate-of-production coefficients to be printed for specified species. The keyword must be followed by one or more names of species. If any ROP (p. 294) keywords are used, all the rate-of-production coefficients will be computed and written to the XML Solution File (for example, XMLdata.zip). However, only those specified by the ROP (p. 294) keyword will be printed in the diagnostic output file. More than one species may be entered per line. If the line is blank after the ROP (p. 294) keyword, then all rate-of-production contributions are computed and written to the XML Solution File, but none are printed.			
	Keyword Usage	Optional keyword. By default, no rate-of-production values are computed.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Closed Multiphase Reactor • Honeycomb Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Multiphase PSR • Plug Flow Reactor • SI Engine Zonal Simulator		
	Notes	• This keyword can be added but not removed from a continuation run. • Rates of production can be calculated for other Reactor Models through the graphical Ansys Chemkin Post-processor		
RPM	Revolutions per minute of the engine crank arm.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Revolutions per minute</i>	Required	rpm	RPM 1200
	Keyword Usage	Optional keyword. By default, the rpm is 1500.		
	Reactor Models	• IC HCCI Engine • SI Engine Zonal Simulator		

Keyword	Definition			
RRAD Reactor Property	Ratio of the upper radiating disk radius to the separation distance between it and the lower substrate. This is used in calculating a surface radiation balance. RRAD (p. 295) is used only if the disk temperature is being calculated by including keyword RADB (p. 286) . See Equation 15.18 of the Chemkin Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Ratio of the upper radiating disk</i>	Required	--	RRAD 3.0
	Keyword Usage	Required keyword only if RADB (p. 286) and RDSK (p. 288) are included.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
RSHK Problem Type	Inclusion of this keyword designates a reflected shock problem.			
	Keyword Usage	Required keyword. See also ISHK (p. 229) .		
	Reactor Models	• Normal Reflected Shock		
RSTR Cluster Property	Inclusion of this keyword causes Ansys Chemkin to read a solution off the XML Solution File (for example, XMLdata.zip) and begin iteration or integration on the current reactor conditions from this solution.			
	Keyword Usage	Optional keyword. By default, a solution is started from the user-specified conditions and no XML Solution File is used.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Partially Stirred Reactor (PaSR) • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • IC HCCI Engine • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor		

Keyword	Definition			
		• Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • SI Engine Zonal Simulator • Stagnation Flow CVD Reactor		
RTIM Solver	Relative tolerance for convergence of Newton iteration as it is used in the pseudo time stepping procedure for steady-state problems employing the <i>Twopnt</i> solver. Since we are not seeking accuracy in a transient solution, this convergence criteria typically does not need to be as stringent as for the Newton iteration on the actual steady-state solution.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Absolute tolerance</i>	Required	--	RTIM 1.E-3
	Keyword Usage	Optional keyword. By default, the relative tolerance is 1.E-4. See also ATIM (p. 155) .		
	Reactor Models	• Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• For a more precise definition, see the description of RTOL (p. 298).		
RTIME Reactor Property	Turn on or off solution of the residence-time equation for a plug-flow simulation.			
	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	<i>String "ON" or "OFF" to toggle the momentum equation</i>	Required	--	RTIME ON RTIME OFF
	Keyword Usage	Optional keyword. By default, the residence-time equation is solved (ON).		
	Reactor Models	• Honeycomb Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		
RTLM Solver	A different relative tolerance can be assigned to moment variables in steady-state calculations. By default, the same relative tolerance given by RTOL (p. 298) is used for all variables.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Tolerance</i>	Required	--	RTLM 1.0E-4
	Keyword Usage	Optional keyword. By default, the absolute tolerance is determined by RTOL (p. 298) .		
	Reactor Models	• Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR		
RTLS Solver	Relative tolerance used by the transient solver, DASPK, as an indicator of the accuracy desired in the solution for the sensitivity coefficients only. Generally, the sensitivity coefficients need not be solved to a great degree of accuracy, so these tolerances should be lower than the tolerances placed on the physical variables.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Relative tolerance</i>	Required	--	RTLS 1.E-2
	Keyword Usage	Optional keyword. By default, the relative tolerance is 1.E-5.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Multiphase Reactor • Closed Plasma Reactor • Honeycomb Reactor • IC HCCI Engine		

Keyword	Definition		
		• Perfectly Stirred Reactor (PSR) • Plasma PSR • Plasma Plug Flow Reactor • Multiphase PSR • Plug Flow Reactor • SI Engine Zonal Simulator	
RTOL Solver	Relative tolerance used by the solver to determine convergence and as an indicator of the accuracy desired in the physical solution. In general the value of RTOL (p. 298) roughly corresponds to the number of significant digits that should be expected from a solution. A typical value should be between 10-3 and 10-6, which would provide roughly three to six significant digits.		
	Parameters	Optional/Reqd.	Units
	Relative tolerance	Required	--
	Examples		
	RTOL 1.E-3		
	Keyword Usage	Optional keyword. The default values are: Open 0-D Reactors run in steady-state mode, Opposed-flow Flame, Premixed Laminar Burner-stabilized Flame, Premixed Laminar Flame-speed Calculation, Shear Flow Reactor: 1.E-4 Normal Incident Shock, Normal Reflected Shock, Plug Flow Reactor, Partially Stirred Reactor (PaSR), CVD: 1.E-6 Closed 0-D Reactors and Open 0-D Reactors run in transient mode: 1.E-8 See also ATOL (p. 157) .	
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Partially Stirred Reactor (PaSR) • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Normal Incident Shock	

Keyword	Definition			
		• Normal Reflected Shock • Opposed-flow Flame • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Multiphase PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • SI Engine Zonal Simulator • Stagnation Flow CVD Reactor		
SCAT Output	Request the scatter plot of a scalar to be output to the file <i>scatter.plt</i> .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Scalar (temperature or species name)</i>	Required	--	SCAT CH4
	Keyword Usage	Optional keyword. By default, no scatter plot is printed.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR)		
SCCM Inlet Property	The volumetric flow rate into the reactor for an optionally specified inlet stream, in standard cubic centimeters per minute assuming that the inlet temperature is 298.15 K and the inlet pressure is 1 atm unless a different value for TSCCM (p. 339) is provided.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Inlet stream name</i>	Optional If there is no stream name than the volumetric flow rate applies to	--	SCCM secondary_air 300

Keyword	Definition			
		the default or all defined streams.		
	Equivalent volumetric flow rate at standard conditions	Required	standard cm ³ /min	SCCM secondary_air 300
	Keyword Usage	PSRs and PaSRs: Optional keyword. If none of TAU (p. 321), FLRT (p. 208) / FPRO (p. 210), SCCM (p. 299) / SCCMPRO (p. 300) are specified or are nonzero, then a closed-system is assumed. FLRT (p. 208) / FPRO (p. 210) or SCCM (p. 299) / SCCMPRO (p. 300) is required for each INLET (p. 226) stream defined. Stagnation Flow CVD Reactors: FLRT (p. 208) / FPRO (p. 210) or SCCM (p. 299) / SCCMPRO (p. 300) or UINL (p. 347) is required for each inlet stream defined. Rotating Disk CVD Reactors: Optional keyword.		
	Reactor Models	• Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	SCCMPRO	Used to specify a transient profile or function of mass flow rate vs. time for an inlet stream, in standard cubic centimeters per minute assuming that the inlet temperature is 298.15 K and the inlet pressure is 1 atm unless a different standard temperature (TSCCM (p. 339)) is entered. The profile specified will be interpolated linearly from the SCCMPRO (p. 300) points provided.		
Inlet Property Profiles	Parameters	Optional/Reqd.	Units	Examples
	Inlet stream name	Optional If no stream name is given, the profile described by the reactant and mole	--	SCCMPRO purge 0.19 300

Keyword	Definition			
		fraction is assumed to apply to all reactors in a cluster.		
	<i>Time</i>	Required	sec (cm for flow reactors)	SCCMPRO 0.19 300
	<i>Equivalent volumetric flow rate at standard conditions</i>	Required	standard cm ³ /min	SCCMPRO 0.19 300
	Keyword Usage	PFRs and Monolith Reactors: Flow specification via one of VEL (p. 354), VDOT (p. 353), VDOTPRO (p. 353) SCCM (p. 299) SCCMPRO (p. 300) FLRT (p. 208), or FPRO (p. 210) is required. PSRs and PaSRs: Optional keyword. If none of TAU (p. 321), FLRT (p. 208) / FPRO (p. 210), SCCM (p. 299) / SCCMPRO (p. 300) are specified or are nonzero, then a closed-system is assumed. FLRT (p. 208) / FPRO (p. 210) or SCCM (p. 299) / SCCMPRO (p. 300) is required for each INLET (p. 226) stream defined. Stagnation Flow CVD Reactors: FLRT (p. 208) / FPRO (p. 210) or SCCM (p. 299) / SCCMPRO (p. 300) or UINL (p. 347) is required for each inlet stream defined. Rotating Disk CVD Reactors: Optional keyword.		
	Reactor Models	• Honeycomb Monolith Reactor • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PFR • Plasma PSR • Plug Flow Reactor • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		

Keyword	Definition		
SCLM Reactor Property	Scaling factor for the particles moments (moments method) or number density (sectional method). A non-unity value for this parameter changes the units of the (internal) solution variable for particle moments or number density. For example, setting it to 1.0E+06 results in micro-moles whereas setting it to 1.0E+09 means that it is nano-moles. A value of 1 would mean that the unit should be moles. A recommended value for typical problems is 1.0E+12. Such scaling helps preserve the positivity of the solution during numerical computation.		
	Parameters	Optional/Reqd.	Units
	Scaling factor	Required	--
	Examples	SCLM 1.0E+12	
	Keyword Usage	Optional keyword.	
SCLS Reactor Property	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Flame-Extinction Simulator • Honeycomb Monolith Reactor • IC HCCI Engine • Multi-Zone HCCI Engine Simulator • Opposed-flow Flame • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • SI Engine Zonal Simulator • Stagnation Flow Flame Simulator	
	Parameters	Optional/Reqd.	Units
	Scaling factor	Required	--
	Examples	SCLS 1.0E+12	
	Keyword Usage	Optional keyword.	

Keyword	Definition	
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Flame-Extinction Simulator • Honeycomb Monolith Reactor • IC HCCI Engine • Multi-Zone HCCI Engine Simulator • Opposed-flow Flame • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • SI Engine Zonal Simulator • Stagnation Flow Flame Simulator
SCOR Solver	Flag instructing that the transient solver, DASPK will use staggered corrector method to solve sensitivity equations. The staggered corrector method is the sensitivity method that was used in previous versions of Ansys Chemkin and is mainly provided for backwards compatibility. It is generally slower than the default sensitivity method in Chemkin (which is the staggered direct method) but sometimes can be more stable and robust than the staggered direct method.	
	Keyword Usage	Optional keyword. By default, DASPK uses staggered corrector method to solve sensitivity equations.
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR

Keyword	Definition			
		• Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator		
	Notes	• SCOR (p. 303) can be changed for a continuation run, but it cannot be removed from one.		
SCOV Output	Analyze the coverage dependence of a surface reaction, that is, create a table of effective reaction rates versus temperature. Surface coverage is assumed to be that of the bath-gas composition. The ALL (p. 149) option is the default and produces tables for every surface reaction. The NONE (p. 250) option suppresses output for all of the reactions. If reaction information is desired for only certain reactions, they may be optionally specified by their number (given in the Pre-processor output) or by typing an exact duplicate of the reaction expression (see example input).			
	Parameters	Optional/Reqd.	Units	Examples
	ALL option	Optional, default is ALL	--	SCOV ALL
	NONE option	Optional, default is ALL	--	SCOV NONE
	Surface reaction number list	Optional, default is ALL	--	SCOV 2 5
	Surface reaction expression	Optional, default is ALL	--	SCOV CH(S)+H<=>C(S,R)+H2
	Keyword Usage	Optional keyword. By default, the table output is determined by the ALL (p. 149) or NONE (p. 250) keyword.		
	Reactor Models	• Mechanism Analyzer		
SDOUT-PUT_WRITE Output	Write output data to a standard (ascii) print-out file.			
	Keyword Usage	Optional keyword. By default, solution data will be written to an ascii output file.		
	Reactor Models	• All		
SENG Output	Inclusion of this keyword causes the calculation of the first-order sensitivity coefficients, with respect to the gas-phase and surface chemistry rate constants,			

Keyword	Definition	
	for the growth rate of all bulk phases. Growth-rate sensitivities will be included in the printed output and the XML Solution File (for example, XMLdata.zip).	
	Keyword Usage	Optional keyword. By default, no sensitivity coefficients are computed. See also ASEN (p. 153) .
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Reactor • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor
	Notes	• This keyword can be added but not removed from a continuation run.
SENT Output	Calculate and store sensitivity coefficients for gas temperature with respect to reaction A-factors. See ASEN (p. 153) .	
	Keyword Usage	Optional keyword. By default, no sensitivity coefficients are computed or printed. Same as ASEN TEMP (p. 153) .
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Reactor • IC HCCI Engine • Multi-Zone HCCI Engine Simulator • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Opposed-flow Flame • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor

Keyword	Definition			
		• SI Engine Zonal Simulator • Stagnation Flow CVD Reactor		
SFAC Reactor Property	This keyword specifies that the rates of all surface reactions will be multiplied (scaled) by the factor SFAC (p. 306). This option is sometimes useful if convergence difficulties are encountered due to unusually large reaction rates. The problem would be first solved with artificially reduced reaction rates, which then can be increased in subsequent continuations or restarts until SFAC (p. 306) is one.			
	Parameters	Optional/Reqd.	Units	Examples
	Multiplier value	Required	--	SFAC 2.0
	Reactor number (PSR clusters only)	Optional If no number is given, value is assumed to apply to all reactors in a cluster.	--	SFAC 2.0 1
	Keyword Usage	Optional keyword. By default, the multiplier value is set to 1.0.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Honeycomb Reactor • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Multiphase PSR • Plug Flow Reactor • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		

Keyword	Definition			
SFLR Solver	Sometimes during the solution procedure some of the very small gas-phase mass fractions, surface site fractions, or bulk species fractions may be calculated as a slightly negative number. No solution component will be allowed to drop below the floor value specified by SFLR (p. 307) .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Minimum bounds on the solution variables</i>	Required	--	SFLR -1.E-5
	Keyword Usage	Optional keyword. By default, the minimum bounds on the solution variables is set to -1.E-4		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation		
SFMN Solver	Set the minimum bounds of the surface species concentration to a slightly negative number to allow the solver more room to search for a solution.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Minimum bound</i>	Required	--	SFMN -1.0d-06
	Keyword Usage	Optional keyword. Usable only with Particle Tracking.		
	Reactor Models	• Opposed-flow Flame • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation		
SGMAXIT Solver	This controls the maximum number of iterations the segregated solver can take per step to solve the problem. The default is 100 and you may increase this value to give the solver greater chance to solve your problem if it is very hard to solve.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Scaling factor</i>	Required	--	SGMAXIT 100
	Keyword Usage	Optional keyword.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Opposed-flow Flame		

Keyword	Definition			
		- Premixed Laminar Burner-stabilized Flame - Premixed Laminar Flame-speed Calculation		
SG-TOL Solver	Absolute tolerance criterion on gas-phase mole fractions in segregated scheme.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Absolute tolerance</i>	Required	--	SGTOL 1.0E-10
	Keyword Usage	Optional keyword. The default value is 1E-10.		
	Reactor Models	- Diffusion or Premixed Opposed-flow Flame - Opposed-flow Flame - Premixed Laminar Burner-stabilized Flame - Premixed Laminar Flame-speed Calculation		
SIDR Solver	Turns on the multi-zone SI Engine Zonal simulation with gas-phase chemistry de-activated. The number of zones is set to 2 by default. SIKN (p. 308) and SIDR (p. 308) are mutually exclusive.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Number of zones</i>	Required	--	SIDR 2
	Keyword Usage	Optional keyword.		
	Reactor Models	SI Engine Zonal Simulator		
SIKN Solver	Turns on the multi-zone SI Engine Zonal simulation with gas-phase chemistry activated. The number of zones is set to 2 by default. SIKN (p. 308) and SIDR (p. 308) are mutually exclusive.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Number of zones</i>	Required	--	SIKN 2
	Keyword Usage	Optional keyword.		
	Reactor Models	SI Engine Zonal Simulator		
SIOA Reactor Property	Specifies the crank angle when the SI Engine Zonal Simulator properties will be saved to the XML solution file.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>crank_angle</i>	Required	degree	SIOA 5.1
	Keyword Usage	Optional keyword.		
	Reactor Models	SI Engine Zonal Simulator		
SIZE Output	Use this keyword to set the data block size in bytes for the XML Solution File (for example, <i>XMLdata.zip</i>). Changing this value may affect the performance of the XML parsing routines in the graphical Ansys Chemkin Post-processor.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Data block size</i>	Required	bytes	SIZE 10000000

Keyword	Definition	
	Keyword Usage	Optional keyword. By default, the data block size is 10 MB.
	Reactor Models	• Chemical and Phase Equilibrium Calculations • Closed Homogeneous Batch Reactor • Closed Partially Stirred Reactor (PaSR) • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • IC HCCI Engine • Mechanism Analyzer • Non-reactive Gas Mixer • Normal Incident Shock • Normal Reflected Shock • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • SI Engine Zonal Simulator • Stagnation Flow CVD Reactor
SLIP Reactor Property	Use the slip velocity model to calculate axial velocity at wall when Knudsen number is large. The model calculates the axial velocity at wall as $U_{wall} = C \cdot L \cdot \left(\frac{2 - \Sigma_v}{\Sigma_v} \right) \cdot \frac{dU}{dy}$ where L is the characteristic length, U is the axial velocity, C is the multiplier, Σ_v is the tangential momentum accommodation coefficient.	

Keyword	Definition			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Multiplier</i>	Required	--	SLIP 3.0 0.9
	<i>Tangential momentum accommodation coefficient</i>	Required	--	SLIP 3.0 0.9
	Keyword Usage	Optional keyword. By default, the slip velocity model is not used.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
SOLUTION _TECHNIQUE Solver	Controls the underlying solution technique. Previous versions of Ansys Chemkin use an older and generally less robust solution method. By default, solution_technique is set to 1, which means the new and generally more robust (and for larger mechanisms often faster) technique is used. Setting solution_technique to 0 uses the older method and you should only use this if you are having convergence issues with <i>Chemkin</i> and are confident you do not have any problems with your mechanism or problem specification.			
	Keyword Usage	Optional keyword. By default, SOLUTION_TECHNIQUE is set to 1.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Reactor • IC HCCI Engine • Multi-Zone HCCI Engine Simulator • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Opposed-flow Flame • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • SI Engine Zonal Simulator		
SP	Constant pressure and entropy constraints.			

Keyword	Definition			
Problem Type	Keyword Usage	Optional keyword. Exactly one problem-type keyword must be included.		
	Reactor Models	Chemical and Phase Equilibrium Calculations		
	Notes	PS (p. 270) keyword.is equivalent.		
SPOS Solver	This keyword provides a (small positive) number that will replace any negative species mass or site fractions. The replacement is made after every successful sequence of time steps, upon adding mesh points, and on restart or continuation. SPOS (p. 311) is often helpful in starting difficult problems when the initial guess is far from the solution. SPOS (p. 311) attempts to force the transient solution away from nonphysical regions that may otherwise be entered due to bad initial conditions and badly conditioned systems.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Species mass fraction</i>	Required	--	SPOS 1.E-14
	Keyword Usage	Optional keyword. By default, no substitution is made for negative fractions during solution for all Reactor Models except for Opposed-flow Flames, where the default value is 1.E-10.		
	Reactor Models	- Diffusion or Premixed Opposed-flow Flame - Non-reactive Gas Mixer - Perfectly Stirred Reactor (PSR) - Plasma PSR - Premixed Laminar Burner-stabilized Flame - Premixed Laminar Flame-speed Calculation - Rotating Disk CVD Reactor - Stagnation Flow CVD Reactor		
SQRX Solver	A pseudo wall thermal conductivity to allow surface enthalpy production to "overflow" in the downstream direction. This keyword is useful when the reactor model fails to converge repeatedly because of stiff surface chemistry and the reactor wall temperature is not fixed. The overall enthalpy of the reactor is still conserved because this pseudo wall enthalpy flux is included in the energy equation.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Pseudo conductivity</i>	Required	--	SQRX 0.001
	Keyword Usage	Optional keyword. By default, no thermal conduction in wall is considered.		
	Reactor Models	Cylindrical Shear Flow Reactor		

Keyword	Definition			
		• Planar Shear Flow Reactor		
SRXN Output	Prints out a table of reaction rates and other pertinent information for a surface reaction. The ALL (p. 149) option is the default and produces tables for every surface reaction. The NONE (p. 250) option suppresses output for all of the reactions. If reaction information is desired for only certain reactions, they may be optionally specified by their number (given in the Pre-processor output) or by typing an exact duplicate of the reaction expression (see example input).			
	Parameters	Optional/Reqd.	Units	Examples
	ALL option	Optional, default is ALL	--	SRXN ALL
	NONE option	Optional, default is ALL	--	SRXN NONE
	Surface reaction number list	Optional, default is ALL	--	SRXN 2 5
	Surface reaction expression	Optional, default is ALL	--	SRXN CH(S)+H<=>C(S,R)+H2
	Keyword Usage	Optional keyword. By default, the table output is determined by the ALL (p. 149) or NONE (p. 250) keyword.		
	Reactor Models	• Mechanism Analyzer		
SS-DR Reactor Property	The nominal value of the Stoichiometric Scalar Dissipation Rate (SSDR). The first flamelet will be computed for this value.			
	Parameters	Optional/Reqd.	Units	Examples
	Nominal value of SSDR	Required	1/s	SSDR 1.0
	Keyword Usage	Optional keyword.		
	Reactor Models	• Diffusion Flamelet Generator		
SS-DR_MAX Reactor Property	The maximum value of the Stoichiometric Scalar Dissipation Rate (SSDR). After computing a flamelet for the nominal value (specified by keyword SSDR), continuations to SSDR_MAX are done in a number of steps as specified by keyword NSTEP_HIGH.			
	Parameters	Optional/Reqd.	Units	Examples
	Maximum value of SSDR	Optional	1/s	SSDR_MAX 100

Keyword	Definition			
	Keyword Usage	Optional keyword.		
	Reactor Models	• Diffusion Flamelet Generator		
SS-DR_MIN	The minimum value of the Stoichiometric Scalar Dissipation Rate (SSDR). After computing a flamelet for the nominal value (specified by keyword SSDR), continuations to SSDR_MIN are done in a number of steps as specified by keyword NSTEP_LOW.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Minimum value of SSDR	Optional	1/s	SSDR_MIN 0.001
	Keyword Usage	Optional keyword.		
	Reactor Models	• Diffusion Flamelet Generator		
SSSKIP	Skip the initial surface site fraction calculation.			
Solver	Keyword Usage	Optional keyword. By default, an initial solution is performed to determine the surface site fractions holding the reagent gas species constant.		
	Reactor Models	• Honeycomb Monolith Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		
SS-MAX-ITER	The maximum number of iterations per steady state search, in the steady-state solver TWOPNT. This is the maximum number of iterations that are allowed each time TWOPNT searches to find the steady state solution. Typically you will not need to change this maximum because TWOPNT will revert to its time stepping algorithm and then re-try searching for the steady state.			
Solver	Parameters	Optional/Reqd.	Units	Examples
	Maximum steady state iterations	Optional	--	SSMAXITER 120
	Keyword Usage	Optional keyword. By default, the maximum number of iterations is 100.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Premixed Laminar Burner-stabilized Flame		

Keyword	Definition			
		• Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• SSMAXITER must be >=1.		
SS-RX Solver	A pseudo diffusivity for surface species to allow them to diffuse along the wall surface in the downstream direction. This keyword is useful when the reactor model fails to converge repeatedly because of stiff surface chemistry and the reactor wall temperature is fixed. The overall mass and element conservations of the reactor are still satisfied because pseudo surface species fluxes are included in the surface species equations.			
	Parameters	Optional/Reqd.	Units	Examples
	Pseudo conductivity	Required	--	SSRX 0.0001
	Keyword Usage	Optional keyword. By default, no surface species flux on wall is considered.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
	Notes	• Typically, the value of SSRX should be kept under 0.01.		
SSTT Solver	Inclusion of this keyword indicates that the local sensitivity analysis will be performed instead of the integrated sensitivity analysis for transient or plug-flow calculations. This may be helpful in speeding up calculations of sensitivity, but we caution that the local sensitivity is less accurate than the integrated sensitivity.			
	Keyword Usage	Optional keyword. By default, the integrated sensitivity analysis will be performed for transient calculations when sensitivity data is requested.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator		

Keyword	Definition			
	Notes	• SSTT (p. 314) can be added to a continuation run, but it cannot be removed from one.		
STAG Problem Type	Specify a Stagnation Flow CVD Reactor model.			
	Keyword Usage	Required keyword. See also OMEG (p. 255) . If the keyword STAG (p. 315) is given and the spin rate OMEG (p. 255) is nonzero, then this inconsistent input will generate an error. A stagnation-point flow can also be specified by using "OMEG 0".		
	Reactor Models	• Stagnation Flow CVD Reactor		
STAG- NA- TION _FLAME Problem Type	Indicates Burner-stabilized Stagnation Flow problem type.			
	Keyword Usage	Required keyword.		
	Reactor Models	• Premixed Laminar Burner-stabilized Stagnation Flow Flame Simulator		
STCH Reactor Property	Parameter to produce a non-uniform grid. For cartesian coordinates the initial grid location for a node J is $X(J)=A*(J-1)**STCH$, where $A=HITE/(NPTS-1)**STCH$, HITE (p. 217) is the reactor height, and NPTS (p. 251) is the total number of grid nodes. If $STCH=1$, a uniform grid is produced. For $STCH > 1$, the grid is more tightly spaced at the lower boundary (cartesian-coordinates) or at the outer boundary (cylindrical coordinates), and consequently the grid is more widely spaced at the other boundary.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Cartesian coordinates</i>	Required	--	STCH 1.2
	Keyword Usage	Optional keyword. By default, the program is set to 1.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
	STCK Output	Analyzes the forward and reverse surface reaction's sticking coefficient, if applicable. The ALL (p. 149) option is the default and produces tables for every surface reaction with a sticking-coefficient formulation. The NONE (p. 250) option suppresses output for all of the reactions. If reaction information is desired for only certain reactions, they may be optionally specified by their number (given in the Pre-processor output) or by typing an exact duplicate of the reaction expression (see example input).		
Parameters		Optional/Reqd.	Units	Examples
<i>ALL option</i>		Optional, default is ALL	--	STCK ALL

Keyword	Definition			
	<i>NONE option</i>	Optional, default is ALL	--	STCK NONE
	<i>Surface reaction number list</i>	Optional, default is ALL	--	STCK 2 5
	<i>Surface reaction expression</i>	Optional, default is ALL	--	STCK CH(S)+H<=>C(S,R)+H2
	Keyword Usage	Optional keyword. By default, the table output is determined by the ALL (p. 149) or NONE (p. 250) keyword.		
	Reactor Models	• Mechanism Analyzer		
STP0 Solver	Initial time step size used by the steady-state solver <i>Twopnt</i> during the initial calculation for the surface conditions at the inlet.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Initial time step</i>	Required	cm	STP0 1.0E-7
	Keyword Usage	Optional keyword. By default, the initial time step is 1.0E-6.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
STPT Solver	The maximum internal time step for the solver in transient calculations. STPT (p. 316) determines the largest time-step the transient solver can take at one time and thereby controls the resolution for interpolation of specified time-profiles.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Time step</i>	Required	sec	STPT 1.0E-4
	<i>Aurora Usage</i>	Optional keyword. If not specified, then If either DELT (p. 182) or DTSV (p. 188) are specified, STPT (p. 316) is set to the smallest of these values. If neither DELT (p. 182) nor DTSV (p. 188) are specified, then STPT (p. 316) is set to the value of the end time divided by 100.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Closed Multiphase Reactor • IC HCCI Engine		

Keyword	Definition			
		• Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • Multiphase PSR • SI Engine Zonal Simulator		
	Notes	• See also: DELT (p. 182) and DTSV (p. 188) keywords.		
STST Reactor Property	The solution will be obtained using a steady-state calculation (with the solver <i>Twopnt</i>) rather than a transient calculation (using the solver <i>DASPK</i>).			
	Keyword Usage	Optional keyword. By default, a steady-state calculation is performed.		
	Reactor Models	• Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• Exclusive toggle with TRAN (p. 336) .		
SURF Reactor Property	Initial values (transient) or estimates (steady-state) for the surface site fraction values for the surface species on each surface site type (surface phase).			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Surface species name</i>	Required	--	SURF Ga(s) 0.001
	<i>Surface fractions</i>	Required	site fractions	SURF Ga(s) 0.001
	Keyword Usage	Optional keyword. By default, the initial or estimated surface-site fractions are 0.0.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Honeycomb Reactor • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor		

Keyword	Definition			
		• Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• The sum of the site fractions should equal one for each surface site type (phase). However, if they do not, a cautionary message will be printed and the site fractions for each surface site type will be normalized so the sum does equal one.		
SVS0	Specify the reference gas viscosity at the reference temperature of the Sutherland's-law for viscosity.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Reference gas viscosity at reference temperature	Required.	g/cm-s	SVS0 1.716E-4
	Keyword Usage	Optional.		
	Reactor Models	• Multi-Zone HCCI Simulator • IC HCCI Engine • SI Engine Zonal Simulator		
SVSS	Specify the Sutherland temperature of the Sutherland's-law for viscosity.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Sutherland temperature	Required.	K	SVSS 114.0
	Keyword Usage	Optional.		
	Reactor Models	• Multi-Zone HCCI Simulator • IC HCCI Engine • SI Engine Zonal Simulator		
SVST	Specify the reference temperature of the Sutherland's-law for viscosity.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Reference temperature	Required.	K	SVST 273.15
	Keyword Usage	Optional.		

Keyword	Definition	
	Reactor Models	- Multi-Zone HCCI Simulator - IC HCCI Engine - SI Engine Zonal Simulator
SYMT Reactor Property	Keyword for temperature boundary condition on the upper wall (only used for non-symmetric cartesian coordinates). The upper wall temperature is set equal to the bottom wall temperature if SYMT (p. 319) is specified.	
	Keyword Usage	Optional keyword. By default, an adiabatic top wall is used.
	Reactor Models	Planar Shear Flow Reactor

10.4. Alphabetical Listing of Keywords [T-Z]

Table 10.4: Alphabetical Listing of Keywords [T-Z]

Keyword	Definition			
T1 Reactor Property	Temperature before the incident shock.			
	Parameters	Optional/Reqd.	Units	Examples
	Temperature	Required	K	T1 300.
	Keyword Usage	Optional keyword. The shock velocity and any two of temperature, pressure, or density must be specified for conditions before the incident shock. See also P1A (p. 257) and RHO1 (p. 291) .		
	Reactor Models	• Normal Incident Shock • Normal Reflected Shock		
T2 Reactor Property	Temperature after the incident shock.			
	Parameters	Optional/Reqd.	Units	Examples
	Temperature	Required	K	T2 1500.
	Keyword Usage	Optional keyword. Any two of temperature, pressure, or density must be specified for conditions after the incident shock. See also RHO2 (p. 291) and P2A (p. 257) .		
	Reactor Models	• Normal Incident Shock • Normal Reflected Shock		
T3 Reactor Property	Temperature after the reflected shock, given as T_5 in the equations.			
	Parameters	Optional/Reqd.	Units	Examples
	Temperature	Required	K	T2 1500.

Keyword	Definition			
	Keyword Usage	Optional keyword. Any two of temperature, pressure, or density must be specified for conditions after the reflected shock. See also RHO3 (p. 292) and P3A (p. 257) .		
	Reactor Models	• Normal Reflected Shock		
TAMB Reactor Property	Ambient temperature for convective or conductive heat transfer out of the system. This keyword is only relevant when the energy equation is being solved.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Optional. If no material is specified, the same value will be used for all materials.	--	TAMB material1 298
	Ambient temperature	Required	K	TAMB 298
	Reactor number (PSR clusters only)	Optional. If no number is given, the keyword is assumed to apply to all reactors in a cluster.	--	TAMB material1 298 1
	Keyword Usage	Optional keyword. This keyword must be used with HTC (p. 219) .		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Monolith Reactor • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • Plasma Plug Flow Reactor		

Keyword	Definition			
		• Multiphase PSR • Plug Flow Reactor		
TAU Reactor Property	The nominal residence time of the gas in the reactor when flow is present.			
	Parameters	Optional/Reqd.	Units	Examples
	Nominal residence time	Required	sec	TAU 1.E-3
	Reactor number (PSR clusters only)	Optional If no number is given, the keyword is assumed to apply to all reactors in a cluster.	--	TAU 1.E-3 1
	Keyword usage	PSRs: Optional keyword. If none of TAU (p. 321), FLRT (p. 208) / FPRO (p. 210), SCCM (p. 299) / SCCMPRO (p. 300) are specified or are nonzero, then a closed-system is assumed. FLRT (p. 208) / FPRO (p. 210) or SCCM (p. 299) / SCCMPRO (p. 300) is required for each INLET (p. 226) stream defined. PaSRs: Optional keyword. Unless the CLSE (p. 170) keyword is used, any two of FLRT (p. 208), STPT (p. 316) and reactor volume (VOL (p. 359)) are required.		
	Reactor Models	• Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Plasma PSR		
TBND Solver	The upper boundary for gas temperature. Setting TBND (p. 321) to the upper limit of thermodynamic data can prevent the Gas-phase Kinetics Pre-processor from getting erratic thermal data by extrapolating the fitting polynomials.			
	Parameters	Optional/Reqd.	Units	Examples
	Upper boundary	Required	K	TBND 10000.
	Keyword Usage	Optional keyword. By default, the upper boundary is 5000.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Diffusion of Premixed Opposed-flow Flame		

Keyword	Definition			
		• Honeycomb Reactor • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
TBTH Reactor Property	Set the bath gas temperature in Kelvin. This temperature is used wherever a single temperature is needed. The default is 298.15 K.			
	Parameters	Optional/Reqd.	Units	Examples
	Bath gas temperature	Required	K	TBTH 900.
	Keyword Usage	Optional keyword. By default, the bath gas temperature is 298.15.		
	Reactor Models	• Mechanism Analyzer		
TDIF Reactor Property	Include thermal diffusion (Soret effect) in the transport calculations.			
	Keyword Usage	Optional keyword. By default, thermal diffusion is not included.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Planar Shear Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
TDEL Reactor Property	Set the temperature increment in all tables where the temperature is varied.			
	Parameters	Optional/Reqd.	Units	Examples
	Temperature	Required	K	TDEL 200.
	Keyword Usage	Optional keyword. By default, the temperature step is 100 K.		
	Reactor Models	• Mechanism Analyzer		

Keyword	Definition			
TDSK Reactor Property	Temperature of the deposition surface. This is a constant value taken as a boundary condition, unless the keyword RADB (p. 286) is given, indicating that the susceptor or disk temperature is calculated from an energy balance. If RADB (p. 286) is specified, TDSK (p. 323) is taken as the initial guess for the susceptor temperature.			
	Parameters	Optional/Reqd.	Units	Examples
	Surface temperature	Required	K	TDSK 1200
	Keyword Usage	Required keyword.		
	Reactor Models	- Rotating Disk CVD Reactor - Stagnation Flow CVD Reactor		
TEBND Reactor Property	The upper boundary for electron temperature. Can be useful for preventing non-plasma solutions in steady state problems.			
	Parameters	Optional/Reqd.	Units	Examples
	Upper boundary	Required	K	TEBND 8000
	Keyword Usage	Optional keyword. By default, the upper boundary is 200000 K (roughly 20 eV).		
	Reactor Models	- Closed Plasma Reactor - Plasma PSR - Plasma Plug Flow Reactor		
TEIN Inlet Property	Electron temperature in the inlet stream. For most cases, there are no free electrons in the inlet stream, in which case the electron inlet temperature is not used.			
	Parameters	Optional/Reqd.	Units	Examples
	Electron temperature	Required	K	TEIN 300.
	Keyword Usage	Optional keyword. By default, the electrons have the same temperature as the inlet gas.		
	Reactor Models	Plasma PSR		
TEMP Reactor Property	The reactor gas temperature. Depending on the Reactor Model and problem type, this is either the user-supplied temperature constraint (TGIV (p. 326)), an initial estimate of the temperature (ENRG (p. 194)), or the initial reactor temperature (for transient cases). See also TPRO (p. 334) .			
	Parameters	Optional/Reqd.	Units	Examples
	Reactor gas temperature	Required	K	TEMP 1000.
	Bulk name (multiphase reactors only)	Optional	--	TEMP Gas 300.0
	Reactor number (PSR clusters only)	Optional If no number	--	TEMP 1000. 1

Keyword	Definition			
		is given, the keyword is assumed to apply to all reactors in a cluster.		
	Keyword Usage	Required keyword. For the multiphase reactors, the keyword is effective for the phase name following the keyword. The name of the bulk phase should be used. "Gas" indicates the gas phase.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations • Closed Homogeneous Batch Reactor • Closed Partially Stirred Reactor (PaSR) • Closed Plasma Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Multiphase PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • SI Engine Zonal Simulator • Stagnation Flow CVD Reactor		

Keyword	Definition			
	Notes	• In previous versions, TINI keyword was used for some Reactor Models.		
TEST	Specifies an estimate of the equilibrium temperature.			
	Parameters	Optional/Reqd.	Units	Examples
	Temperature	Required	K	TEST 2000
	Keyword Usage	Optional keyword. May help convergence to the equilibrium temperature, or assure an appropriate equilibrium temperature is calculated when a second, trivial solution exists (for example, for adiabatic flame-temperature calculations).		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
TEXP	Specifies the average/cylinder temperature that defines the start of the expansion period. This keyword has a lower priority than QEXP (p. 280) .			
	Parameters	Optional/Reqd.	Units	Examples
	temperature	Required	K	TEXP 1150.0
	Keyword Usage	Optional keyword. Default = 1000K.		
	Reactor Models	• Multi-Zone HCCI Simulator • IC HCCI Engine • SI Engine Zonal Simulator		
TFAL	Analyze the fall-off of a gas-phase reaction with respect to changes in the temperature, that is, create a table of reaction rates versus temperature at a constant pressure. The pressure and gas composition are assumed to be that of the bath gas. The ALL (p. 149) option is the default and produces tables for every gas-phase reaction. The NONE (p. 250) option suppresses output for all of the reactions. If reaction information is desired for only certain reactions, they may be optionally specified by their number (given in the Pre-processor output) or by typing an exact duplicate of the reaction expression (see example input).			
	Parameters	Optional/Reqd.	Units	Examples
	ALL option	Optional, default is ALL	--	TFAL ALL
	NONE option	Optional, default is ALL	--	TFAL NONE
	Gas reaction number list	Optional, default is ALL	--	TFAL 2 5

Keyword	Definition			
	<i>Gas reaction expression</i>	Optional, default is ALL	--	TFAL 2CH3(+M)<=>C2H6(+M)
	Keyword Usage	Optional keyword. By default, the table output is determined by the ALL (p. 149) or NONE (p. 250) keyword.		
	Reactor Models	• Mechanism Analyzer		
TFIX Reactor Property	When solving a freely propagating adiabatic flame (FREE (p. 211)), the problem is posed in a flame-fixed coordinate system. In this case the flame speed becomes an eigenvalue. Therefore, an additional constraint is required. Ansys chooses to supply this additional condition by fixing the temperature at one point in the flame, and this input allows the specification of that fixed temperature. Given the fixed temperature, the flame position is determined from the initial temperature profile as specified by the TPRO (p. 334) or TPROF inputs. If the fixed temperature is not one of the temperatures specified in the input, then a linear interpolation of the temperature profile to determine the position of TFIX (p. 326) is used and a mesh point added at that point.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Temperature</i>	Optional.	K	TFIX 500.
	Keyword Usage	Optional keyword. With TPROF, default is the average of unburned gas temperature (TUNBURNT) and mixture equilibrium temperature. With TPRO, the default is the average of the first and last Temperature profile values.		
	Reactor Models	• Premixed Laminar Flame-speed Calculation		
	Notes	• This keyword can be changed for a restart run.		
TGIV Problem Type	Do not solve the gas energy equation, but will instead use a fixed user-supplied temperature (see TEMP (p. 323)).			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Reactor number (PSR clusters only)</i>	Optional If no number is given, the keyword is assumed to apply to all reactors in a cluster.	--	TGIV 2
	<i>Reactor number (PSR clusters only)</i>	Optional.	--	TGIV catalyst

Keyword	Definition			
	<i>Bulk name</i>	Optional	--	TGIV Gas
	Keyword Usage	Optional keyword. Either TGIV (p. 326) or ENRG (p. 194) must be specified, unless CONP (p. 175) , CONV (p. 175) , or COTV (p. 176) problem-types are specified for a closed system. For the multiphase reactors, the keyword is effective for the phase name following the keyword. The name of the bulk phase should be used. "Gas" indicates the gas phase.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Diffusion or Premixed Opposed-flow Flame • Non-reactive Gas Mixer • Honeycomb Reactor • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Multiphase PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• This keyword can be removed or added for a restart run.		
THIG	Set the upper limit of the temperature range (K) in all tables where the temperature is varied. The default is 1500 K.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Temperature</i>	Required	K	THIG 298.15
	Keyword Usage	Optional keyword. By default, the high temperature is 1500.		
	Reactor Models	• Mechanism Analyzer		
THRM	Prints out individual thermodynamics tables for the species in the mechanism. The default is ALL (p. 149) , which generates the tables for all species in the mechanism. The GAS, SUR, and BULK options will cause thermodynamic tables for only species in the specified phase to be printed. Listing individual species by their name or by their number (as listed in the <i>Gas-phase Kinetics</i> or <i>Surface Kinetics</i> Pre-processor output files) will generate			
Output				

Keyword	Definition			
	thermodynamic tables for the specified species. The keyword NONE (p. 250) will suppress all of the species thermodynamic tables.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>ALL option</i>	Optional	--	THRM ALL
	<i>NONE option</i>	Optional	--	THRM NONE
	<i>GAS option</i>	Optional	--	THRM GAS
	<i>SUR option</i>	Optional	--	THRM SUR
	<i>BULK option</i>	Optional	--	THRM BULK
	<i>Species name</i>	Optional	--	THRM CH4
	<i>Species number</i>	Optional	--	THRM 3
	Keyword Usage	Optional keyword. By default, the table output is determined by the ALL (p. 149) or NONE (p. 250) keyword.		
Reactor Models	• Mechanism Analyzer			
TIFP Output	Calculate the ignition delay as the time when the slope of the temperature profile reaches its maximum value. You need to use sufficient number of time points to obtain an accurate temperature profile. Only applicable when you are solving the energy equation with the transient solver.			
	Keyword Usage	Optional keyword. See also TLIM (p. 333) and DTIGN (p. 186) .		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Monolith Reactor • -IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator		
TIM1 Solver	For the steady-state solver, <i>Twopnt</i> , if the Newton method fails to converge, then the application takes some pseudo time steps in order to bring the current iterate within the domain of convergence of Newton’s method. This input specifies how many time steps to take and the initial size of the time step, for the initial fixed-temperature calculation.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Number of time steps</i>	Required	--	TIM1 50 3.E-7

Keyword	Definition			
	<i>Initial size of time step</i>	Required	sec	TIM1 50 3.E-7
	Keyword Usage	Optional keyword. By default, the number of time steps is 100 and the initial size of the time step is 1.E-6. See also TIM2 (p. 329) .		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• In previous versions, TIME (p. 330) keyword was used.		
TIM2 Solver	For the steady-state solver, <i>Twoptn</i> , if the Newton method fails to converge, then the application takes some pseudo time steps in order to bring the current iterate within the domain of convergence of Newton's method. This input specifies how many time steps to take and the initial size of the time step, when the energy equation is being solved.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Number of time steps</i>	Required	--	TIM2 50 3.E-7
	<i>Initial size of time step</i>	Required	sec	TIM2 50 3.E-7
	Keyword Usage	Optional keyword. By default, the number of time steps is 100 and the initial size of the time step is 1.E-6. See also TIM1 (p. 328) .		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor		

Keyword	Definition			
		• Stagnation Flow CVD Reactor		
	Notes	• This input is only used when ENRG (p. 194) or ENGE (p. 193) is included.		
TIME Solver	The total integration time for the transient simulation. If the job is a continuation run and the keyword CNTT (p. 173) is specified, the final time value will be the starting time plus the value of TIME (p. 330) .			
	Parameters	Optional/Reqd.	Units	Examples
	Total integration time	Required	sec	TIME 1.0E-2
	Keyword Usage	Required keyword, except in case of IC HCCI Engine, where NREV (p. 252) can be specified instead.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Partially Stirred Reactor (PaSR) • Closed Plasma Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Normal Incident Shock • Normal Reflected Shock • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Plasma PSR • Multiphase PSR • Rotating Disk CVD Reactor • SI Engine Zonal Simulator • Stagnation Flow CVD Reactor		
	Notes	• See also CNTT (p. 173) keyword.		
TINF Reactor Property	Ambient temperature of the external environment, used for certain heat-transfer options.			
	Parameters	Optional/Reqd.	Units	Examples
	ambient temperature	Required	K	TINF 500
	Keyword Usage	Shear Flow Reactors: Optional keyword. Only used if HTRN (p. 220) option is included. By default, the inlet gas		

Keyword	Definition			
		temperature is used for the ambient temperature (TINL (p. 331)). Premixed and Diffusion Flames: Optional keyword. Only used if the user subroutine QFUN (p. 280) is enabled.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Planar Shear Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation		
TINL	The inlet temperature for an inlet stream.			
Inlet Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Inlet stream name (for PSRs and CVD Reactors only)</i>	Optional If there is no stream name than the inlet temperature applies to all streams.	--	TINL secondary_air 400
	<i>Inlet temperature</i>	Required	K	TINL 400
	Keyword Usage	Required for each inlet stream when then energy equation will be solved.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Non-reactive Gas Mixer • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• In previous versions, TFUE, TOXI, TINF, and GTMP keywords were used.		

Keyword	Definition			
TINL Reactor Property	The temperature of the stagnation plane.			
	Parameters	Optional/Reqd.	Units	Examples
	Stagnation plane name	Optional If there is no stream name than the inlet temperature applies to all streams.	--	TINL StagPlane 600
	Stagnation plane temperature	Required	K	TINL 600
	Keyword Usage	Required for each stagnation plane when then energy equation will be solved.		
	Reactor Models	• Burner-stabilized Stagnation Flow Reactor		
TION Reactor Property	Specified temperature of ions. In this version of the software, there is no separate energy balance that accounts for ion energy gain above the gas temperature. The ions may, however, be much hotter than the neutral species, and this is accounted here as an additional energy loss from the deposited power required to heat the ions to the assumed temperature.			
	Parameters	Optional/Reqd.	Units	Examples
	Specified temperature of ions	Required	K	TION 11500.
	Reactor number (PSR clusters only)	Optional If no number is given, the value is assumed to apply to all reactors in a cluster.	--	TION 11500.1
	Keyword Usage	Optional keyword. By default, the ions have the same temperature as the neutral gas.		
	Reactor Models	• Closed Plasma Reactor • Plasma Plug Flow Reactor		

Keyword	Definition			
		• Plasma PSR		
TJAC Solver	For the steady-state solver <i>TwoPnt</i> , specifies the maximum number of Newton steps that can be taken in performing the pseudo time-stepping before a new Jacobian is evaluated. If TJAC=1, then a full Newton method will result.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Retirement age</i>	Required	--	TJAC 15
	Keyword Usage	Optional keyword. By default, the retirement age is set at 20.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • Planar Shear Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
TLIM Output	For all transient problems in which the temperature is allowed to vary, an "ignition time" is computed, which is defined as the time or distance when the temperature first reaches a value equal to TLIM (p. 333) .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Ignition temperature</i>	Required	K	TLIM 500
	Keyword Usage	Optional keyword. See also DTIGN (p. 186) .		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Monolith Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Plasma PSR • Plasma Plug Flow Reactor		

Keyword	Definition			
		• Plug Flow Reactor • SI Engine Zonal Simulator		
TLOW Reactor Property	Set the lower limit of the temperature range (K) in all tables where the temperature is varied. The default is 300 K.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Temperature</i>	Required	K	TLOW 100.
	Keyword Usage	Optional keyword. By default, the low temperature is 300 K.		
	Reactor Models	• Mechanism Analyzer		
TMAX Reactor Property	Maximum temperature for use with profiles defined by the LINE (p. 233) or PLAT (p. 261) options.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Maximum temperature</i>	Required	K	TMAX 2500.
	Keyword Usage	Optional keyword. By default, the maximum temperature is set at 2200 K.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame		
TOFF Reactor Property	This keyword is used to tell the <i>TwoPnt</i> solver to ignore the temperature when adapting the grid. This can be useful for strained flames, since the temperature gradients can be very steep and, without this option, too many points will be placed in the same place without improving the solution. The flame can be well resolved by basing adaptation only on the species and velocity profiles.			
	Keyword Usage	Optional keyword. By default, the temperature is considered during adaptation.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
TP Problem Type	Constant pressure and temperature constraint.			
	Keyword Usage	Optional keyword. Exactly one problem-type keyword must be included.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
	Notes	• PT keyword is equivalent.		
TPRO Reactor Property Profiles	Reactor gas temperature profile specified as a function of time for transient 0-D homogeneous systems or as a function of distance for channel-flow reactors or reactors where there is a constrained temperature. For 1-D steady-state Reactor Models where the energy equation is being solved, TPRO (p. 334) is used to specify an initial temperature profile estimate.			
	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	<i>Time or Distance value, depending on Reactor Model</i>	Required	sec or cm	TPRO 1.0E-4 1000
	<i>Gas Temperature</i>	Required	K	TPRO 1.0E-4 1000
	<i>Reactor number (PSR clusters only)</i>	Optional If no number is given, the profile described by the first two values is assumed to apply to all reactors in a cluster.	--	TPRO 1.0E-4 1000 1
	Keyword Usage	Optional keyword. By default, no profile is provided.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Multiphase PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor		

Keyword	Definition			
		• Stagnation Flow CVD Reactor		
TPROF Reactor Property	Reactor gas temperature profile estimated as a function of distance for flame speed simulator and pre-mixed burner simulator with the energy equation being solved. It uses unburned gas temperature and mixture equilibrium temperature as corresponding upper and lower bounds. When TPROF (p. 336) is used, user-specified values of estimated center position (XCEN (p. 367)), estimated zone width (WMIX (p. 364)), and optional temperature constraint (TFIX (p. 326)) are ignored and pre-defined values are used. When TPROF (p. 336) is used with no NPTS (p. 251) , a default non-linear 12-point grid is initialized, while TPROF (p. 336) with NPTS (p. 251) initializes a linear NPTS-point grid.			
	Keyword Usage	Optional keyword.		
	Reactor Models	• Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation		
TPRO-FILE_n Reactor Property	Choice for the initial temperature profile. Integer n can be 1 or 2. Option 1 means a dumped energy profile (that is, all internal grid-points at specified maximum temperature) and option 2 means a linear profile from the boundary to grid-point where mixture fraction value is stoichiometric.			
	Keyword Usage	Required keyword. The default value is TPROFILE_1.		
	Reactor Models	• Diffusion Flamelet Generator		
TRAD Reactor Property	Temperature of a radiating disk located above and parallel to the substrate, used in calculating a surface radiation balance. A hot radiating disk may be included in addition to a cool "wall" (TWAL (p. 345)), to represent, for example, a burner inlet. The geometry and location of the radiating disk are controlled by keywords RDSK (p. 288) and RRAD (p. 295) . TRAD (p. 336) is used only if the disk temperature is being calculated by including keyword RADB (p. 286) . See Equation 15.18 of the Chemkin Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	Temperature of a radiating disk	Required	K	TRAD 2500.
	Keyword Usage	Optional keyword. By default, the temperature of a radiating disk is 1000 K.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	TRAN Solver	Perform a transient calculation instead of a steady-state calculation. For flame simulators, this input also specifies how many time steps to take and the initial size of the time step. Perform a transient calculation (with the solver DASPK) instead of a steady-state calculation (using the solver <i>Twopnt</i>).		
Keyword Usage		Required keyword for Closed Homogeneous Batch Reactor, Closed Plasma Reactor, and the IC HCCI Engine. Otherwise, a steady-state calculation is performed by default.		
Reactor Models		• Closed Homogeneous Batch Reactor		

Keyword	Definition			
		• Closed Plasma Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor • Diffusion or Premixed Opposed-flow Flame • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • SI Engine Zonal Simulator		
	Notes	• See also STST (p. 317).		
TRAN Output	Prints out the transport database properties (intermolecular potential parameters) for each gas-phase species in the mechanism. This feature also expands the thermo table to create a table of transport properties as a function of temperature. The NONE (p. 250) option turns off printing of this table. The <i>Transport</i> Pre-processor must have been run successfully, unless the NONE (p. 250) option is used.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>ALL option</i>	Optional	--	TRAN ALL
	<i>NONE option</i>	Optional	--	TRAN NONE
	Keyword Usage	Optional keyword. By default, the table output is determined by the ALL (p. 149) or NONE (p. 250) keyword.		
	Reactor Models	• Mechanism Analyzer		
TRCE Reactor Property	Including this keyword causes the calculation to be run by setting the mass fraction of the last-named <i>Gas-phase Kinetics</i> gas-phase species (or when REOR (p. 291) is used, the species with the largest concentration) to be one minus the sum of the mass fractions of the other species. A conservation equation is not solved for the last (or largest-concentration) species.			
	Keyword Usage	Optional keyword. By default, correction velocity formalism is used.		
	Reactor Models	• Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor		

Keyword	Definition			
		• Stagnation Flow CVD Reactor		
	Notes	• This keyword can be removed or added for a restart run.		
TRES	Assigns a new initial time for a calculation that starts using the solution read from an XML Solution File.			
Restart	Parameters	Optional/Reqd.	Units	Examples
	Initial time	Required	sec	TRES 0.0
	Keyword Usage	Optional keyword. By default, the value of time found on the XML Solution File will be used.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Partially Stirred Reactor (PaSR) • Closed Plasma Reactor • IC HCCI Engine • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Plasma PSR • SI Engine Zonal Simulator		
TRMAX-ITER	The maximum number of iterations time step in TWOPNT's time stepping algorithm. If TWOPNT exceeds this maximum, then it will cut its time step and try again. You may occasionally need to use this option is the time stepping algorithm is having difficulty solving your problem.			
Solver	Parameters	Optional/Reqd.	Units	Examples
	Maximum iterations per time step	Optional	--	TRMAXITER 50
	Keyword Usage	Optional keyword. By default, the maximum number of iterations is 25.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Premixed Laminar Burner-stabilized Flame		

Keyword	Definition			
		- Premixed Laminar Flame-speed Calculation - Rotating Disk CVD Reactor - Stagnation Flow CVD Reactor		
	Notes	TRMAXITER must be >=1.		
TRST	Tells the application which time value in an XML Solution File to use for the initial conditions of the current calculation.			
Restart	Parameters	Optional/Reqd.	Units	Examples
	Time value	Required	sec	TRST 1.0E-5
	Keyword Usage	Optional keyword. By default, the last time value found on the XML Solution File will be used.		
	Reactor Models	- Closed Homogeneous Batch Reactor - Closed Plasma Reactor - Honeycomb Reactor - IC HCCI Engine - Perfectly Stirred Reactor (PSR) - Plasma Plug Flow Reactor - Plasma PSR - Plug Flow Reactor - SI Engine Zonal Simulator		
TS	Constant entropy and temperature constraints.			
Problem Type	Keyword Usage	Optional keyword. Exactly one problem-type keyword must be included.		
	Reactor Models	Chemical and Phase Equilibrium Calculations		
	Notes	ST keyword is equivalent.		
TSCCM	Sets the standard reference temperature used to define the flow rate when it is input in standard cubic centimeters per minute (sccm), that is, when SCCM (p. 299) or SCCMPRO (p. 300) keywords are used.			
Inlet Property	Parameters	Optional/Reqd.	Units	Examples
	Standard temperature	Required	K	TSCCM 300
	Keyword Usage	Optional keyword. By default, the reference temperature is set to 298.15 K.		

Keyword	Definition			
	Reactor Models	• Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
TS-FAC Reactor Property/Model	The maximum liquid/droplet temperature allowed to prevent issues from liquid property evaluation. This maximum temperature value is specified as a fraction of the lowest critical temperature of the liquid component.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Temperature change</i>	Required	K	TSFAC 5.0
	Keyword Usage	Optional keyword. Default is 1 K.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
TS-PL Reactor Property Profiles	This keyword allows an optional specification of a spline-fit surface temperature profile of the lower wall for planar non-symmetric cases or otherwise the surface temperature profile of the upper wall. The data point describing the surface temperature profile is formatted as an (x, T) pair. There is a TSPL (p. 340) keyword line for each desired (x, T) pair. The x coordinates of each TSPL (p. 340) line must be given in ascending order. A spline fit is used to interpolate between points.			
	Parameters	Optional/Reqd.	Units	Examples
	x coordinate	Required	cm	TSPL 0.1 973
	T coordinate	Required	K	TSPL 0.1 973
	Keyword Usage	Optional keyword. By default, for symmetric cases default is specified constant temperature; for non-symmetric cases the wall is adiabatic.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
	Notes	• See also: TPRO (p. 334).		
TS-RF Reactor Property	The temperature of the surfaces in the reactor. Use only if you want the surface temperature, which controls the surface chemistry rates, to be different than the gas temperature.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Material (for 0-D homogeneous and plug-flow reactors only)</i>	Optional If not specified, then the temperature	--	TSRF WAFER 1200.

Keyword	Definition			
		is the same for all materials.		
	Surface temperature	Required	K	TSRF 1200.
	Reactor number (PSR clusters only)	Optional If no number is given, the value is assumed to apply to all reactors in a cluster.	--	TSRF 1200. 1
	Keyword Usage	Closed Homogeneous, PSRs, and Plug Flow Reactors: Optional keyword. If not specified, the surface temperature is assumed to be the same as the gas temperature. Shear Flow Reactors: Required keyword.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor		
	Notes	• In previous versions, STMP keyword was used.		
TSTAU	An artificial damping factor to control how the droplet temperature approaches the maximum temperature value. A large damping factor will result in a smooth droplet temperature profile as it rises towards the maximum value. The damping factor value must be greater than 1K.			
Reactor Property/Model	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	<i>Temperature change</i>	Required	K	TSTAU 5.0
	Keyword Usage	Optional keyword. Default is 1 K.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
TSTP Solver	Initial time step used for integration of the fictitious transient equations used to determine an initial set of surface site fractions for the plug-flow simulation. Steady-state is assumed to be reached when there is no significant change in the surface site fractions over the course of one time step (see RCHG (p. 287)).			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Initial time step</i>	Required	cm	TSTP 0.1
	Keyword Usage	Optional keyword. By default, the initial time step is 1.		
	Reactor Models	• Honeycomb Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		
TSTR Cluster Property	This keyword is valid when using the XMLI (p. 369) , XMLS (p. 370) or RSTR (p. 295) option, when the XML Solution File used for initialization or restart contains transient data. In this case, select the values to use in initialization or restart as those corresponding to the time that is closest to (greater than or equal to) the specified time.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Time</i>	Required	sec	TSTR 0.01
	Keyword Usage	Optional keyword. By default, uses the data from the last time-step found in the XML Solution File.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations • Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • IC HCCI Engine • Mechanism Analyzer • Non-reactive Gas Mixer • Normal Incident Shock • Normal Reflected Shock		

Keyword	Definition			
		• Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • SI Engine Zonal Simulator • Stagnation Flow CVD Reactor		
TSTR Solver	Starting time for the simulation.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Time</i>	Required	sec	TSTR 0.01
	Keyword Usage	Optional keyword. By default, the starting time is 0.0		
	Reactor Models	• Normal Incident Shock • Normal Reflected Shock		
TSUM Output	Controls the printing of summary tables for the thermodynamic functions at the bath gas conditions (see TBTH (p. 322) , PRES (p. 265) , and XBTH (p. 367)). There are three sets of thermodynamic tables: one for the species, one for the gas reactions, and one for the surface reactions. The last three options turn on each table individually. The default is ALL (p. 149) , which will print all three thermodynamic tables. They may all be suppressed with NONE (p. 250) .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>ALL option</i>	Optional	--	TSUM ALL
	<i>NONE option</i>	Optional	--	TSUM NONE
	<i>SPECIES option</i>	Optional	--	TSUM SPECIES
	<i>GAS option</i>	Optional	--	TSUM GAS
	<i>SUR option</i>	Optional	--	TSUM SUR
	Keyword Usage	Optional keyword. By default, the table output is determined by the ALL (p. 149) or NONE (p. 250) keyword.		
	Reactor Models	• Mechanism Analyzer		
	TSWH	Defines when the calculation will be switched from TGIV (p. 326) to ENRG (p. 194) with Woschni correlation as the heat transfer model. The default value is 0 sec (always use energy equation).		

Keyword	Definition			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Time in seconds</i>	Required	sec	TSWH 0.001
	Keyword Usage	Optional keyword.		
	Reactor Models	• Multi-Zone HCCI Engine Simulation		
TTIM	The solution will be obtained with pressure and temperature given as specified functions of time through a user-programmed subroutine. The SUBROUTINE PSTEMPT (TIME, LOU, TEMP, PA) must be provided to specify the temperature and linked to the application program. See the Application Programming Interface Manual for information on how to work with user subroutines.			
Reactor Property	Keyword Usage	Optional keyword. By default, temperature and pressure will be specified by keyword. See also TPRO (p. 334) and PPRO (p. 264) .		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • SI Engine Zonal Simulator		
	Notes	• See also TPRO (p. 334) and PPRO (p. 264) as alternative ways to specify temperature and pressure as functions of time.		
TUN-BURNT	Unburned gas temperature.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Unburned gas temperature</i>	Required	K	TUNBURNT 300.0
	Keyword Usage	Required keyword.		
	Reactor Models	• Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation		
TV	Constant volume and temperature constraints.			
Problem Type	Keyword Usage	Optional keyword. Exactly one problem-type keyword must be included.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
	Notes	• VT keyword is equivalent.		

Keyword	Definition			
TWAB Solver	Absolute error tolerance used by the steady-state <i>Twopnt</i> solver in the initial calculation at the inlet boundary.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Absolute error tolerance</i>	Required	--	TWAB 1.0E-5
	Keyword Usage	Optional keyword. By default, the absolute error tolerance is 1.0E-13.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
TW-AL Reactor Property	Temperature of a neighboring "wall" used in calculating a surface radiation balance. This value is used only if the disk temperature is being calculated by including keyword RADB (p. 286) . See Equation 15.18 of the Chemkin Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Wall temperature</i>	Required	K	TWAL 850.0
	Keyword Usage	Optional keyword. By default, the wall temperature is 500 K.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
TW-PR Output	Specifies print level for the initial steady-state solution of the inlet boundary by the <i>Twopnt</i> solver.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Print level</i>	Required	--	TWPR 0
	Keyword Usage	Optional keyword. By default, the print level is set at 22.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
TWRE Solver	Relative error tolerance used by the steady-state <i>Twopnt</i> solver in the initial calculation at the inlet boundary.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Relative error tolerance</i>	Required	--	TWRE 1.0E-10
	Keyword Usage	Optional keyword. By default, the relative error tolerance is 1.0E-4.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
TWST Solver	Number of time steps before trying another Newton step, used by the steady-state <i>Twopnt</i> solver in the initial calculation at the inlet boundary.			
	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	<i>Number of time steps</i>	Required	--	TWST 50
	Keyword Usage	Optional keyword. By default, the number of time steps is set at 100.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
UFAC Solver	Factor by which to multiply the time step in the steady-state <i>Twopt</i> 's pseudo time stepping procedure when the number of time steps at the current step size reaches the number specified by IRET (p. 229).			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Multiply factor</i>	Required	--	UFAC 2.2
	Keyword Usage	Optional keyword. By default, the multiplication factor is set to 2.0.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
UIGN Output, User Subroutine	Use the ignition delay time definition given in the user routine PSIGNT. Only applicable when you are solving the energy equation with transient solver. See the Application Programming Interface Manual for details on how to work with user subroutines.			
	Parameters	Optional/Reqd.	Units	Examples
	Keyword Usage	Optional keyword.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Monolith Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator		

Keyword	Definition			
UINL Reactor Property	The axial velocity at the inlet boundary. If the rotations rate OMEG (p. 255) is zero, or if the STAG (p. 315) option is used, then UINL (p. 347) is no longer optional, but must be given to specify the problem.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Axial inlet velocity</i>	Required	cm/sec	UINL 23.6
	Keyword Usage	Diffusion or Premixed Opposed-flow Flames: Required keyword for each inlet stream. Rotating Disk CVD Reactor: Optional keyword. The velocity at the outer domain is calculated as a part of the solution. However, using the keyword UINL (p. 347) , one may impose this velocity upon the solution. By default, the axial inlet velocity is 0. Stagnation Flow CVD Reactor: Required keyword.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• In previous versions: UINF, VFUE, or VOXI keywords were used.		
UP-ROF Reactor Property, User Subroutine	Reactor inlet profiles will be given by a user-programmed subroutine. SUBROUTINE CRUPROF must be provided to specify the inlet profiles of all variables and linked to the application program. See the Application Programming Interface Manual for details on how to work with user subroutines.			
	Keyword Usage	Optional keyword. By default, a uniform inlet profile is used for all variables except axial velocity. The axial velocity profile is uniform in the Planar Shear Flow Reactor model and is parabolic (or fully developed) in the Cylindrical Shear Flow Reactor model.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
UREF Reactor Property	For the IC HCCI Engine (ICEN (p. 222)), the heat transfer model (ICHT (p. 223)) evaluates viscosity and thermal conductivity using the instantaneous temperature and pressure inside the cylinder. The UREF (p. 347) keyword is a flag that instructs the heat transfer model to use transport properties evaluated at the initial condition instead. UREF (p. 347) is turned off by default therefore it must be added to old input files in which keyword ICHT (p. 223) is used to reproduce the old results.			
	Keyword Usage	Optional keyword. By default, properties are evaluated using local conditions.		
	Reactor Models	• IC HCCI Engine • SI Engine Zonal Simulator		

Keyword	Definition			
USE _TPRO_GRID Reactor Property	Uses an initial non-uniform grid based on points specified in the estimated temperature profile (TPRO or TPROF).			
	Keyword Usage	Optional keyword.		
	Reactor Models	• Premixed Laminar Burner-Stabilized Flame • Premixed Laminar Flame-Speed Calculation		
USE_TEM- PER- AT- TURE Reactor Property	Use the temperature of another bulk for this phase.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Use same temperature as another phase</i>	Optional	--	USE_TEMPERATURE jetFuel Gas
	Keyword Usage	This keyword indicates that the first phase following the keyword use the same temperature as that of the last phase specified.		
	Reactor Models	• Closed Multiphase Reactor • Multiphase PSR		
USEP Cluster Property	For use with XMLI, XMLS, or RSTR, to override the values of pressure found on the XML Solution File used for restart or initialization with those specified in the user input file.			
	Keyword Usage	Optional keyword. By default, the program uses the pressure from the XML Solution File.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations • Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • IC HCCI Engine • Mechanism Analyzer • Non-reactive Gas Mixer • Normal Incident Shock • Normal Reflected Shock • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor		

Keyword	Definition	
		• Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor
USET Cluster Property	For use with XMLI (p. 369) , XMLS (p. 370) , or RSTR (p. 295) , override the values of temperature found on the XML Solution File used for restart or initialization with those specified in the user input file.	
	Keyword Usage	Optional keyword. By default, the program uses the temperature from the XML Solution File.
	Reactor Models	• Chemical and Phase Equilibrium Calculations • Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • IC HCCI Engine • Mechanism Analyzer • Non-reactive Gas Mixer • Normal Incident Shock • Normal Reflected Shock • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame

Keyword	Definition	
		• Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • SI Engine Zonal Simulator • Stagnation Flow CVD Reactor
	Notes	• In previous versions, USTG keyword was used.
USEV Restart	This keyword is valid when using XMLI (p. 369) or the RSTR (p. 295) options. When this keyword is included, it overrides the values of velocity or flow-rate found on the XML Solution File used for restart or initialization with those specified in the user input file.	
	Keyword Usage	Optional keyword. By default, the program uses the velocity or flow-rate from the XML Solution File.
	Reactor Models	• Honeycomb Reactor • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor
USEV XMLI	When using XMLI (p. 369) , XMLS (p. 370) , or RSTR (p. 295) , overrides the values of velocity or flow-rate found on the XML Solution File used for restart or initialization with those specified in the user input file.	
	Keyword Usage	Optional keyword. By default, the program uses the velocity or flow-rate from the XML Solution File.
	Reactor Models	• Cylindrical Shear Flow Reactor • Honeycomb Reactor • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR

Keyword	Definition			
		• Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
US-RIN Inlet Property	Specification of a reactor inlet stream using a user-programmed subroutine. Use of USRIN requires that a user routine SUBROUTINEUSRINLET (LIUIN, IINWRK, LRUIN, RINWRK, INAME, KNAMES, FLRT, TINL, TEIN, XIN) is written and linked to the application program. Calls to this routine will be used to obtain the corresponding flow rate (FLRT (p. 208)), inlet temperature (TINL (p. 331)), engine-out electron temperature (TEIN (p. 323)), and composition (REAC (p. 288)). See the Application Programming Interface Manual for more information on how to work with user subroutines.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Stream</i>	Required	--	USRIN engineout 2
	<i>Reactor number (PSR clusters only)</i>	Optional, if not defined, then reactor #1 is assumed.	--	USRIN engineout 2
	Keyword Usage	Optional keyword. By default, streams are defined using the INLET (p. 226) and related keyword.		
	Reactor Models	• Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR		
	Notes	• See User Supplemental Programming of the Application Programming Interface Manual for details.		
	UTRN Reactor Property, User Subroutine	Use the mixture average transport properties defined in user-programmed routine CRUTRANS (for Shear Flow reactors), OPUTRANS (for Opposed-flow Flame Simulator) or PRUTRANS (for Premixed Laminar Flame or Flame-speed Calculation). See the Application Programming Interface Manual for details on how to work with user subroutines.		
Keyword Usage		Optional keyword. By default, transport properties will be calculated based on the fundamental transport properties provided in the chemistry set.		
Reactor Models		• Cylindrical Shear Flow Reactor • Opposed-flow Flame Simulator		

Keyword	Definition			
		- Planar Shear Flow Reactor - Premixed Laminar Burner-stabilized Flame - Premixed Laminar Flame-speed Calculation		
UWGT Reactor Property	Grid refinement weighting factor for the axial velocity. A value greater than 1 will increase the grid resolution outside of the reacting zone/wall region to improve the accuracy of velocity solutions near the inlet region.			
	Parameters	Optional/Reqd.	Units	Examples
	Weighting Factor	Optional	--	UWGT 2.0
	Keyword Usage	Optional keyword. Default value is 1.		
	Reactor Models	- Rotating Disk CVD Reactor - Stagnation Flow CVD Reactor		
VCPRO Reactor Property	The cylinder volume is given by a series of CA-volume data points prepended by the keyword VCPRO. The CA data values must be monotonically ascending and must span from the starting crank angle to the ending crank angle. The volume data must be positive.			
	Parameters	Optional/Reqd.	Units	Examples
	CA	Required	degree	VCPRO - 165.0 35.14
	Volume	Required	cm ³	VCPRO -165.0 35.14
	Keyword Usage	Optional keyword (required to turn ON this option).		
	Reactor Models	- Direct Injection Diesel Engine Simulator - IC HCCI Engine - Multi-Zone HCCI Engine - SI Engine Zonal Simulator		
VCOR Reactor Property	Including this keyword causes the calculation to be run using a correction velocity to ensure mass conservation, that is, the sum of the diffusion fluxes is zero. See Equation 15.11 of the Chemkin Theory Manual . If VCOR (p. 352) is not used, then TRCE (p. 337) is in effect.			
	Keyword Usage	Optional keyword. By default, correction velocity is not used.		
	Reactor Models	- Cylindrical Shear Flow Reactor - Planar Shear Flow Reactor - Premixed Laminar Burner-stabilized Flame - Premixed Laminar Flame-speed Calculation - Rotating Disk CVD Reactor - Stagnation Flow CVD Reactor		

Keyword	Definition			
VDOT Inlet Property	Inlet volumetric flow rate.			
	Parameters	Optional/Reqd.	Units	Examples
	Inlet volumetric flow rate	Required	cm ³ /sec	VDOT 100
	Keyword Usage	Optional keyword. Either VDOT (p. 353) or VEL (p. 354) must be specified, unless this is a restart run. PFRs and Monolith Reactors: Flow specification via one of VEL (p. 354) , VDOT (p. 353) , VDOTPRO (p. 353) SCCM (p. 299) SCCMPRO (p. 300) FLRT (p. 208) , or FPRO (p. 210) is required.		
	Reactor Models	• Honeycomb Reactor • Plasma Plug Flow Reactor • Multiphase PSR • Plug Flow Reactor		
VDOTPRO Inlet PropertyProfiles	Specifies a transient profile or function of mass flow rate vs. independent variable (time or position) for an inlet stream, in cubic centimeters per minute. The profile specified will be interpolated linearly from the VDOTPRO points provided.			
	Parameters	Optional/Reqd.	Units	Examples
	Inlet stream name	Optional If no stream name is given, the profile described is assumed to apply to all reactors in a cluster.	-	VDOTPRO purge 0.19 300
	Time (Distance for flow reactor)	Required	sec (cm for flow reactor)	VDOTPRO purge 0.19 300
	Equivalent volumetric flow rate	Required	cm ³ /min	VDOTPRO purge 0.19 300
	Keyword Usage	PFRs and Monolith Reactors: Flow specification via one of VEL (p. 354) , VDOT (p. 353) , VDOTPRO SCCM (p. 299) SCCMPRO (p. 300) FLRT (p. 208) , or FPRO (p. 210) is required. PSRs and PaSRs: Optional keyword. If none of TAU (p. 321) , FLRT (p. 208) / FPRO (p. 210) , SCCM (p. 299) / SCCMPRO (p. 300) , or VDOT (p. 353) / VDOTPRO are specified or are nonzero, then a closed-system is assumed. FLRT (p. 208) / FPRO (p. 210) ,		

Keyword	Definition			
		SCCM (p. 299)/SCCMPRO (p. 300), or VDOT (p. 353)/VDOTPRO is required for each INLET (p. 226) stream defined. Stagnation Flow CVD Reactors: FLRT (p. 208)/FPRO (p. 210), SCCM (p. 299)/SCCMPRO (p. 300) or UINL (p. 347) is required for each inlet stream defined. Rotating Disk CVD Reactors: Optional keyword.		
	Reactor Models	• Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • Multiphase PSR • Plug Flow Reactor (PFR) • Plasma PFR • Honeycomb Monolith Reactor • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
VEL Inlet Property	The gas-phase velocity at the inlet (for plug-flow reactors) or the maximum gas velocity at the inlet (for shear-flow reactors).			
	Parameters	Optional/Reqd.	Units	Examples
	Velocity	Required	cm/sec	VEL 15
	Keyword Usage	Plug Flow Reactors: Optional keyword. Either VDOT (p. 353) or VEL (p. 354) must be specified, unless this is a restart run. Shear Flow Reactors: If the problem is in cartesian coordinates, then the average velocity equals two-thirds of the maximum velocity of the parabolic velocity profile. In cylindrical coordinates, the average velocity is half of the maximum velocity. If the keyword BLTK (p. 162) is given, a flat velocity profile will be used, that is, everywhere the velocity will be set equal to VEL (p. 354) except within a distance BLTK (p. 162) of the wall.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Honeycomb Reactor • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		
VELPRO	Flow velocity along the distance of a plug reactor.			

Keyword	Definition			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Distance value</i>	Required	cm	VELPRO 1.0 10.0
	<i>Velocity</i>	Required	cm/sec	VELPRO 1.0 10.0
	Keyword Usage	Optional keyword. By default, no profile is provided.		
	Reactor Models	• Plug Flow Reactor		
VF-FAC Reactor Property	The fraction of fuel vapor to be retained in the spray parcel after vaporization. If the bulk gas and the spray parcels are traveling at different directions and speeds, a large portion of the fuel vapor could be pushed out of its originating spray parcel. This vaporization rate model parameter can be used to improve the low vaporization rate issue of fuel components with high boiling point. Reducing the value of this parameter will increase the vaporization rate. This model parameter should have a value between 0 and 1 inclusive and will be applied to all injections of the same DI engine simulation.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Retention fraction</i>	Optional	--	VFFAC 0.0
	Keyword Usage	Optional keyword. By default, the vapor retention fraction is set to 0.01.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
VH Problem Type	Constant volume and enthalpy constraints.			
	Keyword Usage	Optional keyword. Exactly one problem-type keyword must be included.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
VFRAC Reactor Property	Volume fraction of a bulk phase in the reactor. This specifies the overall composition of the reactor in terms of different bulk phases including gas, liquid, and solid.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>phase name</i>	Required		VFRAC Gas 0.6
	<i>volume fraction of a bulk phase in the reactor</i>	Required		VFRAC jetFuel 0.4
	Keyword Usage	This keyword is used to specify the composition of the entire reactor. Bulk phase name follows the keyword. "Gas" indicates the gas phase. The composition is normalized to 1 at the start of simulation.		
	Reactor Models	• Closed Multiphase Reactor • Multiphase PSR Reactor		
VIS	Viscosity of the inlet gas mixture.			

Keyword	Definition			
Inlet Property	Parameters	Optional/Reqd.	Units	Examples
	Viscosity	Required	g/(cm · sec)	VIS 0.01
	Keyword Usage	Optional keyword. By default, the viscosity is 0, that is, viscous drag is neglected.		
	Reactor Models	• Honeycomb Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		
	Notes	• A poise is equivalent to g/(cm · sec).		
VISC	Viscosity of the mixture at 300 K. Required input for boundary layer corrections.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Viscosity at 300 K	Required	g/(cm · sec)	VISC 2.65E-4
	Keyword Usage	Optional keyword. By default, the viscosity is not set. This keyword is required for boundary layer corrections.		
	Reactor Models	• Normal Incident Shock		
VLE	Vapor Liquid Equilibrium model for use with the phase transfer process. Additional parameters IDEAL or HENRY, are required to specify the model.			
Reactor Property	• Value of 1, use the form: Henry's Constant=$A \cdot \exp[-B(1/T - 1/C)]$ Here, A, B, C are the three parameters input from following the first parameter. T represents temperature in K. • Value of 2, use the form: $1/\text{Henry's Constant} = \exp[A + B/T + C \cdot \ln(T) + D \cdot T]$ D is the fifth parameter on the input line. This form is available only when pressure units are used specified for Henry's law using the keyword UNITS.			
	Only one species on reactant and product side should be provided. This mapping is unique; a species may participate in only one VLE reaction.			
	Parameters	Optional/Reqd.	Units	Examples
	Model name	Required	--	VLE / IDEAL/
	Model name	Required	--	CO2 = CO2(aq) 1.0 0.0 0. VLE/ HENRY 1 3.34e-05 2400 298.15 /

Keyword	Definition			
		first parameter. HENRY: Henry's law for calculating equilibrium concentration levels in gas and liquid phases. Default form is dimensionless. This can be changed by optional keyword UNITS. IDEAL: Raoult's law for calculating equilibrium concentrations in gas and liquid phases.		
	<i>Model parameters</i>	Required for HENRY parameter For HENRY, four or five parameters may be provided following HENRY. The first parameter,	K	CO2 = CO2(aq) 1.0 0.0 0. VLE/HENRY 1 3.34e-05 2400 298.15 /

Keyword	Definition			
		with an integer value of 1 or 2, indicates the type of temperature dependence for Henry's law. See Table 4.7: Auxiliary Keywords for Liquid Phase Reactions (p. 88)		
	Keyword Usage	Optional keyword. By default, the heat loss from the reactor will be zero. See also QLOS (p. 281) and QPRO (p. 283) .		
	Reactor Models	• Multiphase Reactor		
VOL Reactor Property	The volume of the reactor. In multi-zone models, users can enter zone volume fractions rather than exact zone volumes. The software will calculate the initial cylinder volume, normalize the volume fractions, and compute the exact zone volumes at the start of simulation. VOL (p. 359) is used to give Zone volumes and Zone volume fractions.			
	Parameters	Optional/Reqd.	Units	Examples
	Volume	Required	cm ³	VOL 1200
	Reactor number (PSR clusters only)	Optional If no number is given, the keyword is assumed to apply to all reactors in a cluster.	--	VOL 1200 1
	Keyword Usage	Optional keyword. By default, volume is required input for all PSRs		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Partially Stirred Reactor (PaSR) • Closed Plasma Reactor		

Keyword	Definition			
		• Non-reactive Gas Mixer • Multiphase PSR • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Plasma PSR		
VOL Reactor Property	The fraction of the total volume inside the cylinder for each zone in a Multi-Zone HCCI Engine model.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Zone volume fraction</i>	Required	--	VOL 0.15 4
	<i>Zone number</i>	Required	--	VOL 0.15 4
	Keyword Usage	Optional keyword.		
	Reactor Models	• Multi-Zone HCCI Engine Simulator • SI Engine Zonal Simulator		
VOL Reactor Property	The initial specific volume of the gas mixture.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Specific volume of the gas mixture</i>	Required	cm ³ /g	VOL 1200
	Keyword Usage	Optional keyword. The user must specify two state variables and the composition to define the initial mixture.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
VOLC Reactor Property	Engine cylinder clearance volume.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Engine cylinder clearance volume</i>	Required	cm ³	VOLC 2.0
	Keyword Usage	Optional keyword. Any two of VOLC (p. 359) , VOLD (p. 359) , or CMPR (p. 171) must be specified.		
	Reactor Models	• IC HCCI Engine • SI Engine Zonal Simulator		
VOLD Reactor Property	Engine displacement volume, or the volume swept by the piston during compression.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Displacement volume</i>	Required	cm ³	VOLD 2.0
	Keyword Usage	Optional keyword. Any two of VOLC (p. 359) , VOLD (p. 359) , or CMPR (p. 171) must be specified		

Keyword	Definition			
	Reactor Models	• IC HCCI Engine • SI Engine Zonal Simulator		
VPARI Reactor Property/Model	Initial volume of a single spray parcel.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>initial parcel vol</i>	Required	cm ³	VPARI 5.0
	Keyword Usage	Required keyword.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
VP-MOD Reactor Property/Model	Specify how the droplet surface temperature is determined. If VPMOD=0: uniform droplet temperature model, that is, the droplet surface temperature is the same as the droplet core temperature. If VPMOD=1: two temperature model; the droplet surface temperature is solved by the energy conservation equation at the droplet surface.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Surface temperature model</i>	Required	--	VPMOD 1
	Keyword Usage	Optional keyword. Default: the uniform temperature model is used.		
	Reactor Models	• Direct Injection Diesel Engine Simulator		
VPRO Reactor Property Profiles	Reactor volume profile specified as a function of time.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Time value</i>	Required	sec	VPRO 1.0E-4 1.0
	<i>Volume</i>	Required	cm ³	VPRO 1.0E-4 1.0
	<i>Reactor number (PSR clusters only)</i>	Optional If no number is given, the profile described by the first two values is assumed to apply to all reactors in a cluster.	--	VPRO 1.0E-4 1.0 1
	Keyword Usage	For constrained-volume problems, VOL (p. 359) or VPRO (p. 360) must be specified. Otherwise, a default value of 1.0 is used for the initial reactor volume.		

Keyword	Definition			
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Partially Stirred Reactor (PaSR) • Closed Plasma Reactor • Non-reactive Gas Mixer • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Plasma PSR • Multiphase PSR		
VRS Reactor Property	Reflected shock velocity. If specified, it is used to determine the state of the gas after the shock. The reflected shock velocity is never used unless the incident shock velocity is also given.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Reflected shock velocity</i>	Required	cm/sec	VRS 100
	Keyword Usage	Optional keyword. By default, no shock velocities are computed, but $U_5=0$.		
	Reactor Models	• Normal Reflected Shock		
VS Problem Type	Constant volume and entropy constraints.			
	Keyword Usage	Optional keyword. Exactly one problem-type keyword must be included.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
	Notes	• SV keyword is equivalent.		
VSHK Reactor Property	Incident shock velocity.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Velocity</i>	Required	cm/sec	VSHK 3000.
	Keyword Usage	This input is required for all incident shock problems, and may be used for some reflected shock problems.		
	Reactor Models	• Normal Incident Shock • Normal Reflected Shock		
VTIM Reactor Property	The solution will be obtained with the volume as a function of time specified through a user programmed subroutine. SUBROUTINE PSVOLT(TIME, LOUT, VOL, DVDT) must be provided to specify the volume, and linked to the application program.			

Keyword	Definition			
	Keyword Usage	Optional keyword. By default, volume is specified through VOL (p. 359) or VPRO (p. 360) .		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR		
	Notes	• See also VPRO (p. 360) as an alternative way to specify volume as a function of time. • See the Application Programming Interface Manual for more information on how to work with user subroutines.		
VU	Constant volume and energy constraints.			
Problem Type	Keyword Usage	Optional keyword. Exactly one problem-type keyword must be included.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
	Notes	• UV keyword is equivalent.		
VWALL	Specify a constant axial slip velocity at the walls.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Axial slip velocity</i>	Required	cm/sec	VWALL 1.1
	Keyword Usage	Optional keyword. See also SLIP (p. 309) .		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
WBFB	Specifies the <i>b</i> parameter of the Wiebe function. <i>b</i> must be greater than 0 and is set to 5.0 by default.			
Solver	Parameters	Optional/Reqd.	Units	Examples
	<i>Value of the b parameter</i>	Required	--	WBFB 9.0
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		
WBFN	Specifies the <i>n</i> parameter of the Wiebe function. <i>n</i> must be greater than 0 and is set to 2.0 by default.			
Solver	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	<i>Value of the n parameter</i>	Required	--	WBFN 4.0
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		
WDIF	Use windward differencing on convective terms in the equations.			
Solver	Keyword Usage	Optional keyword. By default, windward differencing is used.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation		
WELL	Flag indicating that a well mixed model will be used to simulate the molecular mixing within the computational particle.			
Reactor Property	Keyword Usage	Optional keyword. By default, a well mixed model is assumed.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR)		
WENG	The reactor wall temperature will be obtained by solving energy conservation equations for the reactor wall. When WENG (p. 363) is used, all the external heat fluxes, that is, heat loss to the environment and heat exchange between the reactors in a network, are applied to the wall energy equation instead of the gas phase energy equation. Also, the heat generated by surface reactions will be included in the wall energy equation. If a surface has more than one material, the wall temperature is always assigned to the first material.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Thermal mass</i>	Required	cal/K	WENG 0.1 500 1
	<i>Heat transfer coefficient</i>	Required	cal/(cm ² · sec · K)	WENG 0.1 500 1
	<i>Reactor number (PSR clusters only)</i>	Optional	--	WENG 0.1 500 1
		If no number is given, the keyword is assumed to apply to all reactors in a cluster.		

Keyword	Definition			
	Keyword Usage	Optional keyword. By default the surface temperature is fixed. The two required numbers on the keyword line specify the thermal mass of the reactor wall and the heat transfer coefficient between the inner wall surface and the gas mixture inside the reactor. The initial wall temperature can be specified by the keyword TSRF (p. 340) otherwise the gas temperature will be used. For Plug Flow Reactors the thermal mass parameter is described in units of cal/(cm · K).		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • SI Engine Zonal Simulator		
WMIX	Width of the mixing region; used in defining the initial profile for the LINE (p. 233) or PLAT (p. 261) options.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Width of mixing region</i>	Required	cm	WMIX 2.0
	Keyword Usage	Optional keyword. By default the width of the mixing region is XEND (p. 367) * 0.5.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
WOSP1	Specify parameters of the Woschni heat transfer correlation for the compression period.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	<i>C11 in the average gas velocity correlation.</i>	Required	--	WOSP1 2.28 0.318 0.0 1.57
	<i>C12 in the Woschni correlation.</i>	Required	cm/(sec - K)	WOSP1 2.28 0.318 0.0 1.57
	<i>C2 in the Woschni correlation.</i>	Required	--	WOSP1 2.28 0.318 0.0 1.57
	<i>Ratio of swirl velocity to mean piston speed.</i>	Required	--	WOSP1 2.28 0.318 0.0 1.57
	Keyword Usage	Optional keyword.		
	Reactor Models	• Multi-Zone HCCI Simulator • IC HCCI Engine • SI Engine Zonal Simulator		
WOSP2	Specify parameters of the Woschni heat transfer correlation for the combustion period.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>C11 in the average gas velocity correlation.</i>	Required	--	WOSP2 2.28 0.318 0.0 1.57
	<i>C12 in the Woschni correlation.</i>	Required	cm/(sec - K)	WOSP2 2.28 0.318 0.0 1.57
	<i>C2 in the Woschni correlation.</i>	Required	--	WOSP2 2.28 0.318 0.0 1.57
	<i>Ratio of swirl velocity to mean piston speed.</i>	Required	--	WOSP2 2.28 0.318 0.0 1.57
	Keyword Usage	Optional keyword.		
	Reactor Models	• Multi-Zone HCCI Simulator • IC HCCI Engine • SI Engine Zonal Simulator		
WOSP3	Specify parameters of the Woschni heat transfer correlation for the expansion period.			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>C11 in the average gas velocity correlation.</i>	Required	--	WOSP3 2.28 0.318 0.0 1.57
	<i>C12 in the Woschni correlation.</i>	Required	cm/(sec - K)	WOSP3 2.28 0.318 0.0 1.57
	<i>C2 in the Woschni correlation.</i>	Required	--	WOSP3 2.28 0.318 0.0 1.57

Keyword	Definition			
	<i>Ratio of swirl velocity to mean piston speed.</i>	Required	--	WOSP3 2.28 0.318 0.0 1.57
	Keyword Usage	Optional keyword.		
	Reactor Models	- Multi-Zone HCCI Simulator - IC HCCI Engine - SI Engine Zonal Simulator		
WPRO	Plasma power deposition profile specified as a function of time.			
Reactor Property Profiles	Parameters	Optional/Reqd.	Units	Examples
	<i>Time value</i>	Required	sec	WPRO 1.0E-4 500
	<i>Plasma power deposition</i>	Required	watts	WPRO 1.0E-4 500
	<i>Reactor number (PSR clusters only)</i>	Optional If no number is given, the profile described by the first two values is assumed to apply to all reactors in a cluster.	--	WPRO 1.0E-4 500 1
	Keyword Usage	Optional keyword. By default, no profile is provided.		
	Reactor Models	- Closed Plasma Reactor - Plasma Plug Flow Reactor - Plasma PSR		
WS-RC	Half-width of the Gaussian source term if the gas is being heated by an optional heat source. See Equation 15.12 of the Chemkin Theory Manual .			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	<i>Half-width</i>	Required	cm	WSRC 0.07
	Keyword Usage	Optional keyword. By default, the half-width is 0.0. This is a required keyword when QDOT is not 0.0.		
	Reactor Models	Rotating Disk CVD Reactor		

Keyword	Definition			
		• Stagnation Flow CVD Reactor		
XBTH Reactor Property	Specifies the bath gas composition. The [Species name] (or number as it appears in the Pre-processor output) and desired mole fraction are required parameters. If at least one species in a phase has been set with the XBTH (p. 367) keyword, then all of the specified mole fractions for that phase are summed and normalized so that they add up to one. If no XBTH (p. 367) parameters have been specified for any species in the phase, then mole fractions for all species in that phase are set equal to one another.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Species name</i>	Optional	--	XBTH H2 1.0
	<i>Species number value</i>	Optional	mole fractions	XBTH CH(S) 0.5
	Keyword Usage	Optional keyword. By default, the table output is determined by the ALL (p. 149) or NONE (p. 250) keyword.		
	Reactor Models	• Mechanism Analyzer		
XCEN Reactor Property	Center of the mixing region; used in defining the initial profile for the LINE (p. 233) or PLAT (p. 261) options. Note that the fuel inlet is assumed to be located at $x=0$.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Center of mixing region</i>	Required	cm	XCEN 3.0
	Keyword Usage	Optional keyword. By default the center of the mixing region is XEND (p. 367) * 0.35.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	XEND Reactor Property	Physical length of the computational domain, or value of x at the end of the domain. Depending on the reactor, the beginning of the domain is either 0.0 or the value of XSTR (p. 372).		
Parameters		Optional/Reqd.	Units	Examples
<i>Channel length</i>		Required	cm	XEND 25
Keyword Usage		Required keyword.		
Reactor Models		• Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • Planar Shear Flow Reactor		

Keyword	Definition			
		• Plasma Plug Flow Reactor • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
XEST Reactor Property	For steady-state calculations, these are the estimated gas-phase mole fractions to begin the iteration. For transient problems, this keyword provides the initial values for the gas-phase mole fractions in the reactor. For example, XEST H2O 0.5 assigns an initial mole fraction of 0.5 to water vapor in the reactor.			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	XEST H2O 0.5
	Initial fraction	Required	mole fractions	XEST H2O 0.5
	Keyword Usage	Transient cases: Required keyword; Steady-state cases: Optional keyword. By default, the initial or estimated gas-phase mole fractions are 0.0. For steady-state cases, if no XEST (p. 368) keywords are given, then an equilibrium calculation is performed to determine the initial estimates for the reactor composition.		
	Reactor Models	• Perfectly Stirred Reactor (PSR) • Plasma PSR • SI Engine Zonal Simulator		
	Notes	• The sum of all the estimated mole fractions should equal one. If they do not sum to one, they will be normalized and a warning message will be printed to the output file.		
XIMN Reactor Property	Minimum mass or mole fraction value applied to intermediate species estimates, when the (default) equilibrium is used to determine product estimates. Ignored in the case that INTM (p. 227) keywords are present. In this case, the intermediate species fraction is initialized to be the average of its PROD2 (p. 267) and REAC (p. 288) values; or XIMN (p. 368) , if XIMN (p. 368) is greater than this average.			
	Parameters	Optional/Reqd.	Units	Examples
	Intermediate fractions	Required	mole fractions	XIMN 1.0E-10
	Keyword Usage	Optional keyword. By default, the intermediate fraction is set to 0.		
	Reactor Models	• Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation		

Keyword	Definition			
XINL Inlet Property	Inlet mole fraction of a species in the specific phase.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>inlet stream name</i>	Required	--	XINL C1_Inlet1 N2 1.0 1.0
	<i>species name</i>	Required	--	XINL C1_Inlet1 N2 1.0
	<i>inlet mole fraction</i>	Required	K	XINL C1_Inlet1 N2 1.0
	Keyword Usage	Required keyword for the specific phase if the inlet flow of the specific phase is non-zero.		
Reactor Models	• Multiphase PSR Reactor			
XML_OUT- PUT_WRITE Output	Write output data to XML file.			
	Keyword Usage	Optional keyword. By default, solution data will be written to XML file.		
	Reactor Models	• All		
XMLI Cluster Property	Read a solution from the XML Solution File used for initialization (<i>XMLdata.zip</i>), which may be a solution from any other Reactor Model (see also RSTR (p. 295)). When initialization (XMLI (p. 369)) is used from an XML Solution File with spatial profiles (that is, 1-D or channel-flow models), the initial values are actually averages of the profiles stored in the XML Solution File. The integral averages are calculated using trapezoidal integration rules.			
	Keyword Usage	Optional keyword. By default, the program does not look for an XML Solution File used for restart or initialization.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations • Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • IC HCCI Engine • Mechanism Analyzer • Non-reactive Gas Mixer • Normal Incident Shock • Normal Reflected Shock • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR)		

Keyword	Definition	
		• Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • SI Engine Zonal Simulator • Stagnation Flow CVD Reactor
	Notes	• For shear-layer flow solutions, we use the value integrated over the height (or radius) and divided by the cross-sectional area for the specified axial-distance location. • For Opposed-flow Flames and CVD Reactors, we use the value integrated over the spatial domain, divided by the total axial distance.
XMLS Cluster Property	Use a previously stored XML Solution File or the XML Solution File from an upstream reactor to initialize the inlet conditions of this inlet.	
	Keyword Usage	Optional keyword. By default, the program does not look for an XML Solution File used restart or initialization.
	Reactor Models	• Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • Non-reactive Gas Mixer • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame

Keyword	Definition			
		• Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
XRES Restart	Force the starting distance for the new solution to be this value and ignore the value of distance from the XML Solution File used for restart or initialization.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Initial distance</i>	Required	cm	XRES 10
	Keyword Usage	Optional keyword. By default, the value of the XML Solution File is used during a continuation or restart run.		
	Reactor Models	• Honeycomb Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		
XRST Restart	This keyword is valid when using RSTR (p. 295) option. In this case, select the values to use in restart as those corresponding to the distance that is closest to (greater than or equal to) the specified distance.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Distance</i>	Required	cm	XRST 5.0
	Keyword Usage	Optional keyword. By default, the point where the previous solution ended is used.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
XSDF Reactor Property	Default value for a momentum-transfer cross-section between electrons and each species. This value is used for all species not specified with the XSEK (p. 371) keyword.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Momentum-transfer cross-section</i>	Required	cm ²	XSDF 1.0E-16
	Keyword Usage	Optional keyword. By default, the cross-section value is 0. In a plasma problem the user must either specify XSDF (p. 371) or include an XSEK (p. 371) keyword for all species except electrons.		
	Reactor Models	• Closed Plasma Reactor • Plasma Plug Flow Reactor • Plasma PSR		
XSEK	Momentum-transfer collision cross-section between electrons and a specified species. For example, "XSEK AR 1.0E-16" would indicate a momentum-transfer cross-section of			

Keyword	Definition			
Reactor Property	10 ⁻¹⁶ cm ² between electrons and argon atoms. For any species not specified by the XSEK (p. 371) keyword, a user-specified default value will be used.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Species</i>	Required	--	XSEK AR 1.0E-16
	<i>Momentum-transfer cross-section</i>	Required	cm ²	XSEK AR 1.0E-16
	Keyword Usage	Optional keyword. By default, the cross-section value is 0. In a plasma problem the value for every species is specified by the XSDF (p. 371) keyword.		
	Reactor Models	• Closed Plasma Reactor • Plasma Plug Flow Reactor • Plasma PSR		
XSRC Reactor Property	Height above the disk which is the center of a Gaussian-shaped power source. See Equation 15.12 of the Chemkin Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Height</i>	Required	cm	XSRC 0.6
	Keyword Usage	Optional keyword. By default, the height is 0.0.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
XSTR Reactor Property	The beginning of the computational domain. For burner-stabilized flames, this is the burner location.			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Inlet axial position</i>	Required	cm	XSTR 1.5
	Keyword Usage	Optional keyword. By default, the starting or inlet axial position is 0.		
	Reactor Models	• Honeycomb Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		

Keyword	Definition			
XT-MP Reactor Property	If TSRF (p. 340) is used to specify the surface temperature, the application will set the surface temperature to TINL (p. 331) at $x=0$ and smoothly ramp the temperature up to TSRF (p. 340) at a distance of XTMP (p. 373) .			
	Parameters	Optional/Reqd.	Units	Examples
	<i>Distance between TINL point and TSRF point</i>	Required	cm	XTMP 0.25
	Keyword Usage	Optional keyword. By default, the distance is set to 0.5.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
ZNDB Reactor Property	Calculates the ZND structure behind the incident shock with the boundary layer correction. The gas-mixture properties before the incident shock must be provided. The speed of the incident shock is set to the Chapman-Jouguet detonation wave speed, which is determined from the gas properties before the shock.			
	Keyword Usage	Optional keyword.		
	Reactor Models	• Normal Incident Shock reactor model		
ZNDC Reactor Property	Calculates the ZND structure behind the incident shock. The gas mixture properties before the incident shock must be provided. The speed of the incident shock is set to the Chapman-Jouguet detonation wave speed which is determined from the gas properties before the shock.			
	Keyword Usage	Optional keyword.		
	Reactor Models	• Normal Incident Shock reactor model		
ZONEAVG Output	Flag to store only the zone-average solution data in the Multi-Zone HCCI Engine Simulator.			
	Keyword Usage	Optional keyword. By default, all solution data is stored in the Multi-Zone HCCI Engine Simulator output.		
	Reactor Models	• Multi-Zone HCCI Engine Simulator • SI Engine Zonal Simulator		

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