Ansys Chemkin Visualization Manual

Ansys

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: About This Manual

This manual describes visualization features in Ansys Chemkin, the Visualizer, and other post-processing alternatives. The Graphical Post-Processor (p. 7) focuses on the Chemkin Visualizer, which is launched from the Chemkin Interface. Post-Processing Alternatives (p. 27) provides additional post-processing options, including the Export Solution Utility (*GetSolution.exe*) and the Export to Excel options. Reaction Path Analyzer (p. 37) discusses the Chemkin Reaction Path Analyzer, which provides visualization of the inner workings of the chemistry model and fundamental understanding of reaction mechanism dependencies.

1.1. Overview of Solution Data Available from CHEMKIN

The objective of post-processing is the analysis and/or extraction of data obtained from the Ansys Chemkin simulations. The analysis may be as simple as comparing a set of scalar values or may require 2-D and 3-D plotting and contour capabilities. In some cases, we want to make derived calculations based on the raw Chemkin outputs.

There are three types of outputs produced by the Ansys Chemkin reactor simulations:

- Solution File (zip file).

  This file, which by default is named XMLdata_<project_name>.zip, is a compressed, XML-formatted text file comprised of multiple blocks of information. The information includes the independent and dependent variables in the system as well as any sensitivity data that was requested in the problem setup.

  By using an XML format, we provide a generalized format that all of our reactor models can read and write. Each Solution File is comprised of a header block and multiple data blocks. Each block (*XMLdata1.zip*, etc.) is compassed, separately, but the blocks must be read consecutively and seamlessly to process the entire file as an XML-formatted stream. The Ansys Chemkin installation includes such a SAX-based XML parser program which is used by our simulation, export, and post-processing programs when working with the Solution File. The purpose of breaking the file into multiple zipped blocks is to allow large data sets to be compressed into smaller files without overwhelming the machine resources for memory during the file operations.

  There are a number of derived values calculated as part of the post-processing. These values are not found within the Solution File itself and are created on the fly, using the solution data and the Ansys Chemkin utilities. Table 1.1: Output Variables Created by Derived Calculations in the Visualizer (p. 2) lists the derived variables that are routinely or optionally calculated for the applicable reactor models.

- Diagnostic Output File (*.out*).

  A text file listing the simulation inputs, the progress of the solution and some or all of the outputs. This is useful for a quick inspection/review and also contains any error messages generated by the application. The diagnostic output file should not be used for any post-processing or batch processing, as the format of the output is not a fixed format and may vary from one solution to another.

- Pre-parsed, comma-separated input files for the Visualizer (*.ckcsv*).

  These files are created by the post-processing step of the Parameter Study facility. They contain the aggregation of results from multiple parameterized runs of the simulation. These files are in a special format that is easily loaded by the Visualizer. They contain the derived values, as requested, that are detailed in Table 1.1: Output Variables Created by Derived Calculations in the Visualizer (p. 2) .

Note:

Note that including sensitivity data or rate-of-production data during post-processing may result in problems involving too much memory requirements during the solution processing. For large mechanisms, consider reducing the amount of sensitivity data using the "SEN" option as described in the Chemkin Input Manual and selecting only a subset of sensitivity or ROP data during data selection for solution post-processing.

Note:

If your objective is to extract the Ansys Chemkin results as an intermediate step to pass to an external program or scripting step, we provide data extraction utilities that can extract all or a subset of Solution File data into either a parsed file (*.ckcsv*) or further into multiple comma-separated values files that are easily loaded into Excel or other 3rd-party utilities. Please refer to the information on command-line and batch-programming options for extracting solution file information.

Table 1.1: Output Variables Created by Derived Calculations in the Visualizer

Variable	Definition	Applicable Reactor Models
Dry Mass Fraction	Gas-phase species mass fractions, based on the total moles of the gas minus water vapor.	All
Dry Mole Fraction	Gas-phase species mole fractions, based on the total moles of the gas minus water vapor.	All
IMEP	The indicated mean effective pressure. IMEP considers only the work done between IVC and EVO in the IMEP calculation. The definition is consistent with indicated work and indicated power. There is no assumption about the cycle. IMEP is calculated as: $$IMEP=\frac{W_{(IVC\,to\,EVO)}}{V_{dis}} \quad (1.1)$$ in which W is indicated work, V_{dis} is the displacement volume, calculated as: $$V_{dis}=\frac{\pi\times Bore^2}{4}\times Stroke \quad (1.2)$$	IC Engine

Variable	Definition	Applicable Reactor Models
Indicated Work	The indicated work of a cylinder is given by the average product of the normal force on the face of the piston and the piston velocity. It is calculated as the integral of *PdV*, where *P* is the pressure and *dV* is the differential volume. For a description of cycle/gross indicated work, see the tutorial,"Spark-Ignition Engine Simulation for Knock," in the *Chemkin Tutorials*.	IC Engine
Mixture Enthalpy	Mass averaged enthalpy of mixture	All
Molar Conversion	Percentage conversion of gas-phase species based on: (1) initial and final mole fraction in the case of a closed reactor, or (2) inlet and outlet mass flux in the case of an open reactor.	All Closed Homogeneous, PSR, PFR, and Shear Flow Reactors
Net Heat Production from Gas-Phase Reactions	The net heat production from a gas-phase reaction is the sum of the rate of heat production from all gas-phase species involved in this reaction. The rate of heat production from a gas-phase species in a reaction is the product of the contribution of the reaction to the production rate of the species and the enthalpy of the species.	All
Normal Strain Rate	Local rate of change in the axial velocity with respect to distance.	Opposed Flow Flame and CVD Reactors
Parts Per Million CO Dry Basis	The Gas-phase volumetric fraction of CO expressed in parts per million, after removing the volumetric contribution of water. $PPM_{CO}=1.E6\frac{X_{CO}}{1-X_{H_2O}}$	All Closed Homogeneous, PSR, PFR, and Premixed Flame Reactors
Parts Per Million CO Dry Basis 15% O2 Correction	The Gas-phase volumetric fraction of CO expressed in parts per million, after removing the volumetric contribution of water and correcting to 15% Oxygen $PPM_{CO}\left(15\%O_2\right)=1.E6\frac{X_{CO}}{1-X_{H_2O}}\frac{0.21-0.15}{0.21-\frac{X_{O_2}}{1-X_{H_2O}}}$	All Closed Homogeneous, PSR, PFR, and Premixed Flame Reactors
Parts Per Million NO Dry Basis	The Gas-phase volumetric fraction of NO expressed in parts per million, after removing the volumetric contribution of water. The defining equation is the analogous to the equation for CO.	All Closed Homogeneous, PSR, PFR, and Premixed Flame Reactors
Parts Per	The Gas-phase volumetric fraction of NO expressed in parts per million, after removing the volumetric	All Closed Homogeneous,

Variable	Definition	Applicable Reactor Models
Million NO Dry Basis 15% O2 Correction	contribution of water and correcting to 15% Oxygen. The defining equation is the analogous to the equation for CO.	PSR, PFR, and Premixed Flame Reactors
Parts Per Million NOx Dry Basis	The Gas-phase volumetric fraction of NOx expressed in parts per million, after removing the volumetric contribution of water. The defining equation is the analogous to the equation for CO, but NOx includes the volumetric contributions of NO, NO2 and N2O.	All Closed Homogeneous, PSR, PFR, and Premixed Flame Reactors
Parts Per Million NOx Dry Basis 15% O2 Correction	The Gas-phase volumetric fraction of NOx expressed in parts per million, after removing the volumetric contribution of water and correcting to 15% Oxygen. The defining equation is the analogous to the equation for CO., but NOx includes the volumetric contributions of NO, NO2 and N2O.	All Closed Homogeneous, PSR, PFR, and Premixed Flame Reactors
Rate of Production	Species rates of production are calculated based on the local chemical state at each time or position point in the solution. Values are given in per-volume units for gas-phase reactions and per-surface-area for surface reactions. Contributions to net species production rates by each reaction or total production rates can be selected. Note that selecting to include contributions from all reactions may result in too much data to process in the Visualizer, so should be used with caution when the mechanism is large.	All
Sensible Enthalpy	Mass averaged enthalpy minus mass averaged enthalpy at STP.	All
Shear Strain Rate	Local rate of change in the "scaled" radial velocity (*v/r*) with respect to distance.	Opposed Flow Flame and CVD Reactors
Speed of Sound	The speed of sound traveling through the mixture.	All
Unburned Hydrocarbons	The Unburned Hydrocarbons (UH) value is defined as $UH(ppmC) = 10^6 \times \sum_{\substack{\text{species} \\ \text{containing} \\ C, H \text{ elements} \\ \text{only}}} nC_i X_i$	All Closed Homogeneous, PSR, and PFR Reactors

Variable	Definition	Applicable Reactor Models
	where nC_i is the number of carbon atoms per molecule in species *i*, and X_i is the mole fraction of species *i*. Here, hydrocarbons are those molecules that contain one or more of both the elements carbon (C) and hydrogen (H), and no other elements.	
Volatile Organic Compounds	The Volatile Organic Compounds (VOC) value is defined as: $(VOC)(ppmC) = 10^6 \times \sum_{\substack{\text{all species} \\ \text{containing} \\ C,H \text{ elements}}} nC_i X_i$ where nC_i is the number of carbon atoms per molecule in species *i*, and X_i is the mole fraction of species *i*. Here, a volatile organic compound is defined as a species containing one or more of both the elements carbon (C) and hydrogen (H), but the molecule may include other elements, such as oxygen (O) or nitrogen (N).	All

Chapter 2: The Graphical Post-Processor

The Visualizer is launched from within the Ansys Chemkin interface from the Analyze Results panel, using the **Plot Results** option, with the **Use Chemkin Visualizer** option checked. The basic workflow for visualization is to load `.ckcsv` or `.csv` file(s), display plots, and optionally export a subset of data for subsequent use. The Chemkin Visualizer does not directly read or process Chemkin solution files (XMLdata.zip) because the Analyze Results capability in the Chemkin interface handles this task. This chapter describes how to operate the Visualizer to accomplish these tasks:

- Choose data for graphical display
- Edit the properties of a plot
- Choose from available data sources

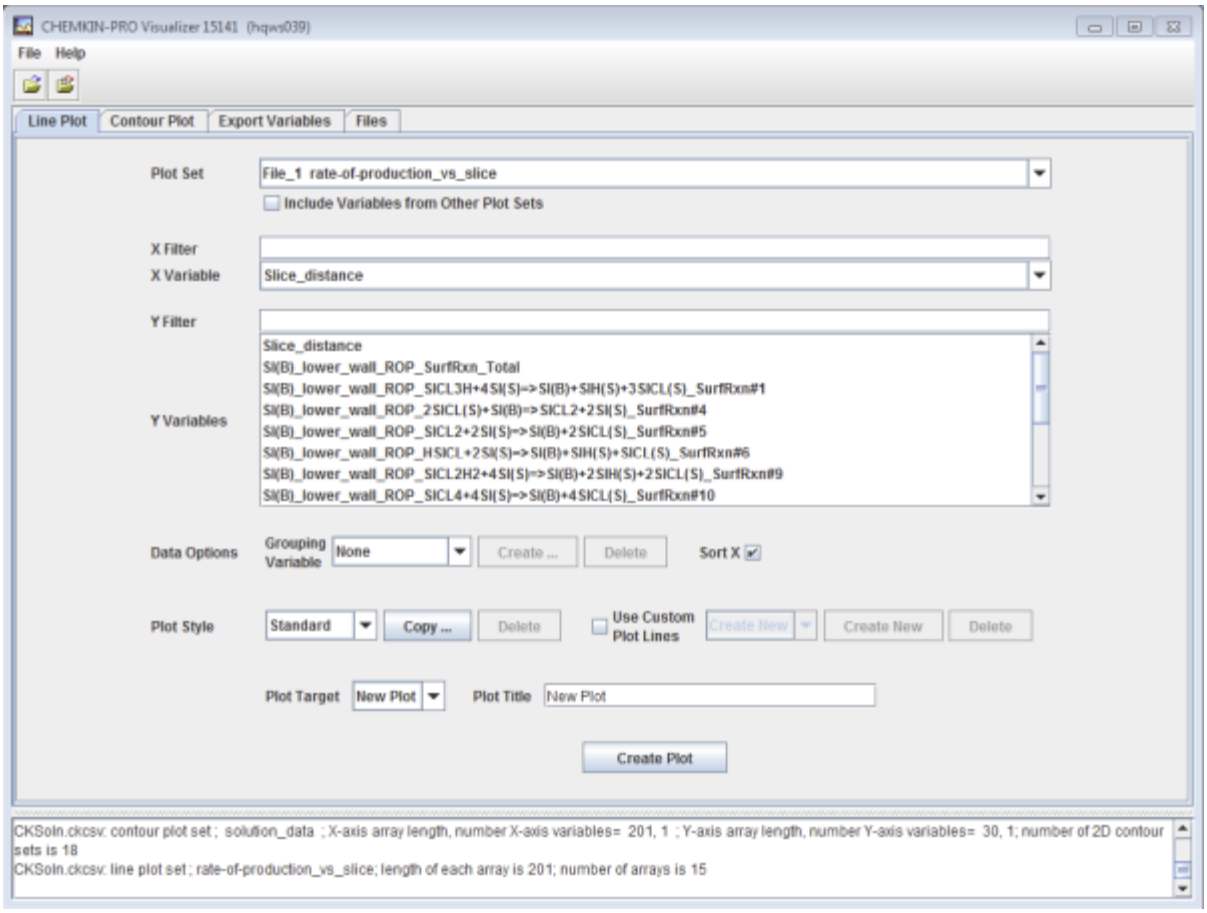
This section provides a more complete description of the elements of the Ansys Chemkin Graphical Visualizer. The information here includes descriptions of menus and buttons as well as hints on program features.

2.1. Overview of Interface

2.1.1. Control Panel

The Ansys Chemkin Visualizer provides a control panel for creating line and contour plots, including defining the plot style criteria, and exporting the plot data. Once plot data have been loaded, the tabs of this plot control panel are displayed, as shown in Figure 2.1: Line Plot Tab (p. 8). If you Cancel during the initial load of plot data, the panel's tabs are not shown until you use the **File > Open** or **File > Import CSV Data Plot** command.

Figure 2.1: Line Plot Tab



Once data are loaded, the control panel's tabs are presented with the Line Plot tab active. This panel is described in detail in the following sections. In addition to these tabs, there are drop-down menus (**File** and **Help**) and a data-loading status window at the bottom of the control panel.

2.1.1.1. Menus/Navigation

The menu bar located at the top of the control panel has two menus: **File** and **Help**. These are described in the following sections.

2.1.1.1.1. File Menu

The **File** pull-down menu is located at the left end of the Ansys Chemkin Visualizer menu bar. There are three operations available in the Visualizer: **Open**, **Import CSV Data**, and **Exit**. These are described below.

- *Open Option*

  The **Open** option allows you to open an exported solution data set having a *.ckcsv* file extension. These files are described in Overview of Solution Data Available from CHEMKIN (p. 1). Selecting the **Open** option displays a file browser on your computer for selecting an existing solution file. Once the file (or multiple files) is selected, the program will attempt to read the data in the file. If there are any difficulties reading the file, a message will appear in the Message Box at the bottom of the Chemkin Visualizer window.

- *Import CSV Data Option*

  You can import x-y data from plain text files into the Ansys Chemkin Visualizer using the **Import CSV Data** option in the **File** menu. The import utility expects to find columns of data, delimited by commas. Selecting the **Import** option opens a dialog box where you can identify how the file header information is provided. If you click **OK** to read in the data and the import utility encounters errors reading the specified format, you will receive a message in the Message Box, and the data will not be imported.

- *Exit option*

  The **Exit** option will exit the Ansys Chemkin Visualizer.

2.1.1.1.2. Help Menu

The **Help** menu contains a link to open Ansys Chemkin Online Help and documentation at the Ansys Help site.

2.1.1.2. Messages

The Message Box, located at the bottom of the control panel, helps you to follow the progress of the post-processing steps. The messages tell you what command is being executed, when it has finished executing, and whether or not the process has completed successfully.

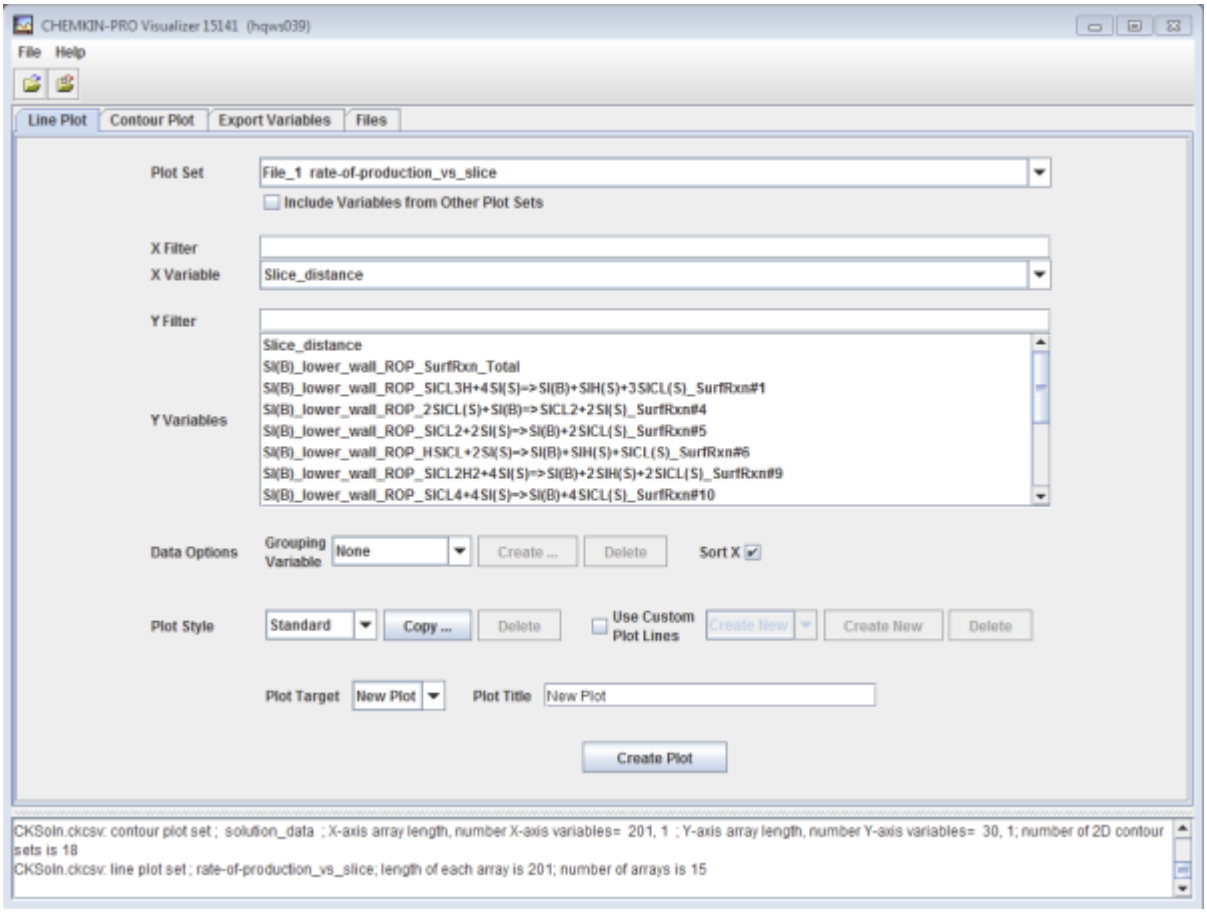
2.1.2. Control Tabs

Within the Control panel, below the menu toolbar, are a series of Control Tabs from left to right that allow switching between different control panels. The default control tab is the Line Plot tab. The Contour Plot tab allows 3-D contour data to be displayed. The remaining Control Tabs allow export of the data that is being considered in the plotting session and a read-only display of the data files that have been opened for use. Details on the inputs for each of these Control Tabs are in the following sections.

2.1.2.1. Line Plot Tab

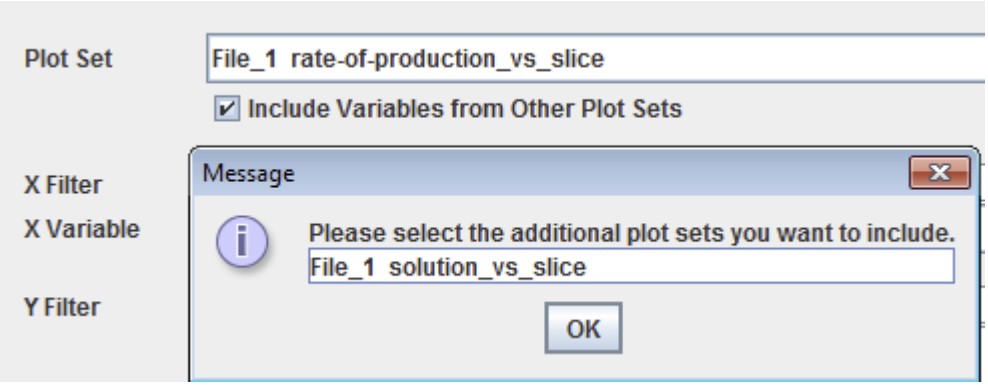
Line Plot Type

Figure 2.2: Line Plot Tab



- **Include Variables from Other Plot Sets** - By default, only variables for a single plot set are available for selection. For instance, slice1 may contain distance (or time) and several dependent variables, such as mass fractions, temperature, pressure, etc. Any 2 variables can be used to create an XY line plot. In some of the 1-D reactor models and in parameter studies, there may be many plot sets created; such as slices at varying distances along a shear-layer flow channel or a solution set that just contains wall data as a function of axial distance. As long as the dimensions of the solution sets are compatible, you can plot solutions from different solution sets on the same plot. To do that, use the **Include Variables from Other Plot Sets** check box near the top of the tab. Clicking this box will activate a message dialog that allows you to specify more than one plot set from which to select XY variables. Only those plot sets with the same number of items will be available for selection, as shown in Figure 2.3: Select Additional Plot Sets dialog (p. 11):

Figure 2.3: Select Additional Plot Sets dialog



- **X Filter** - Narrows the list displayed for X Variable to only those variables whose names start with the string typed into the filter.

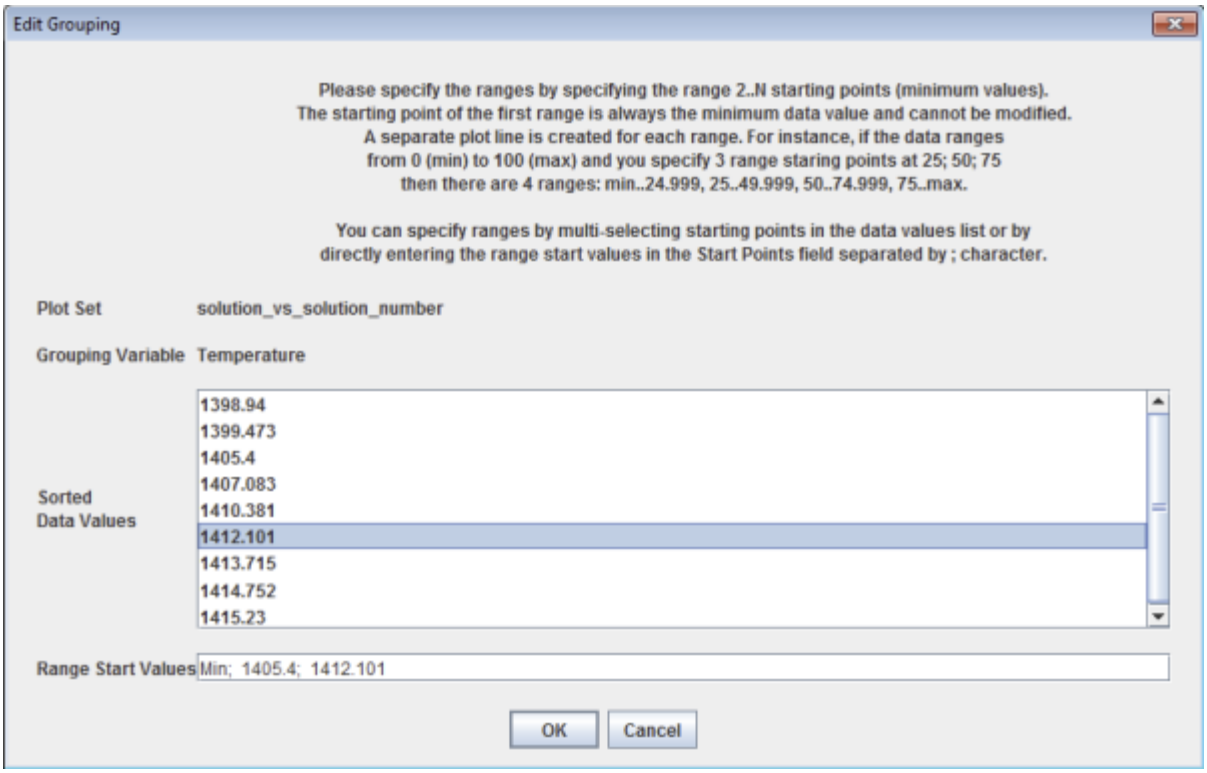
  X Variable - The independent variable for the XY line plot.

  Y Filter - Narrows the list displayed for Y Variable to only those variables whose names start with the string typed into the filter.

  Y Variable - The dependent variable(s) for the XY line plot(s). You can select one or multiple Y variables to plot against the X variable.

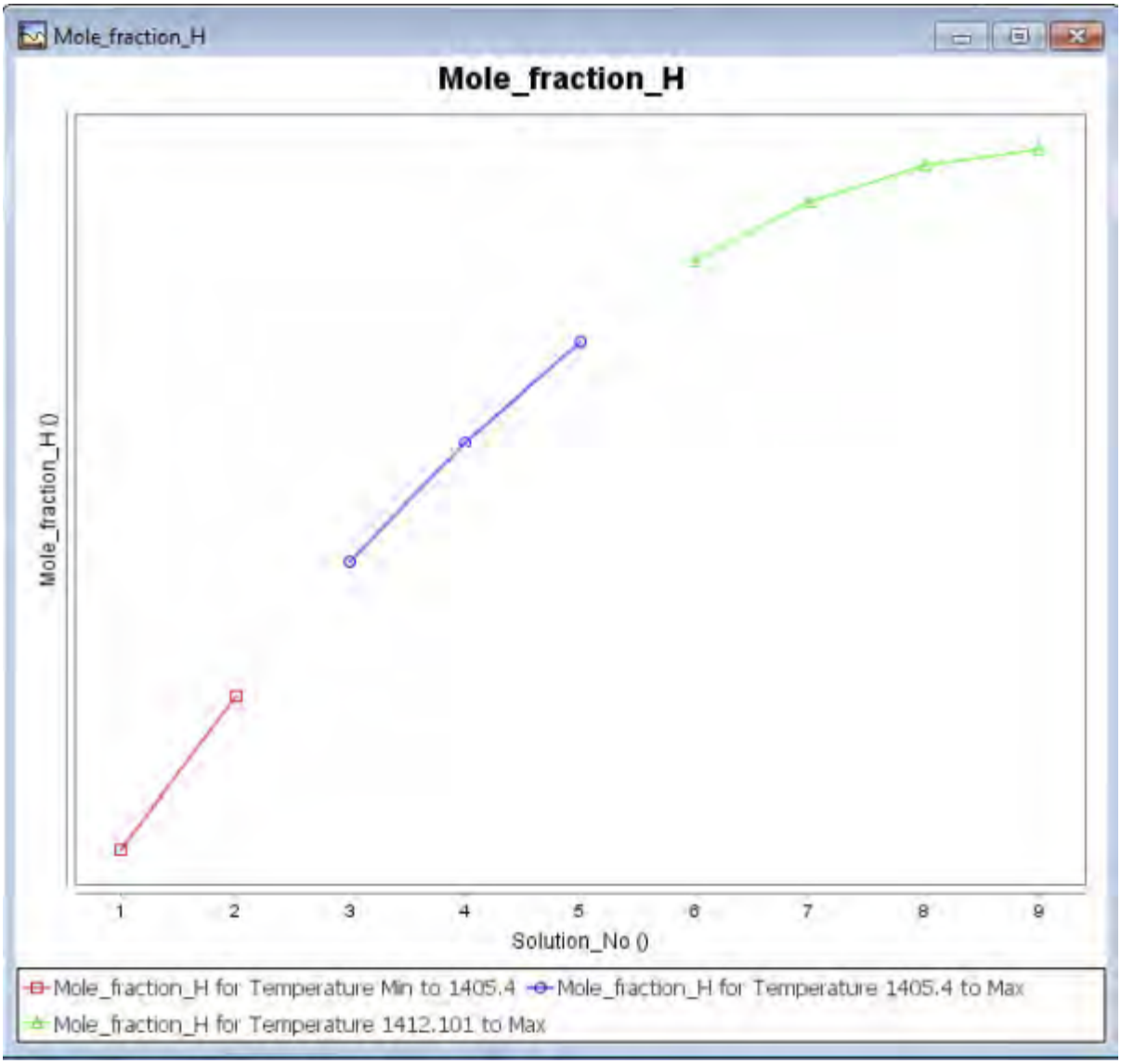
  Grouping Variable - This drop list allows you to select a 3rd variable (neither X nor Y) from the same plot set (or merged plot sets), which will be used to subdivide the XY plot points into multiple plot line segments. Use the **Create New** option within the drop list to define a new grouping variable. Figure 2.4: Select Grouping Ranges dialog (p. 12) shows an example dialog with **Temperature** selected to be the grouping variable.

Figure 2.4: Select Grouping Ranges dialog



- The resulting plot of Solution No. versus Mole fraction H Figure 2.5: Plot lines resulting from multiple range start points (p. 13) (Figure 2-4) shows that adding two range start points (in addition to the Min value, which always starts the first range) results in three plot line segments.

Figure 2.5: Plot lines resulting from multiple range start points



- **Sort on X** - Check this box to cause the X variable to be sorted (only for this plot). Most Ansys Chemkin independent variables are already sorted, but imported data may not be sorted. Since the line plot is essentially a connection of line segments from one XY point to the next, you may need to sort the X variable in some cases.

  Plot Style - The default Standard plot style can be supplemented by as many alternative plot styles as you would like using either Create New style or the Copy button to make a copy of the Standard style and then modify it. The Plot Style dialog is described more fully in Section 2.1.2.2.

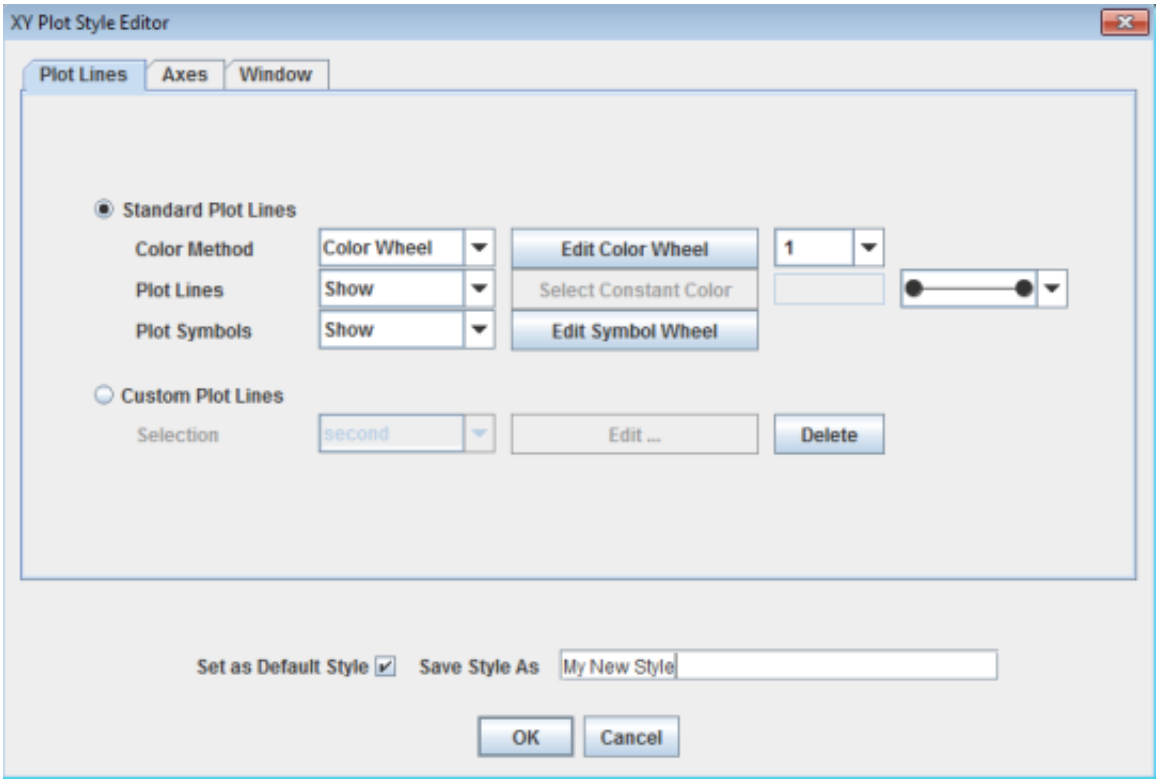
  Use Custom Plot Lines - This setting supplements the Plot Style and allows even more control over how each plot line is displayed. This dialog is also described more fully below.

  Plot Target - By default, each plot is displayed in a new window. For line plots, you can select to have the plot line(s) added into an existing plot window by selecting the specific plot name from this droplist. If you choose a different Plot Style or Custom Plot Lines setting, these style and settings are applied to all the plot lines including those previously plotted.

2.1.2.2. Plot Style Dialog

The Plot Style dialog allows you to define the way your plot lines, axes, labels, and other elements are rendered. You have much more ability to control the rendering as the plot is being generated than once the plot window is created, and you can save your style choices for reuse. The Plot Style dialog panel has three tabs, as shown in Figure 2.6: Plot Style dialog (p. 14).

Figure 2.6: Plot Style dialog



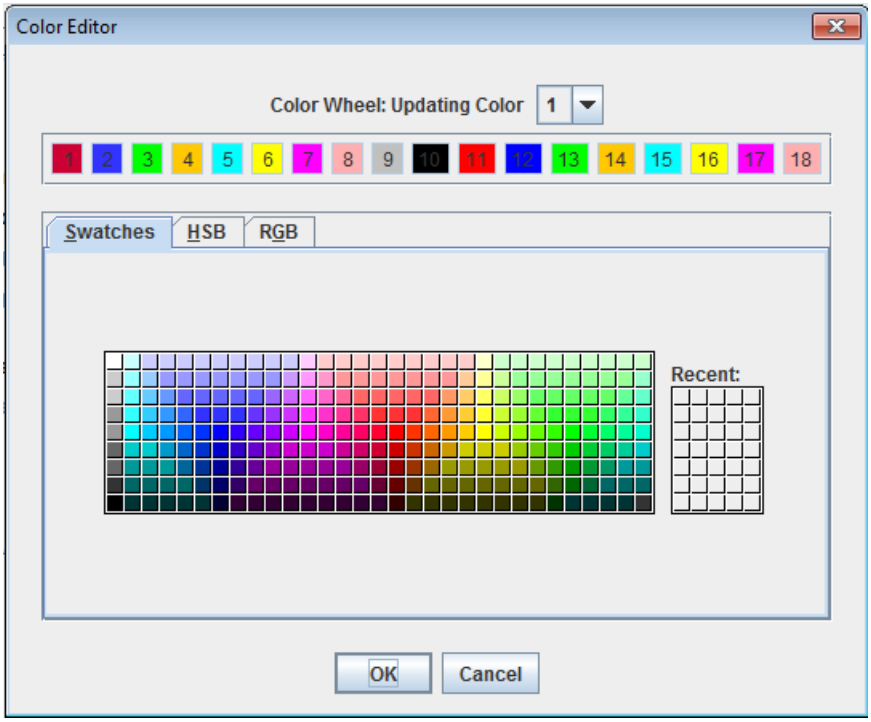
2.1.2.2.1. Plot Lines tab

Standard Plot Lines or Custom Plot Lines - The first choice is whether to use **Standard Plot Lines** or **Custom Plot Lines**. The standard plot lines style option allows you to select either constant colors or select a color "wheel" (a list of colors that are used in succession for the 1st, 2nd, … lines of a plot). You can choose whether lines, symbols, or both are displayed and control the line thickness. The symbol wheel behaves analogously to the color wheel. The **Custom Plot Lines** option uses a special custom plot lines style (a named **Custom Plot Lines** style) defined in a separate dialog. This controls the color, symbol, line style, etc., for each plot line separately and gives you maximum control in defining your plot appearance.

- **Color Method** - This drop-list allows you to select from either a constant color or using the color wheel. The **Edit Color Wheel** button allows you to modify the color wheel values and select different colors to be used. There is only one color wheel, so this change affects all future plots generated using the color wheel. The **Integer** drop-list on the right is the starting point within the Color Wheel for the first plot line. You can specify this differently within each **Plot Style** if you wish to do so. Since the Color Wheel has 18 colors and you are unlikely to create plots with that many lines, you can use this to employ different segments of the Color Wheel in different Plot Styles. Click on the Color Swatch you prefer for each of the 18 colors shown in the numbered list. You can select 18 different colors or reuse colors by clicking on the same

swatch. You can use the HSB or RGB tabs to specify the colors numerically. See Figure 2.7: Color Editor (p. 15).

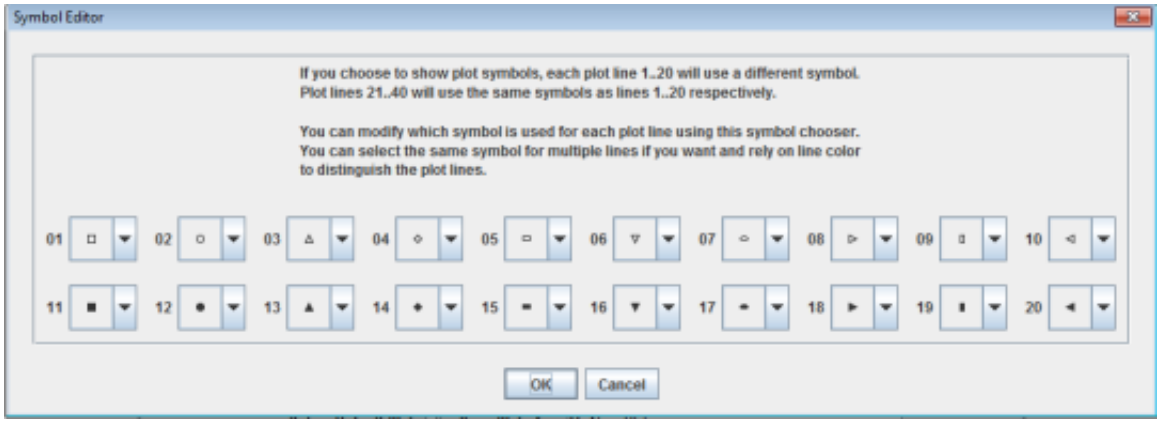
Figure 2.7: Color Editor



Plot Lines - Use this to show or hide the plot lines. If you selected the **Constant Color** option for **Color Method**, then specify that color here. You can also choose the line style that will be used for all plot lines when this Plot Style is used.

Plot Symbols - Use this to show or hide the plot symbols. Use the **Edit Symbol Wheel** button to show a dialog that allows you to select the order in which the plot symbols are assigned to plot lines.

Figure 2.8: Symbol Editor



- **Selection (of Custom Plot Lines)** - Use this to select an existing **Custom Plot Lines** style element or use **Create New** to define a new **Custom Plot Lines** style. This custom style element allows a different plot line style for each plot line, as shown here:

Figure 2.9: XY Custom Plot Line Style Editor

2.1.2.3. Contour Plot Tab

Contour Plot Type

Contour Set - The set contains a consistent set of data that can be used for constructing a contour plot. Specify the X, Y, and Z dimension values.

X Filter - Narrows the list displayed for X Variable to only those variables whose names start with the string typed into the filter.

X Variable - The first independent variable for the contour plot. For contour plots, the X and Y axis choices are vectors and the Z choice is a 2-D plane of points corresponding to the X/Y values. Only one choice may be made for the X variable from a drop-list of choices.

Y Filter - Narrows the list displayed for Y Variable to only those variables whose names start with the string typed into the filter.

Y Variable - The second independent variable for the contour plot. As shown above, this is a drop-list field for selecting the Y axis of a contour plot.

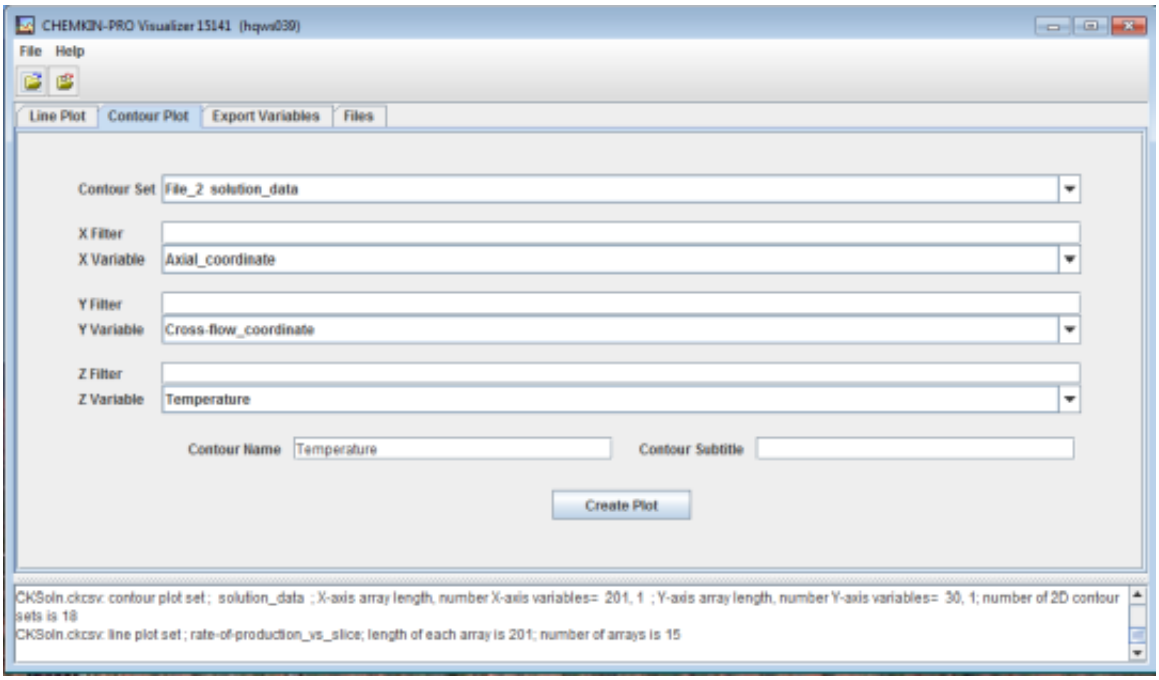
Z Variable - The dependent variable for a contour plot. This is a 2-D plane for contour plot and only one selection can be made per contour plot. No over-plotting of contour plots is allowed.

Contour Name - The name of the plot created for display on the plot and for contour plot history file.

Contour Subtitle - A smaller font subtitle can also be displayed on the contour plot.

Create Contour - This button triggers the creation of a new window containing the requested plot.

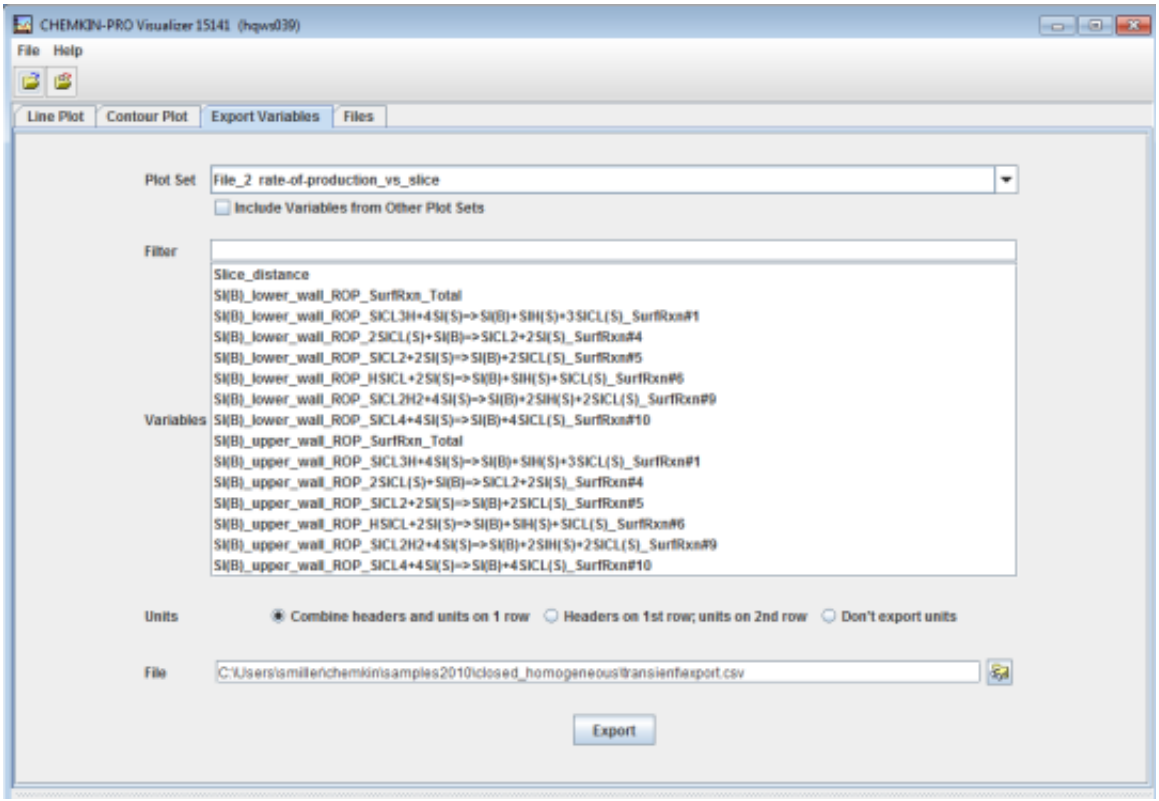
Figure 2.10: Contour Plot tab



2.1.2.4. Export Variables Tab

The Export Variables tab allows you to export subsets of XY line plot data from the current session. An example of the Export Variables tab is shown in Figure 2.11: Export Variables Tab - Export Line Plot data to CSV file (p. 18). The possible operations that can be performed on the data from this panel are described in the following descriptions.

Figure 2.11: Export Variables Tab - Export Line Plot data to CSV file



Include Variables from Other Plot Sets - By default, only variables for a single plot set are available for selection. Clicking this box will activate a message dialog that allows you to specify more than one plot set from which to select variables. Only those plot sets with the same number of items will be available for selection, as shown in Figure 2.3: Select Additional Plot Sets dialog (p. 11).

- **Filter** - Narrows the list displayed for Variable to only those variables whose names start with the string typed into the filter.
- **Variables** - Variables to export from the plot set(s)
- **Data Type and Variable choices** - The choices displayed here are the same choices as those provided in the **Line Plot Tab** (Plot Lines tab (p. 14)): Line Plot or Contour Plot, along with selecting Plot Sets and variables.
- **Units** - The header row and units format choice determines the format of the exported file.
- **Export** button - Launches a file selection dialog that allows selection of the file (new or existing) that will receive the exported data. If the file already exists, it will be overwritten, not appended.

2.1.2.5. Files Tab

This tab simply presents a reference list of the data files that have been loaded into the Visualizer session. If all of the plot/contour sets loaded from a file are freed from memory, the file will still be listed. This information is provided here as a cross-reference to the file numbers used when displaying the **Contour Set** and **Plot Set** choices.

2.1.3. Selecting Results to Load from a Solution File

When you click the **Analyze Results** option on the Ansys Chemkin Interface (see Post-process the Solution in the *Chemkin Getting Started Guide*) or when you open a solution file from within the Chemkin Visualizer, the Select File and then the Select Results to Load from Solution File dialogs will appear. This dialog (see Figure 2.12: Results to Import—Solution Sets (p. 20)) is divided into three tabs: **Solutions Sets**, **Species/Variables** and **Units of Measure**.

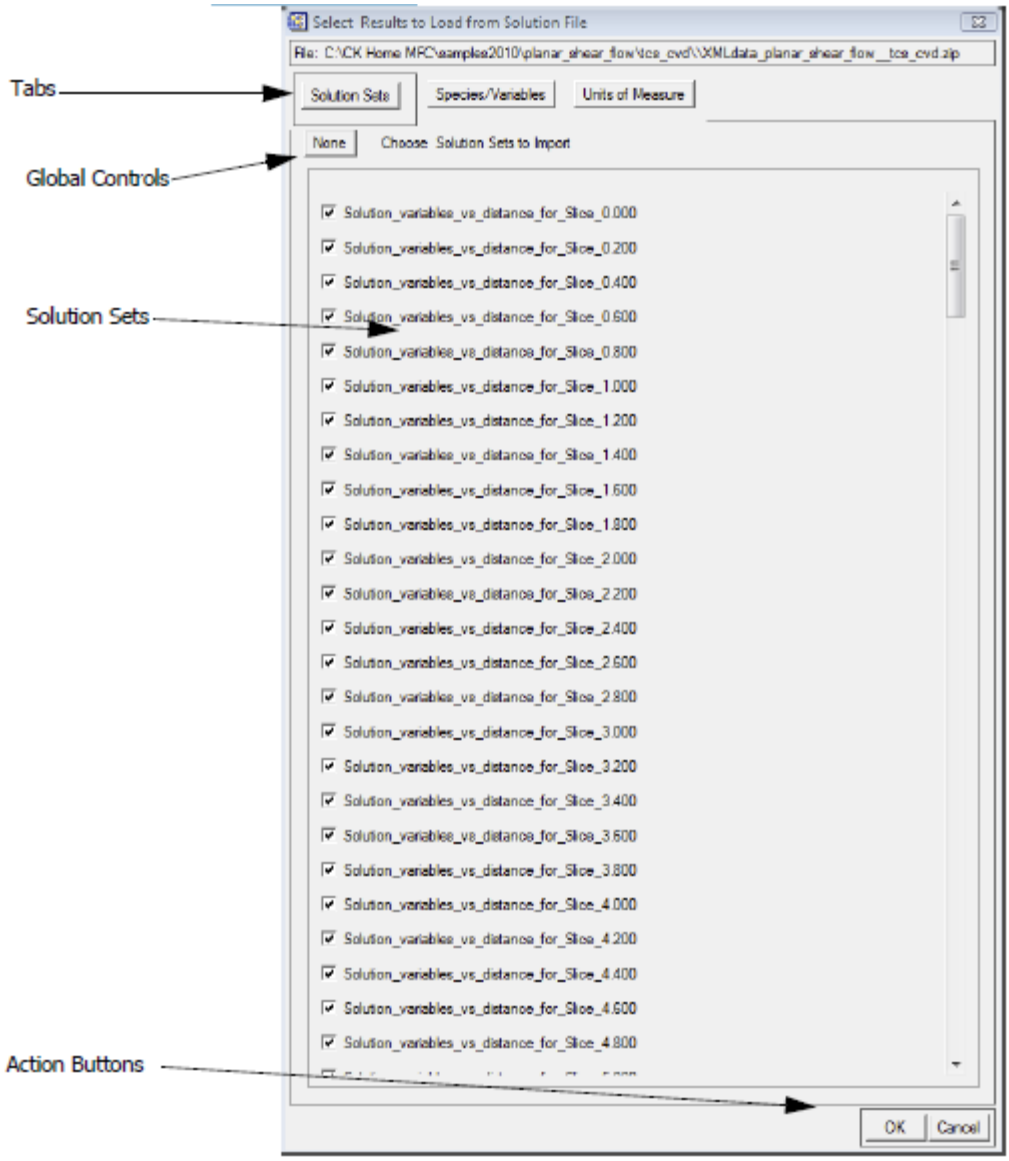
The dialog also contains two action buttons, **OK** and **Cancel**. **OK** will proceed to the Visualizer Control Panel. **Cancel** will exit out of the Ansys Chemkin Visualizer.

The Solutions Sets tab is displayed by default. If Ansys Chemkin produces only one solution set, the dialog will instead display the Species/Variable tab and the Solutions Sets tab will be disabled. Each tab is described in the sections below.

2.1.3.1. Solution Sets Tab

The Solutions Sets tab shown in Figure 2.12: Results to Import—Solution Sets (p. 20) allows you to choose which solution set you would like to plot.

Figure 2.12: Results to Import—Solution Sets

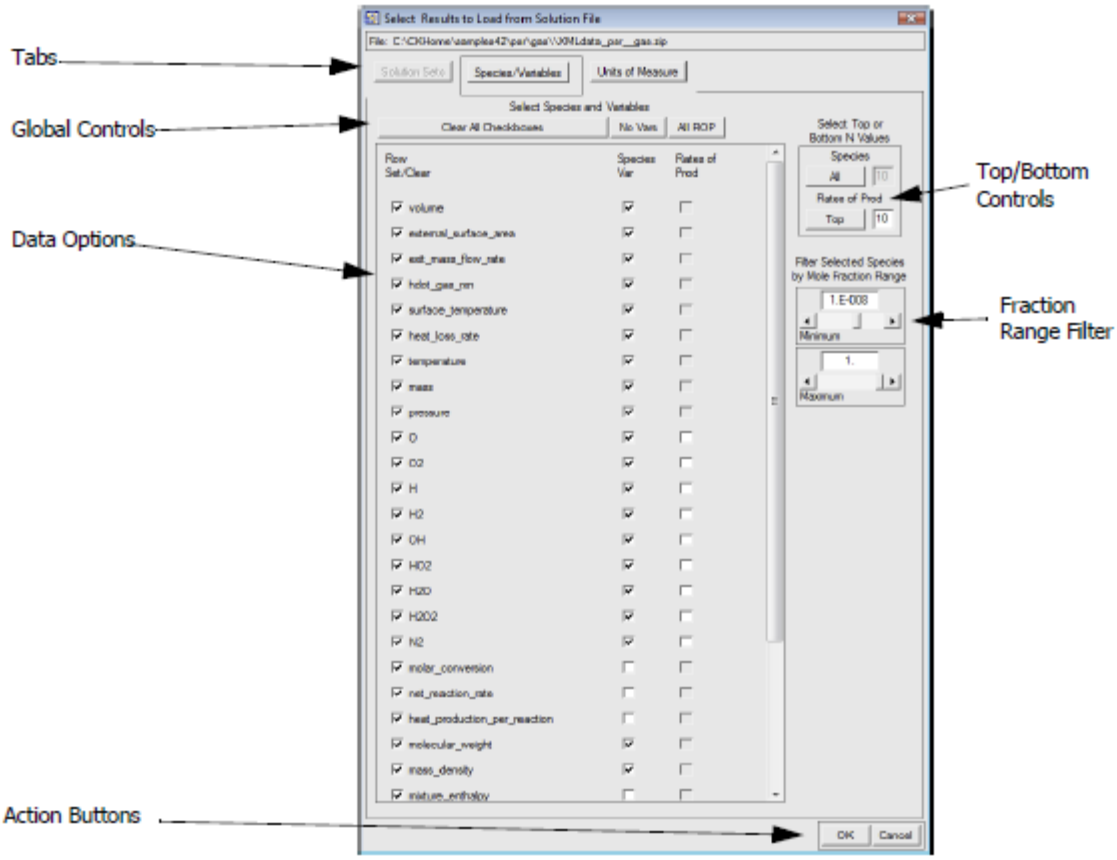


The **None/All** toggle button allows you to select or deselect all the solution sets at one time. Additionally, there is a series of check boxes next to each of the individual solution sets available from the Ansys Chemkin solution. The check boxes can be selected individually or the **None/All** toggle button can be used for global selections.

2.1.3.2. Species/Variables Tab

The Species/Variables tab shown in Figure 2.13: Results to Import—Species/Variables (p. 21) allows you to select the specific data to be loaded into the Ansys Chemkin Visualizer. The tab includes several methods for selecting data, including the **Global Controls**, Data Options check boxes, **Top/Bottom Controls** and the **Fraction Range Filter** areas.

Figure 2.13: Results to Import—Species/Variables



2.1.3.2.1. Global Controls

The global controls consist of toggle buttons that allow you to quickly select or deselect species and variables you wish to plot. Depending on the Ansys Chemkin reactor model there will be four toggle buttons:

- **Clear All** Check boxes toggle button deselects all the species and variables. This can be useful if you only want to select a few items.
- **No Vars/All Vars** toggle button selects or deselects all items in the Species/Variable column. The Species/Variable column lists all the available species or other variable data.
- **No Sens/All Sens** toggle button select or deselects all items in the Sensitivity column, when sensitivity data are available.
- **No ROP/All ROP** toggle button selects or deselects all the items in the Rate of Production column. This column allows selection of rates of production contributions of reactions to each species by name. You may need to scroll the dialog to find a specific species in the list.

Depending on the output created by an Ansys Chemkin reactor model, some of the columns may not appear. For example, if sensitivity output was not selected in the Chemkin interface prior to generating the Chemkin Solution, the dialog will not include a Sensitivity column (as in Figure 2.13: Results to Import—Species/Variables (p. 21)).

2.1.3.2.2. Data Options Check Boxes

The Species/Variables tab lists all the data that can be plotted by the Ansys Chemkin Visualizer with a check box to the left of each row or item within the row that can be selected or deselected to produce a specific data element. The first column allows selection or deselection of a row in the data set and the other check boxes can the be selected or deselected on an individual basis.

In addition to the variables calculated as part of the Ansys Chemkin solution, there are many derived calculations listed. These include species net rates of production (ROP), net rate of progress of reactions (net_reaction_rate), and in some cases, molar conversion of principal components. When ROP is selected for a species, the net rates of production of that species for each reaction will be included in the data for post-processing, subject to the filters in the **Top/Bottom Controls**. When net_reaction_rate is selected, the net rate of progress of all reactions will be included in the data for post-processing (these are not subject to the **Top/Bottom Controls)**. Rates of production and rates of progress of reactions are defined in detail in the Chemkin Theory Manual.

Selecting molar conversions will result in the calculation of molar conversion rates for any species that has an initial or inlet mole fraction greater than 1.E-9. The molar conversions are simply defined as the percent change in mole fraction and therefore do not account for changes in total moles of the system due to large temperature or pressure changes. This latter calculation is useful in isobaric systems where gas-phase temperature changes are small. For reactor models that provide temporal or spatial data, the molar conversions are also provided as a function of time or distance.

2.1.3.2.3. Top/Bottom Controls

The Top/Bottom Controls allow filtering of the values of species fractions (**Species**), reaction sensitivity (**Sens**) or species rates of production (**Rates of Prod**) that will be brought into the Visualizer. You may select the Top (or Bottom) values (for example, the 10 species with the largest mole fractions). The number can be specified in the available text box (default is **10**), while the **All/Top/Bottom** toggle button determines how the data will be filtered.

Note:

When you select top/bottom #N species in the post-processor for a transient problem, it picks the N number of species based on their maximum values throughout the reaction time. For example, at one point in time, species A may be present in very high amounts but species B may be high later in the reaction. Then maximum levels of both A and B will be used to order the top or bottom order of species.

2.1.3.2.4. Mole Fraction Range Filter

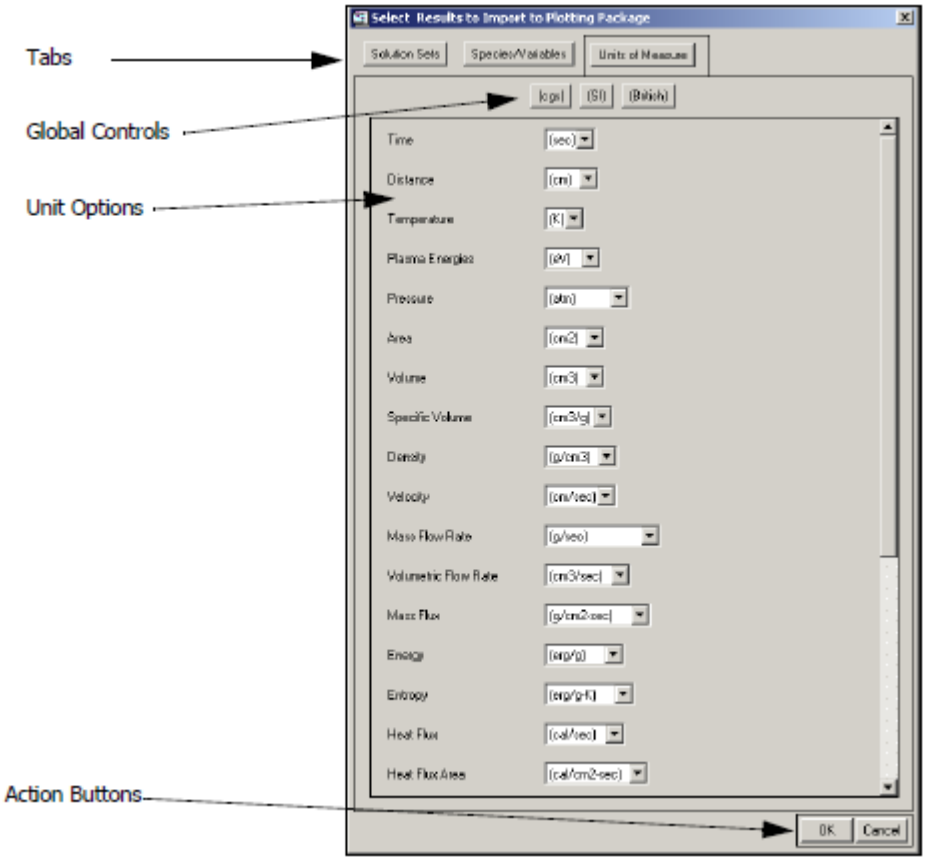
The **Mole Fraction Range Filter** provides an alternate method to selecting species for importing data into the post-processor. Here, you can select the range of species mole fractions in decades. Use either the **Minimum** and **Maximum** slider controls or type directly into the text boxes.

2.1.3.3. Units of Measure Tab

The Units of Measure tab shown in Figure 2.14: Results to Import—Units of Measure (p. 23) allows selection of the units of measure for the plot data. This tab consists of some Global Controls, as

well as controls of individual items. The default settings are based on User Preferences set in the Ansys Chemkin Preferences panel for the Visualizer.

Figure 2.14: Results to Import—Units of Measure



2.1.3.3.1. Global Controls

The global controls allow selection of a global system of units based on centimeter/gram/second (**cgs**), Système International d'Unités (**SI**) or British Units standards of measurement. Choose either one by clicking the **(cgs)** or **(SI)** or British buttons. These buttons will select a predetermined set of unit options in the list below, overriding any custom selections that were previously made.

2.1.3.3.2. Unit Options

You can customize the units of measure using a series of drop-down lists in the **Unit Options** area. These options temporarily override your default settings during the post-processing session. Default settings are controlled by the Preferences panel in the Ansys Chemkin Interface, as described in Managing Preferences.

2.2. Modifying Plot Displays

You can modify a line plot, once displayed, by using mouse motions to reposition the plot or using the context menu that appears when you right-click on the plot display. The context menu is not sensitive to your mouse position within the plot; there is only one context menu for line.

The context menu offers the following choices:

Figure 2.15: Line Plot—Context menu

2.2.1. Properties…

The **Properties…** choice brings up a multi-tab properties panel that allows you control over the axes displays and the plot title. The ability to modify the plot axes tick marks is especially useful and is not offered within the plot style options. Since these options are very straightforward, no further description is provided here. Briefly experiment with these options to see their impact. However, note that the context menu is only aware of the first plot line and hence the first Y axis. If you have selected to plot multiple Y values, you will need to use the style option of the plot selection panel to exert control over all the Y axes.

2.2.2. Save as…

The **Save as…** option allows you to save the plot as a .png format file.

2.2.3. Print…

The **Print…** option allows you to print the plot.

2.2.4. Selecting the Data Range (Region of Interest)

The remaining three options of **Zoom In**, **Zoom Out**, and **Auto Range** all control the region of interest. You can use a mouse rubber banding motion to select a region of interest. You can continue to refine that region of interest in successive rubber banding motions. You can undo those selections using the context menu's **Zoom Out** or **Auto Range**.

2.3. Modifying Contour Plot Displays

You can modify a contour plot, once displayed, by using mouse motions to reposition the plot or using the context menu that appears when you right-click the plot display. The context menu is not sensitive to your mouse position within the plot; there is only one context menu for contour plots. Contour plots also offer a toolbar because the mouse movements to control the 3-D positioning of the plot are less intuitive.

2.3.1. Zoom Options

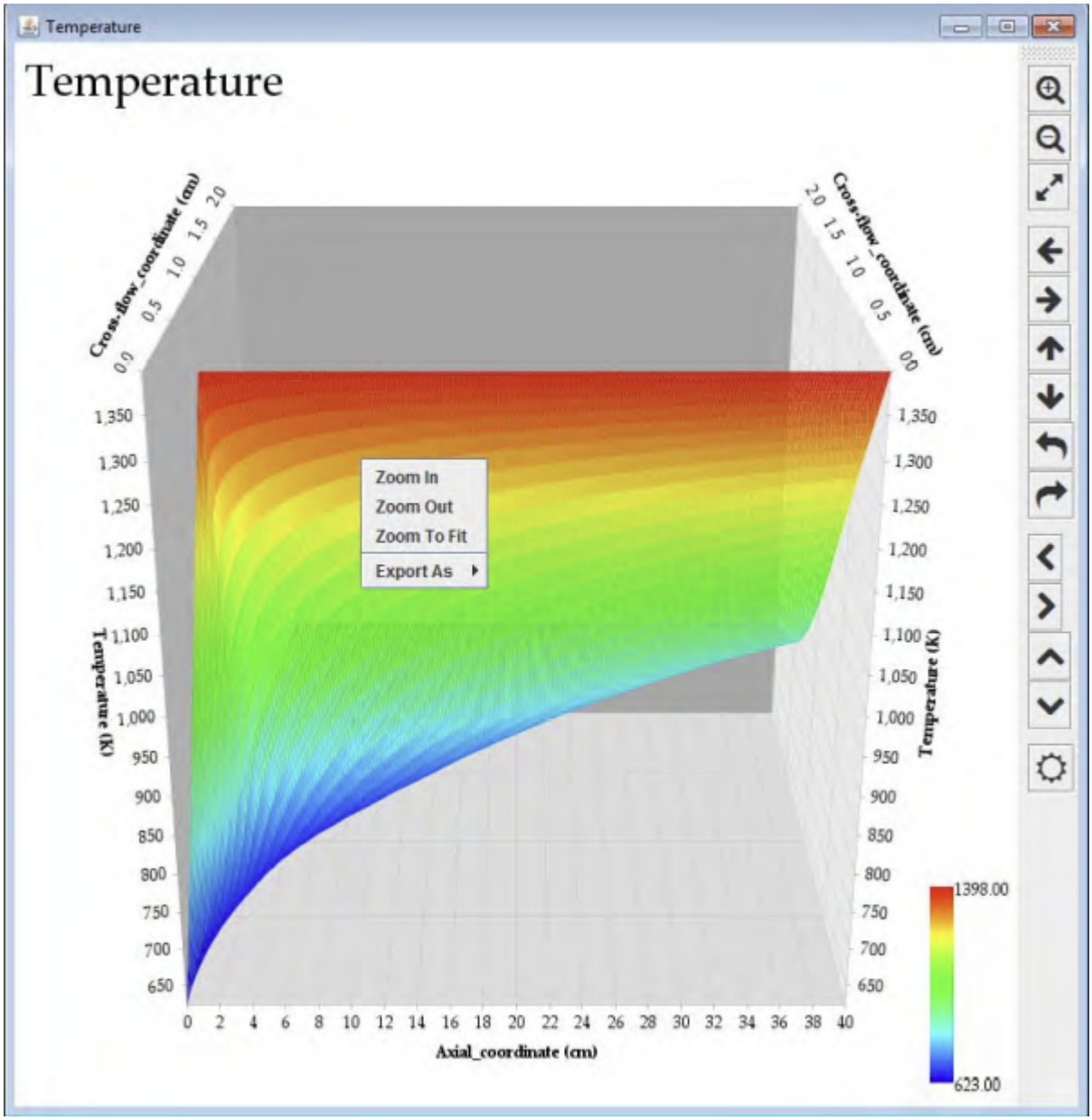
The zoom options on a contour plot are limited to a stepwise zoom-in or zoom-out operation. The **Zoom to Fit** option restores the contour plot to the initial sizing.

2.3.2. Export As

The **Export As** option allows you to export your plot to a pdf, jpg or png format file.

2.3.3. Tool Bar Options

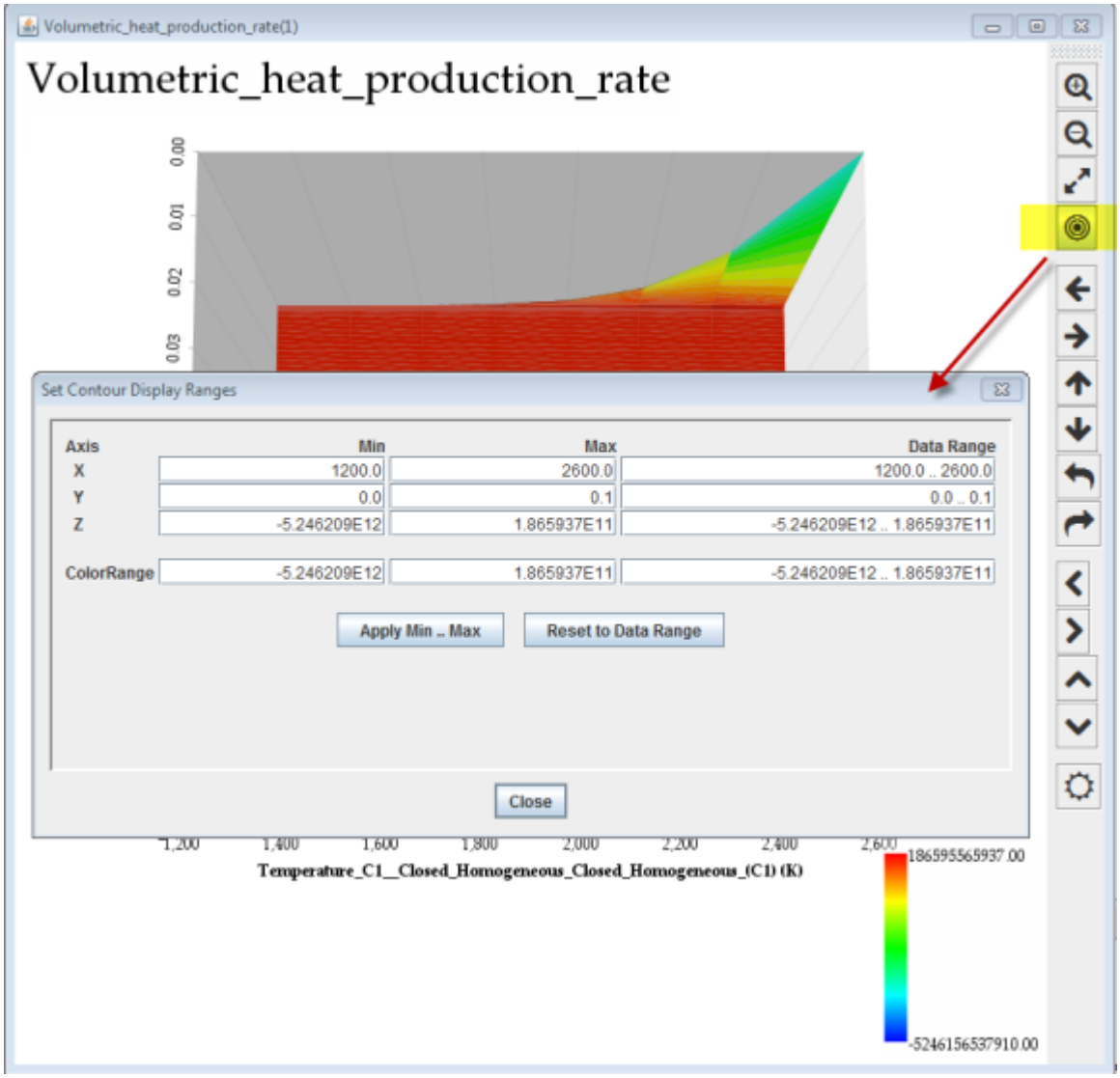
Figure 2.16: Contour Plot—Context menu displayed



From top-to-bottom as displayed in Figure 2.16: Contour Plot—Context menu displayed (p. 25), the tool bar options are broken into 4 groups. All of the tool bar buttons have mouse-over tool tips. The first 3 buttons provide the same Zoom In, Zoom Out, Zoom to Fit operations as the context menu.

The fourth button, as highlighted in Figure 2.17: Contour Plot—Set Contour Display Ranges (p. 26), opens a dialog to adjust the X, Y, Z, ranges displayed and the bounds of the color scale associated with the Z values.

Figure 2.17: Contour Plot—Set Contour Display Ranges



The next group of 6 buttons control the rotation of the 3-D image in the 3 dimensions. These operations are also performed with the mouse by clicking and holding the left mouse button while moving the mouse.

The next 4 buttons control the translation of the 3-D image in the X and Y directions. You can also perform these operations by clicking the left mouse button and moving the mouse—while holding down the **Alt** key.

The bottom button gives you access to control the light source used to light the contour. There is only one light source; multiple light sources are not currently supported.

Chapter 3: Post-Processing Alternatives

This chapter discusses alternative methods for processing results other than the Ansys Chemkin Visualizer or the Reaction Path Analyzer. Export to Microsoft Excel (Windows Only) (p. 27) discusses exporting the data to Microsoft Excel for analysis and GetSolution Data Conversion Utilities (p. 29) discusses the GetSolution utilities to prepare the data from Chemkin output for some other form of analysis.

3.1. Export to Microsoft Excel (Windows Only)

An option in the Ansys Chemkin Visualizer allows you to export all the selected solution data to an Excel workbook so Excel can be used to generate custom plots. This option serves as an alternative to Chemkin's native Visualizer on Windows platforms. The **Use Excel to Post-Process** option is available on the Select Post-Processing Variables panel after you have chosen to plot results using the Analyze Results node. If the option is selected when the **Process Solution Data** button is used, all the solution data will be collected in a single unsaved workbook in Excel. For a nominal run, the workbook includes the following worksheets:

- Basic solution data as selected by user in the Select Post-Processing Variables panel
- Single-point data (such as ignition delay time and flame speed) in a transient simulation or 1-D steady-state simulation if selected
- Sensitivity data if selected
- Rate-of-production data if selected

For a parameter study, the workbook includes the following worksheets:

- Basic solution data collected from each parameter study run
- Single-point data collected from each parameter study run if selected
- Sensitivity data collected from each parameter study run if selected
- Rate-of-production data collected from each parameter study run if selected
- Single-point data vs. the parameters varied in the parameter study
- End-point data in a transient simulation or 1-D steady-state simulation vs. the parameters varied in the parameter study

All the solution data loaded into Excel is in column-based format. Because Excel imposes a limit on the number of columns in a single worksheet, data sets that exceed this limit will be automatically divided up into subsets so that each subset will satisfy the limit. Please note that the contour data sets available to Ansys Chemkin's native Visualizer are not available to Excel because it cannot handle that type of data.

3.1.1. Excel Settings

Microsoft Excel security sometimes blocks processing Ansys Chemkin results. Follow these steps to enable Chemkin processing in your Excel installation. From Excel, access File > Options and select Trust Center and then Trust Center Settings. In the next screen, set the options to match those shown in Figure 3.2: Adjusting Excel security settings for Chemkin results post-processing, step 2 (p. 29).

Figure 3.1: Adjusting Excel security settings for Chemkin results post-processing, step 1

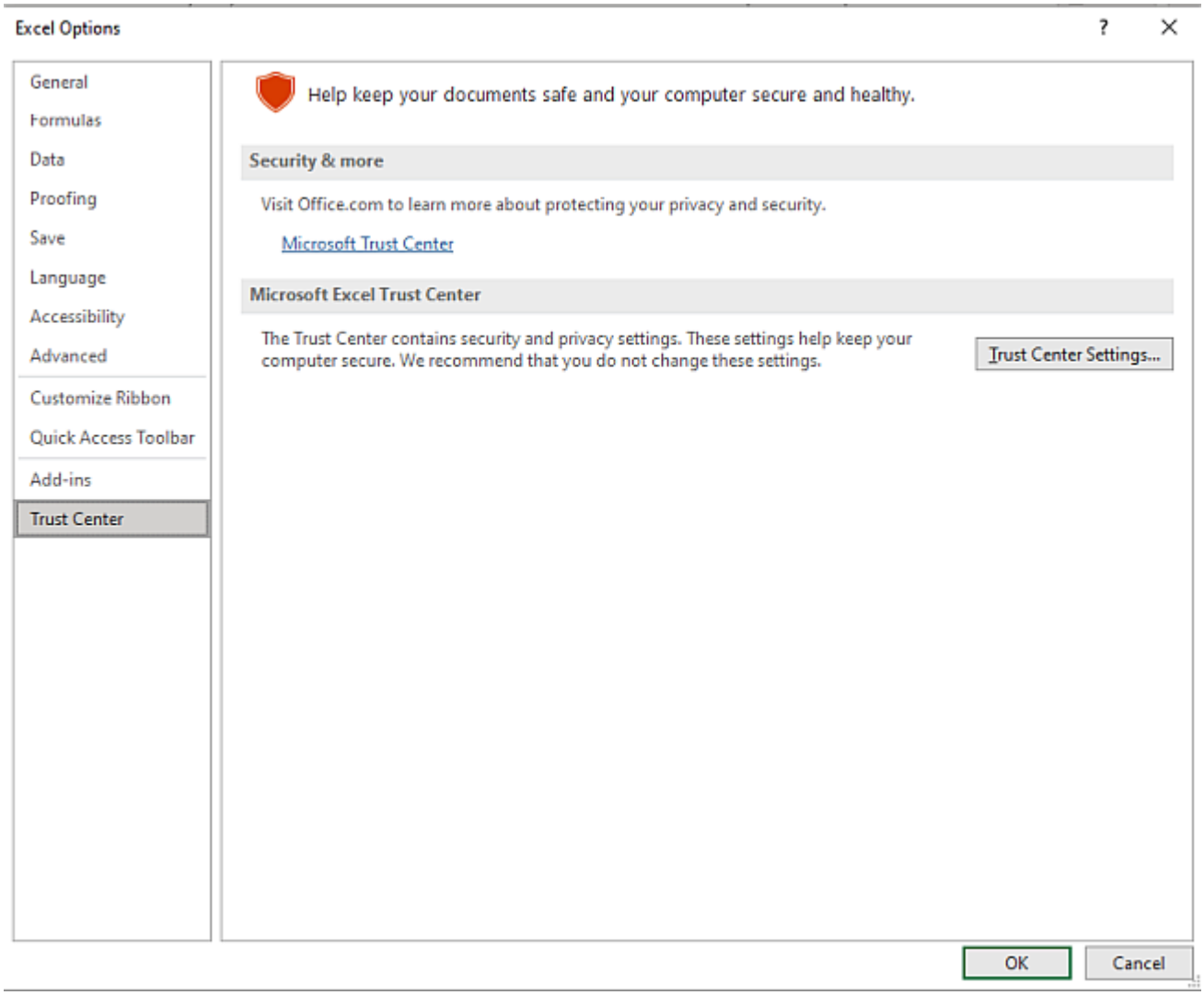
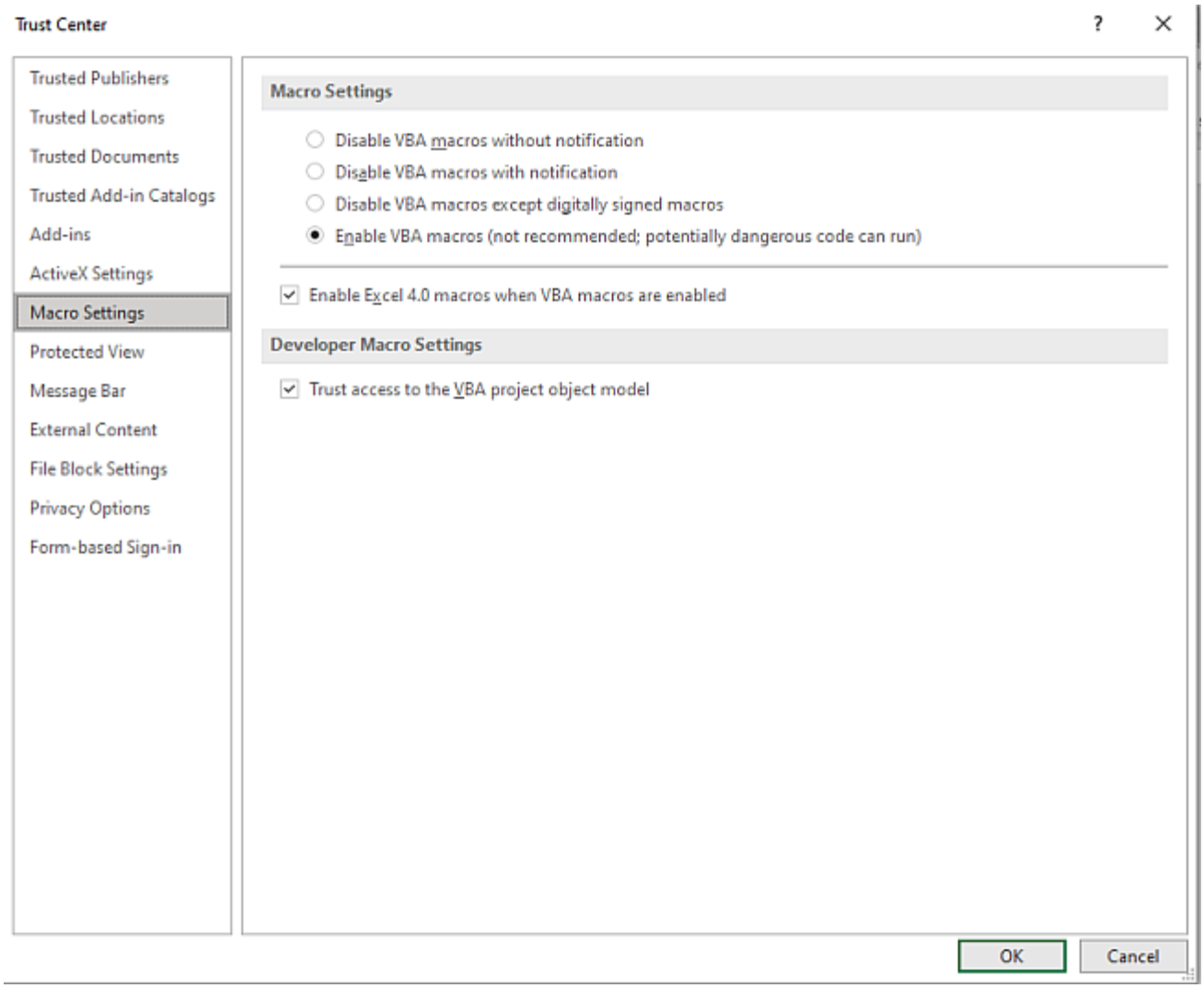


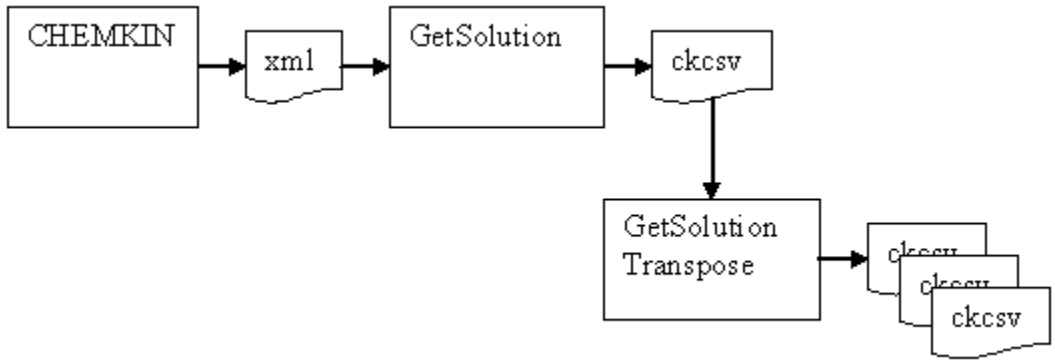
Figure 3.2: Adjusting Excel security settings for Chemkin results post-processing, step 2



3.2. GetSolution Data Conversion Utilities

As described in About This Manual (p. 1), post-processing of Ansys Chemkin simulations involves extracting and analyzing the data contained in the Solution Files (one per cluster in the reactor network) and in the pre-parsed post-processor files (*.ckcsv*) produced by the Run Parameter Study Facility. The Solution File is not directly readable, but there is a provided utility program called *GetSolution[.exe]* that reads it and converts it into *.ckcsv* format. The *.ckcsv* format is a comma-separated text file that is directly readable by scripts, but is organized in block structures for efficient use by the Visualizer. We also provide the *GetSolutionTranspose[.exe]* utility to further convert the *.ckcsv* file format into a set of separate plot set files with a more accessible column-based *.csv* format, compatible with Excel and other third-party packages. The GetSolution utility (and transpose option) can be run from either the command-line or from within the Chemkin Interface (under the **Utility** group or menu).

Figure 3.3: GetSolution Data Flow



The post-processing arguments for GetSolution are described in Table 3.1: GetSolution Arguments (p. 30). All arguments listed in the table are optional.

Table 3.1: GetSolution Arguments

Argument	Description
`-help`	GetSolution will display the help information.
`-listonly`	GetSolution will create a **CKSolnList.txt** file for user selections. For more details about *CKSolnList.txt*, see text below.
`-nosen`	GetSolution will skip the sensitivity data in XML solution file.
`-norop`	GetSolution will skip the rate-of-production data in XML solution file.
`-mass`	GetSolution will use mass fraction instead of mole fraction for species composition (by default mole fraction is used).
`-all`	GetSolution will export all species data sets including those consisting of only zero values (by default the all-zero data sets are skipped).
`-p`	GetSolution will specify a preference file that holds preferred units.
`preference_file`	The name of the preference file used with the -p argument. You will need to use the full path if the file is not in the working directory.
`XML_zipfile`	The name of the XML solution file, which must contain a **.zip** suffix. You must use the full path if the file is not in the working directory. If a file is not specified, the *XMLdata.zip* file located in your working directory will be used.
`abbrevi ation_file`	The name of a text file containing abbreviations of all variable names, which must contain a **.csv** suffix. This allows you to change the default labels of the variables used in the output file's data rows. You will need to use the full path if the file is not in the working directory. An example file named *abbreviations.csv* is provided in the *data* directory of your Ansys Chemkin installation.

3.2.1. Using the GetSolution Utility with Command Line Arguments Only

Please follow these instructions to run the GetSolution utility only:

1. Open a Command prompt or UNIX shell.
2. Make sure the full path to your Ansys Chemkin bin directory is included in your PATH environment variable (see Ansys Chemkin Windows Environment or Chemkin Linux Environment in the *Chemkin Getting Started Guide*).
3. Navigate to your working directory.
4. At the command line, type (one continuous line):

   ```
   GetSolution [-help] [-listonly] [-nosen] [-norop] [-mass] [-all] [-p] [preference_file] [XML_zipfile] [abbrev
   ```

   The bracketed words represent optional commands. See Table 3.1: GetSolution Arguments (p. 30) for further details.
5. GetSolution generates a comma-delimited text file named *CKSoln.ckcsv* and places it in your working directory. *CKSoln.ckcsv* can be imported into third party software such as Microsoft® Excel®.

3.2.2. Using the GetSolution Utility with CKSolnList.txt File

Please follow these instructions to run the GetSolution utility with a *CKSolnList.txt* file:

1. Open a Command prompt or UNIX shell.
2. Make sure the full path to your Ansys Chemkin bin directory is included in your PATH environment variable (see Ansys Chemkin Windows Environment or Chemkin Linux Environment).
3. Navigate to your working directory.
4. At the command line, type `GetSolution -listonly` to create a *CKSolnList.txt* file.
5. Edit the *CKSolnList.txt* file to make user selections. See The CKSolnList.txt File (p. 32) for a detailed look at the syntax of *CKSolnList.txt*.
6. At the command line, type (one continuous line):

   ```
   GetSolution [-help] [-nosen] [-norop] [-mass] [-all] [-p] [preference_file] [XML_zipfile] [abbreviation_file]
   ```

   The bracketed words represent optional commands. See Table 3.1: GetSolution Arguments (p. 30) for further details.
7. GetSolution generates a comma-delimited text file named *CKSoln.ckcsv* and places it in your working directory.

If command-line arguments and the *CKSolnList.txt* are used together, command-line arguments will override selections made in the *CKSoln.txt* file.

Note:

You can also create a *CKSolnList.txt* with only the selections you need and run GetSolution to generate a *CKSoln.ckcsv*.

3.2.3. The CKSolnList.txt File

The *CKSolnList.txt* file allows you to create a detailed filter for the GetSolution file. Table 3.2: Summary of Syntax Rules (p. 32) shows the syntax rules for a *CKSolnList.txt* file.

Table 3.2: Summary of Syntax Rules

Rule	Description
1	Any text after a # character is considered comments.
2	The following keywords are reserved: `VARIABLE`, `UNIT`, `SPECIES`, `VAR`, `SEN`, `ROP`, `FILTER`, `TOP`, `BOTTOM`, `MAX`, `MIN`, `ALL`, `NONE`.

The initial section of the file handles variable selections. There are three global selection options:

VARIABLE VAR ALL/NONE `- select all variables or none`

VARIABLE SEN ALL/NONE `- select all sensitivities or none`

VARIABLE ROP ALL/NONE `- select all rate-of-productions or none`

There are also selection options on a per-variable base:

VARIABLE `var_name var_flag sen_flag rop_flag`

The flags can have three types of value:

```
0  - there is no data, so can not be selected

1  - is selected already, can be de-selected

3  - is de-selected already, can be selected
```

These two types of selection options can be used together to make the process more efficient. The example below shows to extract temperature and its sensitivity and NO2 and its rate-of-production but nothing else from a variable:

VARIABLE VAR NONE

VARIABLE SEN NONE

VARIABLE ROP NONE

VARIABLE temperature 1 1 0

VARIABLE NO2 1 0 1

The next section handles unit selections. Each unit choice can be set using:

UNIT `var_type unit_choice`

An example of variable types and their unit choices are shown below:

Time `(sec) (min) (hr)`

Distance `(cm) (m) (inch) (ft) (mil)`

Temperature `(K) (C) (F)`

A full list of unit choices can be seen in GetSolution help.

The next section handles the filter for top/bottom selection. You can pick the top *n* or bottom *n* species, reaction sensitivities, and species rate-of-productions. Only one of the three choices, `ALL`, `TOP n`, `BOTTOM n`, can be selected.

SPECIES ALL/TOP n/BOTTOM n

SEN ALL/TOP n/BOTTOM n

ROP ALL/TOP n/BOTTOM n

The next section handles the filter for species data based on mole fraction. The `MAX` and `MIN` specifies the range of mole fraction. The default is `MAX = 1.0` and `MIN = 0.0`.

FILTER MAX `max_value`

FILTER MIN `min_value`

3.2.4. The CKSolnTranspose Utility

The CKSolnTranspose utility can be used to convert the row-based *CKSoln.ckcsv* file to a set of column-based **.csv* files. A column-based file format is often easier to import into third-party plotting packages. It is also necessary for use with the Import utility of the graphical Ansys Chemkin Visualizer. The CKSolnTranspose executable located in the *bin* directory of your Chemkin installation. If you have already appended the *bin* directory to your local PATH environment variable, type the following command to run CKSolnTranspose:

```
%CKSolnTranspose [-help] [-column N] [CKSolnFile]
```

where `-help` displays the command syntax information and `-column N` specifies the maximum number of columns per output file. The default is 100 columns per file. We note that the Microsoft Excel limit is 256.

`CKSolnFile` is an optional file name for the row-based solution file generated by GetSolution. The full path has to be included if it is not in the working directory. By default the file name is *CKSoln.ckcsv*.

Note:

Please note that 2-D contour data sets are ignored if they exist. Only 1-D (line) plot data is included.

3.2.5. The CKSoln.ckcsv File

The *CKSoln.ckcsv* file produced by the GetSolution utility is composed of blocks of data. These blocks are either rows of 1-D arrays of data or 2-D data structures. Each block begins with a label row that provides either a plot set or a contour set name and then specifies the number of elements in the 1-D array or 2-D matrix (for contour data). Array block labels are then followed by 1 or more rows of array data with the data name, units (or empty parentheses), and data values. Contour block labels are followed by 2 axis-rows and then the Z values for each (X,Y) tuple on a row by row basis. The Z-variable and units are specified on the label_2D line.

For instance, these are two 1-D array block labels:

```
label, solution_no_1, 334
label, rate-of-production_for_solution_no_1, 334
```

These is one 2-D contour block labels and axes data (truncated):

```
label_2D, Temperature, (K), 5, 15
Axial_coordinate, (cm), 0.000000e+000, <4 more data values>
Cross-flow_coordinate, (cm), 2.220446e-016, <14 more data
values>
```

Note:

When there are more than 256 values (labels, units, data) per row, Microsoft® Excel® will complain that it cannot completely load the data because it runs out of columns. You can transpose the data, reduce it, etc., to eliminate this problem.

There is not a 1-to-1 correspondence between the Solution Sets listed in the Data Selection dialog of the Ansys Chemkin Visualizer and the resulting label blocks in the *CKSoln.ckcsv* file; when adjacent 1-D arrays in different Solution Sets have the same length, we continue to append to the same block. This results in fewer plot sets in the Plot X-Y selector, which makes it easier to plot data from different Solution Sets at the same time.

The *XMLdata.zip* file is composed of a set of zipped files. Each zipped data file contains an *.xml* file; but these *.xml* files are interdependent insofar as an xml **<tag>** may begin in one file and be closed in the following file. For this reason, they may not display properly if examined one at a time. Each of these *.xml* files is roughly 10 MB prior to zipping. The overall processing sequence is to extract the zip files, sequentially open them one at a time to process the xml contents, and then to re-zip them back into *XMLdata.zip*. If this process is interrupted (for instance, runs out of memory or disk space), it can leave *.zip* and *.xml* files in the Working Directory. For this reason, the GetSolution utility always does a "cleanup" step first. You may see messages saying `Could Not Find XMLdata*.xml`, or similar. These are normal and mean there were no stray files needing to be deleted.

Since the overall process is sequential, the data is extracted in blocks when the *CKSoln.ckcsv* file is constructed. If we were only extracting one block of data, and it was not too large, it might have been practical to transpose the data into columnar format in the *.csv* file. However, the different blocks do not necessarily have the same length. At the time of writing block 1, we do not know how many more blocks we will be writing. Therefore, it is not feasible to output the multiple blocks in columnar format. This may not be immediately obvious to anyone who is looking at a simple problem with only one block of data. See the *cylindrical_shear_flow__cvd.ckprj* sample problem for an example of the complexity of having both 1-D and 2-D blocks of data in a *.csv* file.

Chapter 4: Reaction Path Analyzer

The Reaction Path Analyzer is a feature that has been incorporated into Ansys Chemkin to provide visualization of the inner workings of the chemistry model and to provide fundamental understanding of reaction mechanism dependencies. The pathways leading to the formation of species are presented in a single graphical interface that displays the relative importance of each reaction. The Reaction Path Analyzer is available as a post-processing option in the Analyze Results panel, for any Chemkin reactor model. After a successful simulation run, the option to select the Reaction Path Analyzer is available from the Analyze Results node on the project tree.

4.1. Overview of Reaction Path Analyzer Display Panels

When the Reaction Path Analyzer is opened, a large primary window is visible which displays data and has a side-panel that controls which data are displayed and how they are presented. The large primary window is composed of three sections, as shown in Figure 4.1: The main Reaction Path Analyzer panel, showing the Reaction Path Diagram, the Rate of Production area, and the Sensitivity area, and the Solution tab of the Control panel. (p. 38): the Reaction Path Diagram, the Rate of Production Bar Graph, and either the Sensitivity bar graph or the Forward and Reverse Rate-of-progress bar graph. Figure 4.2: The Reaction Path Analyzer Control Panel, which controls what data is being displayed in the Reaction Path Diagram. (p. 39) shows the control panel that displays on the right side, with options to change the constraints used in generating and displaying the path diagram, based on the current Ansys Chemkin solution. These components are described briefly below, while Using the Reaction Path Analyzer (p. 43) contains instructions on how to modify the display characteristics.

Figure 4.1: The main Reaction Path Analyzer panel, showing the Reaction Path Diagram, the Rate of Production area, and the Sensitivity area, and the Solution tab of the Control panel.

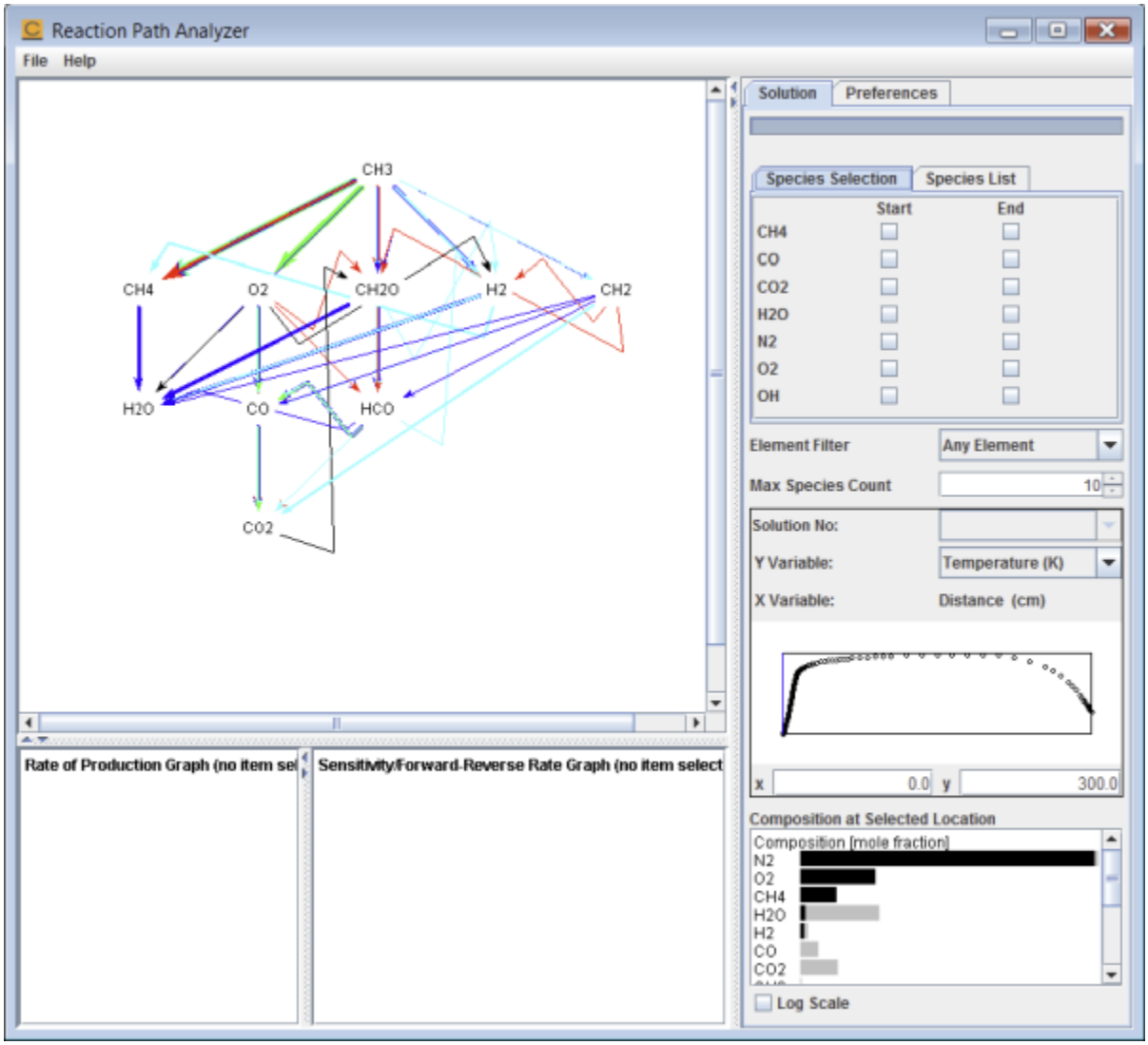
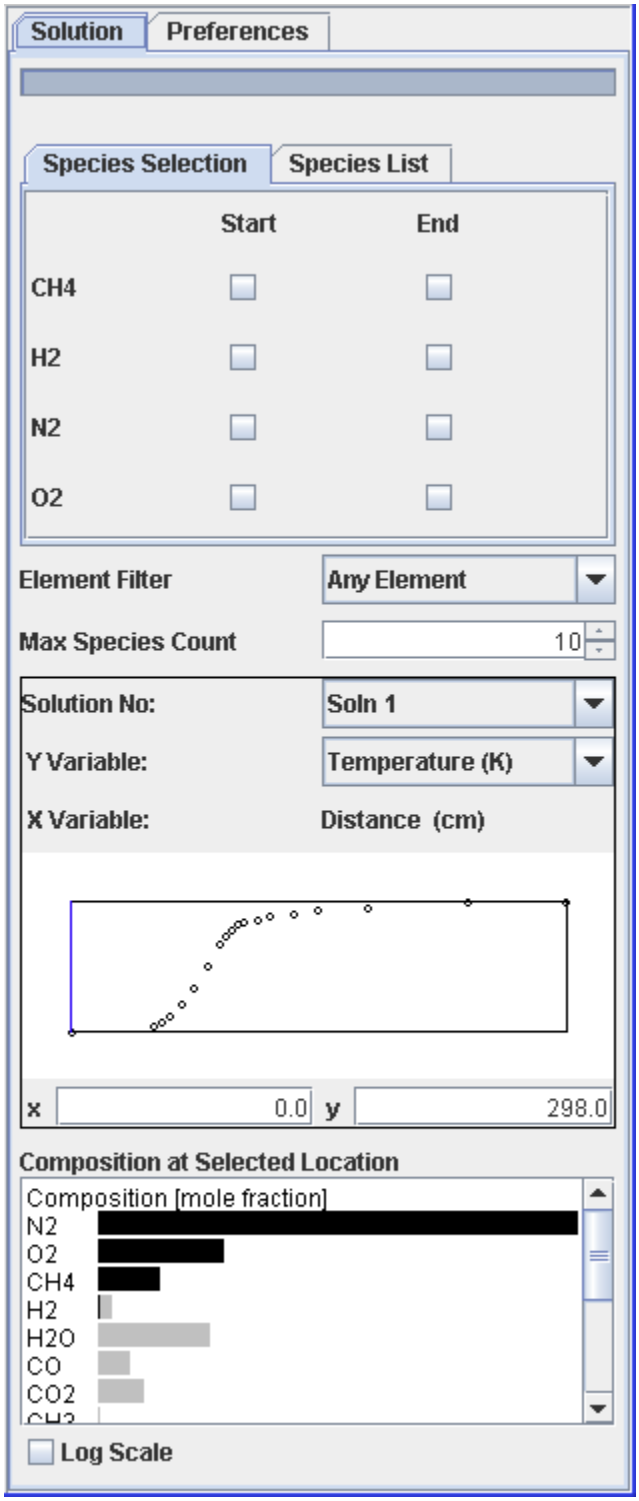


Figure 4.2: The Reaction Path Analyzer Control Panel, which controls what data is being displayed in the Reaction Path Diagram.



4.1.1. Reaction Path Diagram

The Reaction Path Diagram displays species as well as reaction pathways connecting the species. The relative sizing of the connecting pathways is related to the relative contribution of that pathway to the net rate of production of the species. Path widths with the minimum rate of production corres-

ponding to a line thickness of one, and the maximum rate of production scaled to the largest allowed line thickness. Intermediate line thicknesses are determined on a log scale.

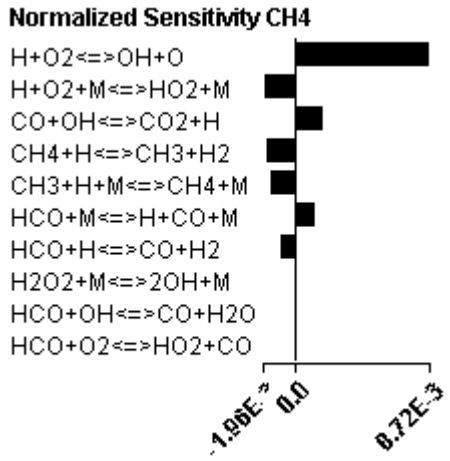
4.1.2. Rate of Production Bar Graph

Selecting either a species or a connecting pathway between species in the Reaction Path Diagram will activate the lower left panel, reserved for the display of species rates of production. Selecting a species will display all rates of production for the selected species whether it is a product or a reactant in the reaction. Selecting a connecting pathway between any two species will populate the contents of the graph with the contributing rates of production for all reactions contributing to the path selected. All Rate of Production data are displayed in bar graphs as seen in the lower left region of Figure 4.1: The main Reaction Path Analyzer panel, showing the Reaction Path Diagram, the Rate of Production area, and the Sensitivity area, and the Solution tab of the Control panel. (p. 38), showing the relative contributions of each reaction on a linear scale.

4.1.3. Sensitivity Bar Graph

Selecting a species in the Reaction Path Diagram will activate the lower right panel, displaying all sensitivity coefficients that have been calculated for the selected species. If there are no sensitivity data in the Ansys Chemkin solution file, no sensitivity bar chart will be displayed. When available, data is displayed in bar-graph form, providing the normalized, relative sensitivity of the species to each reaction, as shown in Figure 4.3: Sensitivity plot for the H2O2 species (p. 40).

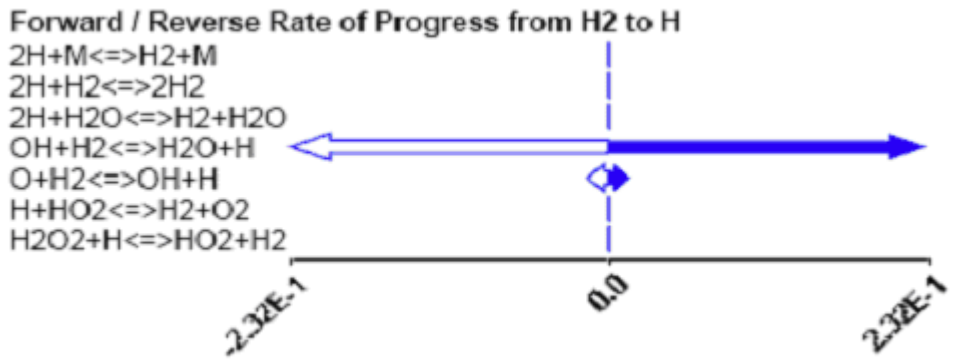
Figure 4.3: Sensitivity plot for the H2O2 species



4.1.4. Forward and Reverse Rate Chart

Selecting a connection path in the Reaction Path Diagram will activate the lower right panel, displaying all forward and reverse reaction rates for each reaction that is a contributor to the selected connection path. As shown in Figure 4.4: Forward and reverse rate of progress chart (p. 41), the forward and reverse rates are charted to show their relative sizes.

Figure 4.4: Forward and reverse rate of progress chart



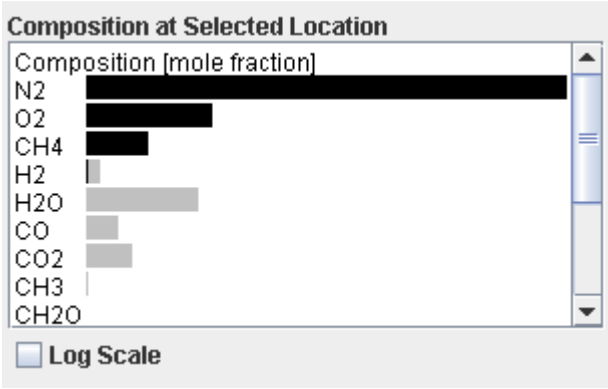
4.1.5. Control Panel

The Control Panel contains access to elements that modify the form of the Reaction Path Diagram being displayed, as well as graphical tools to help determine which time or space solution point is currently being displayed. These components of the Control Panel are described briefly below, while instructions on how to use these components is provided in Using the Reaction Path Analyzer (p. 43).

4.1.5.1. Composition Bar Graph

The Composition display is a graphical representation of the local values for species at the selected point in the Ansys Chemkin solution. The relative contribution of each species is displayed in a bar graph chart as shown in Figure 4.5: Composition display (p. 41). The maximum species fraction that occurs at any point in the Chemkin solution is displayed as a gray bar behind the black bar showing the local value. By default, the composition bar chart is displayed on a linear scale, but this can be changed to a log scale.

Figure 4.5: Composition display

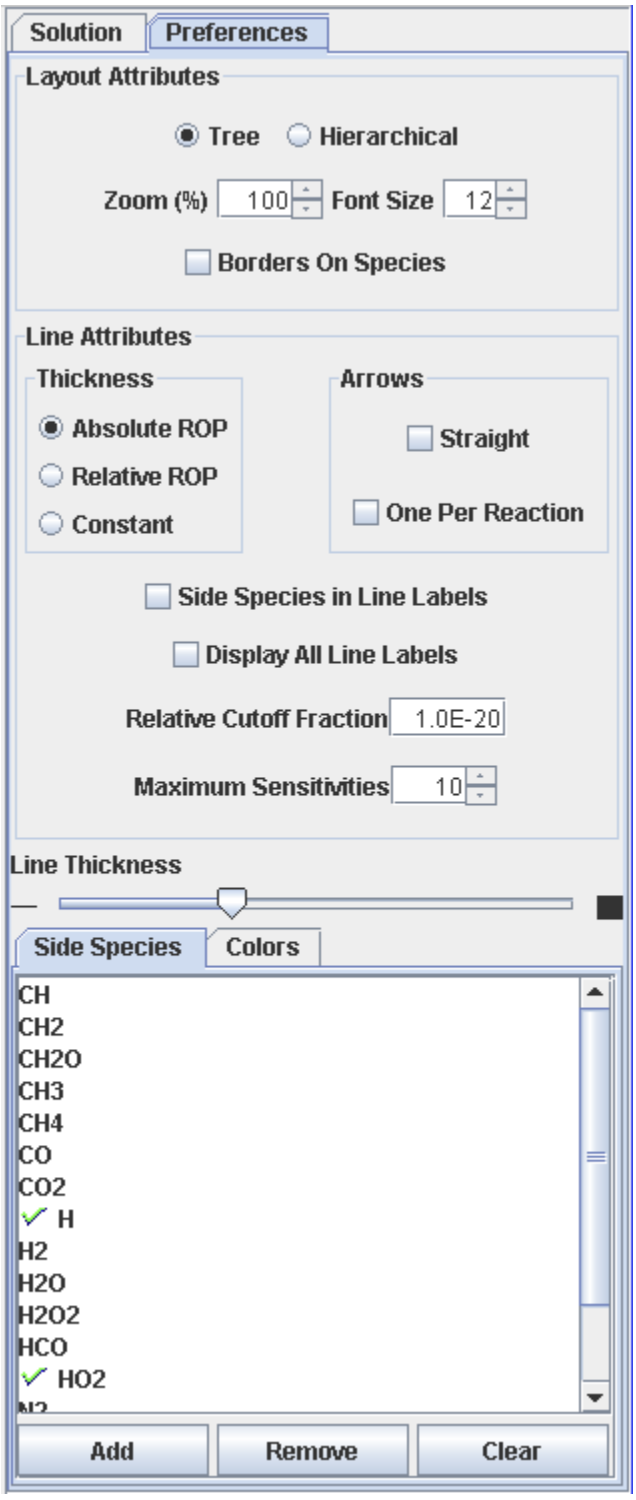


4.1.5.1.1. Preferences Selection

To change user preferences for the Reaction Path Analyzer, click the Preferences tab, shown in Figure 4.6: Preferences panel (p. 42). The Preferences panel allows the setting of options that

dictate the behavior of the Reaction Path Diagram. The purpose of these options is described in more detail in the following section.

Figure 4.6: Preferences panel



4.2. Using the Reaction Path Analyzer

The Reaction Path Analyzer provides you with many options to control the way the reaction network is generated and displayed in the Reaction Path Diagram. The purpose and impact of each control is described briefly here.

4.2.1. Maximum Number of Species Displayed

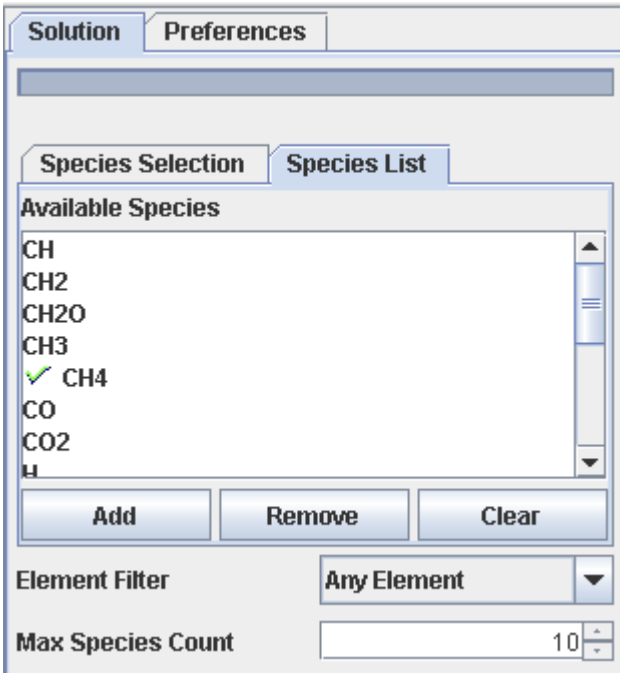
This control sets a maximum number of species displayed in the Reaction Path Diagram. By default, species are ranked according to the maximum rate of depletion of all species at the particular point selected in the Ansys Chemkin solution. The species with the maximum depletion rate determines the top of the "tree" for the Reaction Path Diagram. Other species that will be included in the display are then chosen according to a similar ordering, with the added constraint that they be connected to the first species selected. In addition to this default behavior, the target (top of the tree) species can be selected explicitly in the Control Panel, through several options described below. However the tree is determined, no more than the **Maximum Number of Species** will be displayed on the Reaction Path Diagram at any one time. In this way, the size of the diagram can be controlled by this option.

4.2.1.1. Start and End Species

Species of interest can be selected in the Species List tab as shown in Figure 4.7: The Species List tab for selecting species available for start and end. Preferred species persist beyond the application lifetime. (p. 44). By default the reactants are available for selection. Species highlighted in the Species List tab on the Solution panel are available in the Species Selection tab, where they can be dynamically selected and deselected as the **Start** and/or **End Species** used to generate the Reaction Path Diagram. There are three options to determining the Reaction Path Diagram using the Species Selection **Start** and **End Species** :

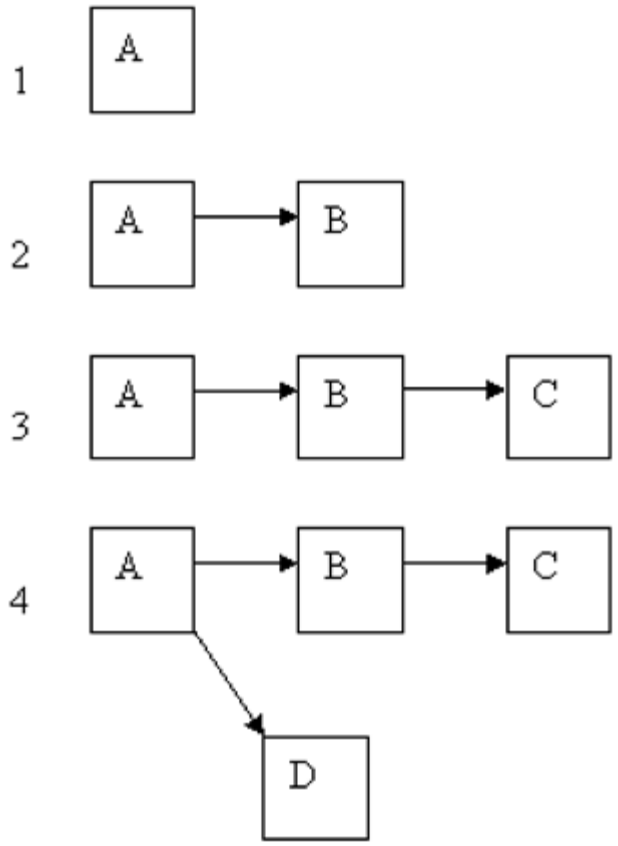
- Select only a **Start Species**
- Select only an **End Species**
- Select both a **Start** and **End species**

Figure 4.7: The Species List tab for selecting species available for start and end. Preferred species persist beyond the application lifetime.



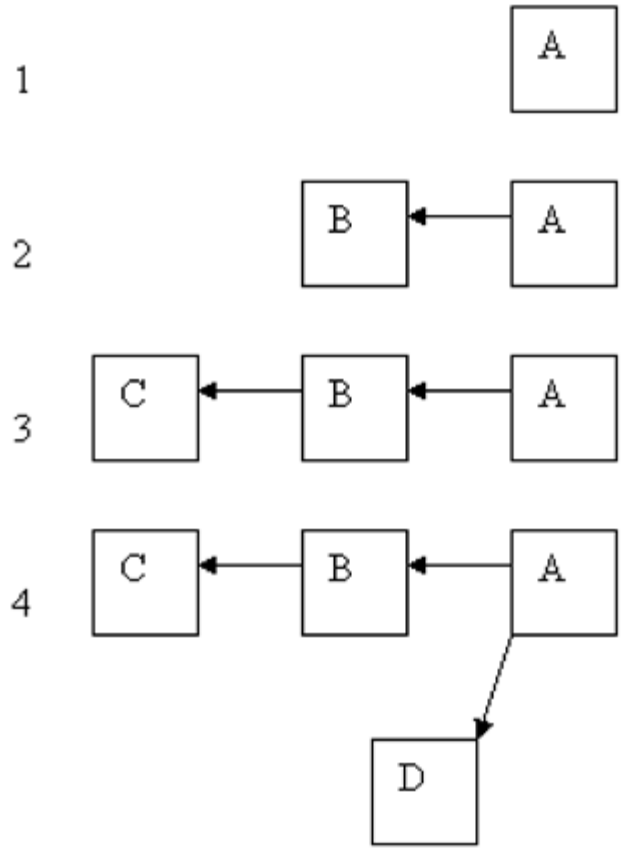
Selection of only a **Start Species** will generate a diagram with the given species as the origin, and additional species are added to the diagram according to the magnitude of the rate-of-production (ROP) of species that can be connected to one of the existing species on the diagram. This growth of the tree is continued until the maximum number of species displayed is reached. A schematic of this procedure is provided in Figure 4.8: The first four steps when generating a diagram from the Start Species (p. 45).

Figure 4.8: The first four steps when generating a diagram from the Start Species



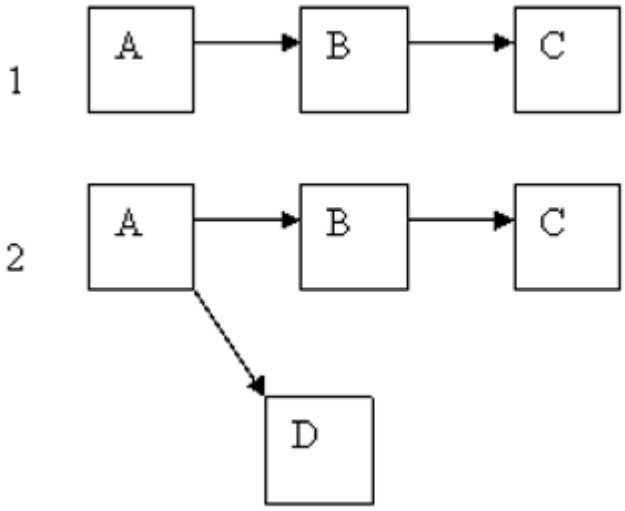
Selection of only an **End Species** results in analogous behavior to the **Start Species** selection, except that the species will be added to the Reaction Path Diagram according to ROP channels leading to the formation of the existing species on the Diagram. The steps for building the tree in this case is shown in Figure 4.9: The first four steps when building a diagram from an End Species (p. 46).

Figure 4.9: The first four steps when building a diagram from an End Species



The selection of both **Start** and **End Species** will cause the inclusion of species connecting the maximum ROP route from **Start** to **End**. Additional species are added to the Diagram according to maximum ROP pathways originating from the species already in the Diagram and that are along the trail connecting the **Start** and **End Species**. This is illustrated in Figure 4.10: The first two steps when building a diagram from the Start and End Species (p. 47).

Figure 4.10: The first two steps when building a diagram from the Start and End Species



4.2.2. Elemental Restriction

The species displayed in the Reaction Path Diagram can be restricted to the ones containing a specified element. The only pathways that will be displayed in the Diagram will also be similarly restricted to following the given element. By default, all elements are allowed in the Reaction Path Diagram construction.

4.2.3. Maximum Line Thickness

The maximum line thickness slider control will set the maximum line thickness displayed in the Reaction Path Diagram. Since ROP values vary over orders of magnitude, the scaling of lines is logarithmic. The power of the logarithm is chosen so that the minimum corresponds to one pixel width, and the maximum ROP corresponds to the user-specified maximum line width.

4.2.4. Solution Data Point Selection

Solution data points are selected from a sub-section of the Control Panel, below the **Line Thickness** slider bar. Ansys Chemkin generates solutions that vary with one or more independent variable (for example, time, distance or some varied parameter). The Reaction Path Analyzer therefore provides a Solution selection interface that allows dynamic selection of a point along a solution varying in one dimension. The Solution point selected will determine the local values of ROP that are used to generate the Reaction Path Diagram. Sub-components of the Solution panel include Solution Selection, Dependent Variable Selection, and the Data Point Display and Selection. These are described briefly below.

4.2.4.1. Solution Number Selection

The Solution Selection interface allows the selection among several solutions that may be contained in a single solution file. For example, if a 1-D simulation was run with continuations, is allows the selection of which continuation solution will be analyzed. In the Multizone model it will allow the selection of an individual zone, as well as the zone average. Similarly for the Spark Ignition (SI)

model, the unburned, burned, and average zones are available here for selection. IIf there is only one solution contained in the Ansys Chemkin solution file, this option will be disabled.

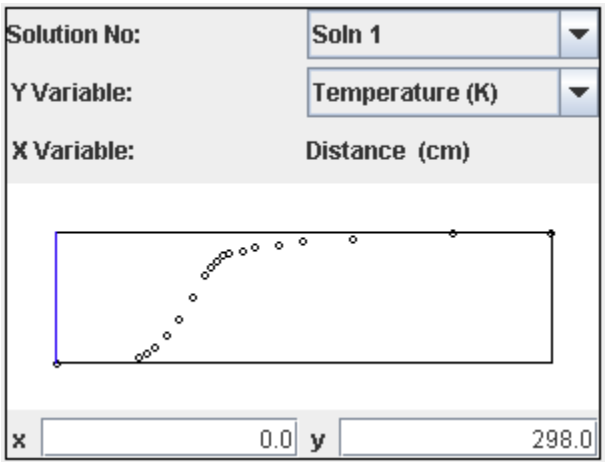
4.2.4.1.1. Y Variable Selection

The **Y Variable** pull-down menu allows selection of the dependent variable that will be displayed in the graph window below the **Selection** menu. By default, this is set to temperature, but any other solution variable that is usually available in the Ansys Chemkin Visualizer can be selected instead.

4.2.4.1.2. Data Point Display and Selection

Within the graph that displays the selected Y Variable plotted as a function of the independent variable, an "X" location for the solution can be selected. Clicking inside of the X-Y plot window, shown in Figure 4.11: Data Selection window (p. 48), will set the point of interest, and a new Reaction Path Diagram will be generated for that location. In addition, pressing the right or left arrows on your keyboard will increment or decrement the point of interest by one stored solution point, when the Control Panel is in focus on your screen. This allows finer control of the location. By default, the location selected is at the start of the solution, for example, at X (time or distance)=0.0. The location selected, in terms of (X,Y) values is displayed below the graph.

Figure 4.11: Data Selection window



4.2.5. Preferences

There are several User preferences that can alter the way the automatic generation of the Reaction Path Diagram is performed and displayed. The three panels of the Preferences dialog are shown in Figure 4.6: Preferences panel (p. 42), and the details of each option are described below.

4.2.5.1. General Preferences

General preferences are organized into three categories: How the species are laid out in the diagram, how the reaction connections are assembled in the diagram, and how the compositions of associated bar charts are organized.

4.2.5.2. Layout Options

This group of controls alters the layout and dimensions of the Reaction Path Diagram. Controls are available for setting the layout manager, the zoom, font size, and borders on species.

4.2.5.3. Layout Attributes

The layout manager dictates the method used to determine the position of the species in the Reaction Path Diagram. This fundamental layout technique alters the format of the display, and can either improve or hamper the visualization of reaction paths, depending on the chemistry and results of the model. There are two options for layout handling, either the **Tree Method** or the **Hierarchical Method**.

The Tree layout uses a generated ancestor tree to determine the primary layout of the diagram panel. Each child is determined by a positive ROP leading from a chosen species to another species. The layout of the panel is chosen so that the progeny that can be reached by one species is maximized. In the ancestor tree layout, all depleting pathways exit from the bottom of a species, and all formation pathways enter at the top of a species.

GraphViz [1] (p. 57) is open-source graph visualization software. The program used by the Reaction Path Diagram for this type of layout is `Dot`. The `Dot` executable makes hierarchical, or layered drawings of directed graphs. The layout algorithm aims edges in the same direction (top to bottom, or left to right) and then attempts to avoid edge crossings and reduce edge length. GraphViz is open source, CPL-licensed software. It may be redistributed, without cost, and in other software distributions, as long as the license terms are met. The Reaction Path Analyzer assumes that the `Dot` executable is accessible on the path. If that is not the case, then add the GraphViz bin directory to your `path` environment variable.

4.2.5.4. Zoom (%)

The zoom level will change the relative sizing of all components in the Reaction Path Diagram.

4.2.5.5. Font Size

Changing font size will alter the size of font for labels displayed in the Reaction Path Diagram.

4.2.5.6. Borders on Species

This option will put boxes around the species in the Reaction Path Diagram.

4.2.5.7. Reaction Connection Options

There are several settings to modify how the reactions connecting species are displayed within a reaction path diagram. These controls modify the reaction line thickness, whether or not joints are added in a line, line labels, and the maximum magnitude of the displayed line.

4.2.5.8. Line Thickness

Changing from Absolute ROP to Relative ROP will alter the relative sizing of the connecting pathways between species. The relative size of each arrow will be normalized by the sum of all ROPs exiting

a source species. The Constant ROP line thickness will leave all lines at a constant thickness independent of their magnitude.

4.2.5.9. Straight or Jointed Lines

Selecting Straight lines will make all reaction pathways connecting species into single lines within the Reaction Path Diagram, making direct connections between the source and destination species. The (default) **Jointed Line** option causes lines to be wrap around the species and avoid overlap. This option applies to both the Tree and GraphViz layouts.

4.2.5.10. Line Labels

The labels on reaction lines can be composed of either the absolute magnitude of the rates in a connection or a relative magnitude of the rates. Additionally, the label can include information about side species associated with a reaction pathway. The concept of a side species is explained in Side Species Preferences (p. 50). These labels appear with mouse hovering, mouse selection, or can be turned on for all reaction connections.

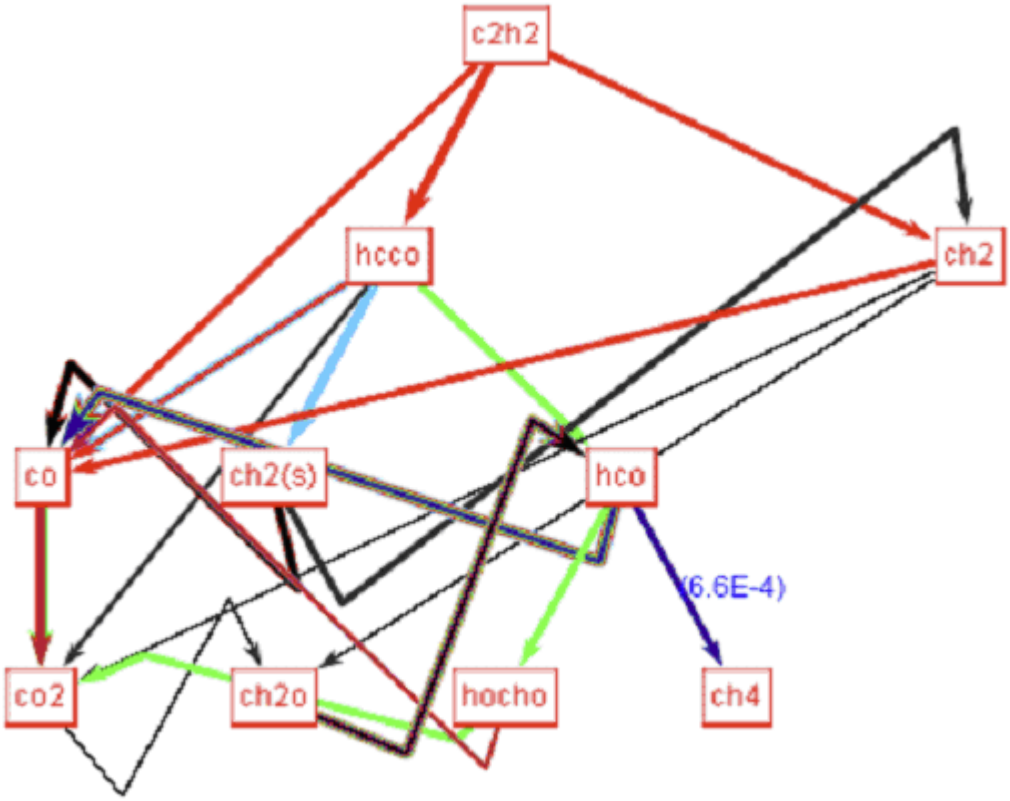
4.2.5.11. Composition Options

Composition controls set the data limitations of bar charts. The maximum species and maximum reactions set the number of entries in sensitivity, rate of production, or composition bar charts. Log scale will scale the bars on the Composition Bar Chart on the Control Panel using a logarithmic, rather than linear, scale. For this option, the minimum composition value is represented by a zero-length bar.

4.2.6. Side Species Preferences

Side species are components such as radicals that are important in the reactions connected on the path analysis diagram, but should not be characterized as source or target species on the reaction-path diagram. Common examples of such side species include the hydrogen radical, hydroxide radical, oxygen radical, and the peroxy radical. You can select which species should be designated as side species in the diagrams, using the tabs shown in Figure 4.6: Preferences panel (p. 42).

Figure 4.12: Path diagram. With connections colored according to the presence of a side species in a reaction



4.2.7. Color Preferences

The arrow color and species color can be set as a preference. Changing these colors alters the coloring scheme of the Reaction Path Diagram. The second color option will color a reaction connection logarithmically according to heat rate of production, with positive heat being red, and negative heat being blue. The remaining color choices indicate which of these side species are involved in a reaction line that connects two species in the diagram. An example of a diagram colored by side species is shown in Figure 4.12: Path diagram. With connections colored according to the presence of a side species in a reaction (p. 51).

4.2.8. Help Menu

The commands under **Help** on the Control Panel include a link to user documentation as well as an **About** menu.

4.2.9. Export Options

Exporting raw data from the ROP bar chart, the Sensitivity bar chart, or the Forward/Reverse Rate of Progress chart is available from the **File > Export** menu or ribbon. Data in the chart are saved to a new file in comma-space-delimited (csv) format.

4.2.10. Printing Options

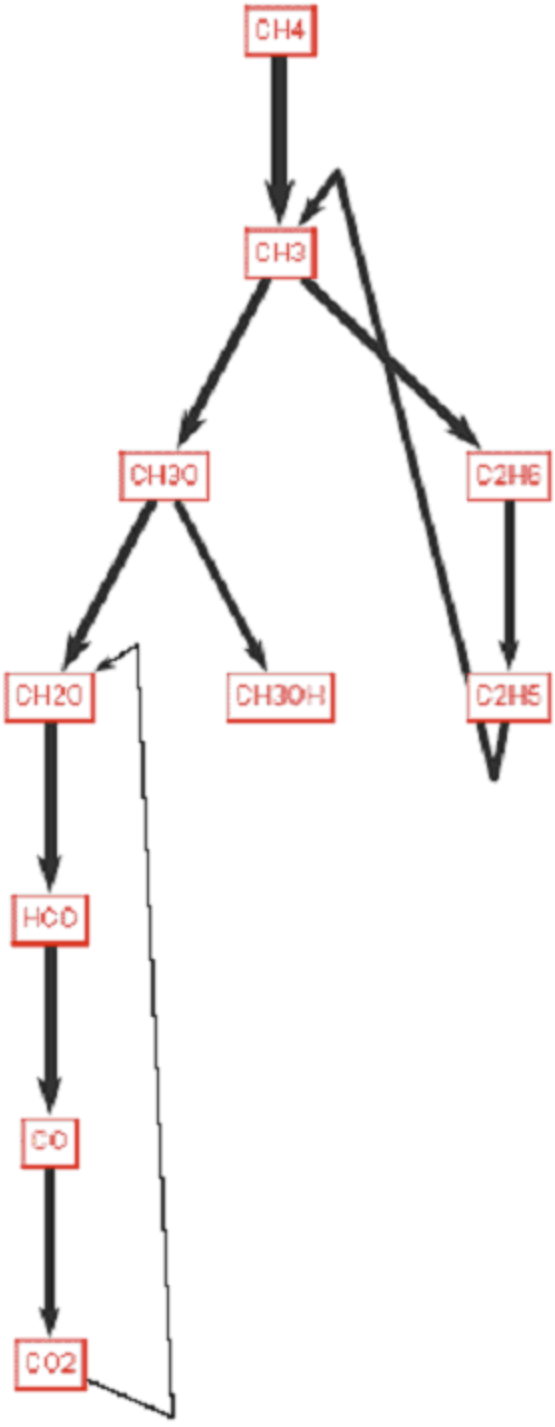
Printing of the Reaction Path Diagram, the ROP bar chart, the Sensitivity bar chart, or the Forward/Reverse Rate of Progress chart is available in the **File > Print** option of the Control Panel. All charts are automatically scaled to fit a single page.

4.3. Reaction Path Analyzer Example

In the evaluation of a mechanism, the Reaction Path Analyzer provides graphical descriptions of the pathways of formation in a mechanism. A common example of the use of reaction pathway analysis is in studying the decomposition in a methane air flame. To verify the Reaction Path Analyzer against such a benchmark, then, a methane combustion mechanism [2] (p. 57) was investigated with assistance from the Reaction Path Diagram. A Burner Stabilized Flame simulation was performed with Chemkin using the USC mechanism from Wang [2] (p. 57). Conditions are: atmospheric pressure, 300-K inlet temperature, and a methane-air equivalence ratio of one. From previous studies, it is expected that depletion of methane species in the pre-flame region occurs primarily through hydrogen abstraction by hydroxy radical. Later in the warmer region of the flame other hydrogen abstraction reactions begin to match the magnitude of the hydroxyl radical hydrogen abstraction reaction.

A Reaction Path Diagram for this case is shown in Figure 4.13: Methyl decomposition pathways (p. 53). The diagram is displayed at a temperature of 1400 K. Analysis of the diagram indicates that the main pathways of decomposition of methyl radical is to the formation of the excited CH_2 species, which then decomposes to form CH_2 O and CH_3 O. Other channels lead directly from methyl radical to the radical-radical recombination to ethane. The primary depletion of ethane is through the hydrogen abstraction to ethyl radical, which through radical-radical recombination with a methyl radical leads to the formation of propane. In the hotter region of the flame, these molecular-weight growth reactions are less favored. All of this is consistent with previous, published findings.

Figure 4.13: Methyl decomposition pathways



Appendix A. Auxiliary Information

A.1. Solution File Format

The *XMLdata.zip* is a standard zip file (you can open it with WinZip or any other zip utility) that contains the following files:

- *chemkindata.dtd* -- A DTD document defining the structure of an XML file
- *XMLdata-1.xml.zip* -- A zipped XML document which serves as a checkpoint for GetSolution utility (internal use only)
- *XMLdata0.xml.zip* -- A zipped XML document containing solution size information and solution header
- *XMLdata1.xml.zip* -- A zipped XML document containing chemistry mechanism data
- *XMLdata2.xml.zip* -- A zipped XML document containing solution data
- And possibly many more solution-data zipped XML documents

The purpose of a DTD (Document Type Definition) is to define the legal building blocks of an XML document. It defines the document structure with a list of legal elements. The *chemkindata.dtd* file documents the file format for the Ansys Chemkin *.xml* output files. For more information on DTD files, the web tutorial at https://www.w3schools.com/xml/xml_dtd_intro.asp is a good resource.

If the XML file's contents were small, we would simply store a single XML file. However, since solution files can be quite large (sometimes exceeding 100 MB even when zipped), we process what is logically and conceptually a single XML file as a series of separate files. Each of those files is kept zipped until needed.

Breaking a single XML file into a series of separate files poses some problems for standard XML file readers because each file is not, by itself, a proper XML file (because opening or closing tags may be in different files). So, we have a more complex XML file reader module that drives the open/parsing/closing of the XML files. Since XML files store information in character mode, the processing of an XML solution file is slower than processing of binary data stored in *save.bin*. In exchange for the slower performance, we get cross-platform portability, improved size scalability, and, most-importantly, cross-application file format consistency. This lays the foundation for creating networks of heterogeneous reactor models, which we have made much more accessible since Ansys Chemkin 4.

Occasionally an XML file will require more RAM/swap space than the system has available and our XML reader module (part of GetSolution) will abnormally terminate. Or, for some reason, the user will kill an *Aurora* or other application executable job; or the *Aurora* or other application executable will die due to a bug or system limitation. Any of these reasons can leave *XMLdata*.xml* files in unzipped states. These files are essentially temp files and need to be deleted prior to the next use of the XML reader module contained in GetSolution and in Ansys Chemkin.

This XML reader (and writer) module is a complex, internal part of our Ansys Chemkin program suite and can not be invoked directly by any user-written programs. We make the GetSolution program available for use in scripting/batch applications. If for some reason you want more details about the internal XML structure contained in the *XMLdata.zip* files, please consult the DTD document.

Bibliography

[1] Ellson, J., E. Gansner, et al. GraphViz - Graph Visualization Software, http://www.graphviz. org..

[2] Qin, Z., V. V. Lissianski, et al. (2000). "Combustion chemistry of propane: A case study of detailed reaction mechanism optimization." Proceedings of the Combustion Institute 28: 1663- 1669..