CHAPTER ONE

INTRODUCTION TO ASPEN PLUS

1.1 BASIC IDEAS

Aspen Plus is based on techniques for developing flowsheets that were used by chemical engineers many years ago. Computer programs were just beginning to be used, were of the stand-alone variety, and were typically used for designing single units. Solution of the material and energy balances for even the simplest flowsheet without recycle required an engineer to design each unit one-at-a-time and, manually, introduce the solution values of a previously designed unit into the input of the next unit in the flowsheet. When it became necessary to deal with a recycle, the calculations began with a guess of the recycle values and calculations ended when the values produced by the last unit in the loop matched the guesses. This involved much repetitive work and was not guaranteed to converge. This procedure evolved through the construction of rating models of units, as opposed to design models, which could be tied together by software in a way that emulated the above procedure and employed robust mathematical methods to converge the recycle elements of the process. This type of system is termed a sequential modular simulator. An excellent example of such software was Monsanto Corporation's Flowtran (1974), which eventually became the kernel upon which Aspen Plus was built.

Subsequently, Aspen Plus, though still basically a sequential modular simulator, has grown considerably and has many advanced functionalities with links to specialized software such as, detailed heat exchanger design, dynamic simulation, batch process modeling, cost estimation, and others. It also has a facility for using an equation-based approach in some of its models that permits convenient use of design specifications in process modeling and solving problems with tight specifications.

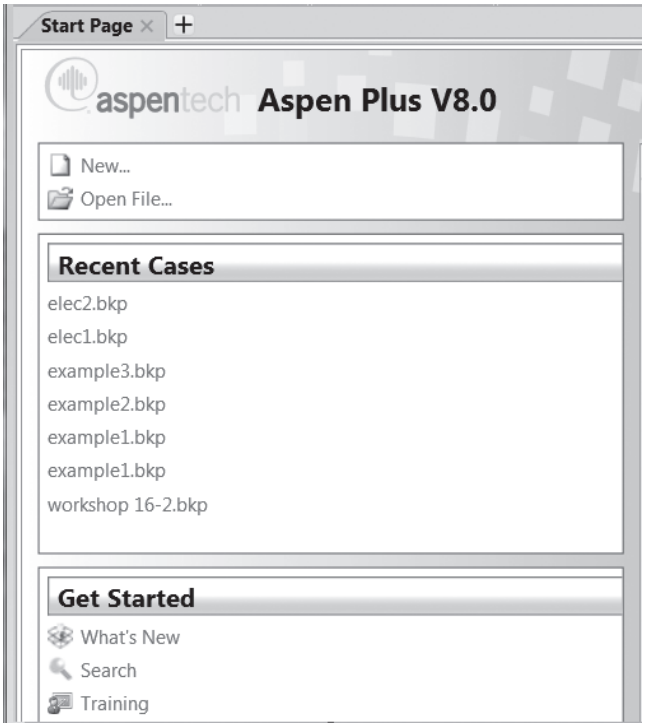
Teach Yourself the Basics of Aspen Plus™, Second Edition. Ralph Schefflan.

Companion Website: www.wiley.com\go\schefflan\AspenPlus2e

The Aspen Engineering Suite, which incorporates Aspen Plus, can be installed in a variety of ways using network servers or on a stand-alone personal computer. Installation is the responsibility of either the user, with tools provided by Aspen Technology, or the information technology department that services the user. This is done only once and modified, typically annually, with future releases. Whether the user's installation is by network downloads or by CDs it is necessary that the user select desired modules, at a minimum, Aspen Plus and its required add-ons, and associated documentation. All other modules are not necessary.

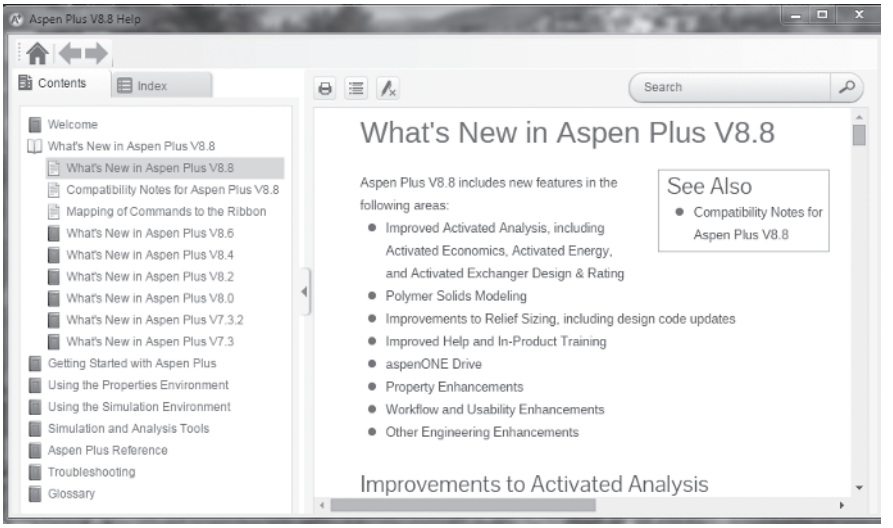
There has been a significant change in the way Aspen Plus software has been organized and accessed by users. All property-related activities, such as property models, regression of experimental data as well as component selection and new component additions, and more, have been incorporated into an environment designated Properties. Similarly, all process simulation activities are organized in the Simulation environment. For Aspen Plus release 8.8 access to What's New is shown in Figure 1.1a and various documentation links are shown in Figure 1.2a, including the Aspen Plus Reference. If using earlier 8.x releases, documentation can be found in the link, What's New from the Aspen Plus Start Page. For

(a)



(b)

Figure 1.1. (a) Aspen Plus Start Page release 8.8. (b) Aspen Plus Start Page release 8.x.



(a)

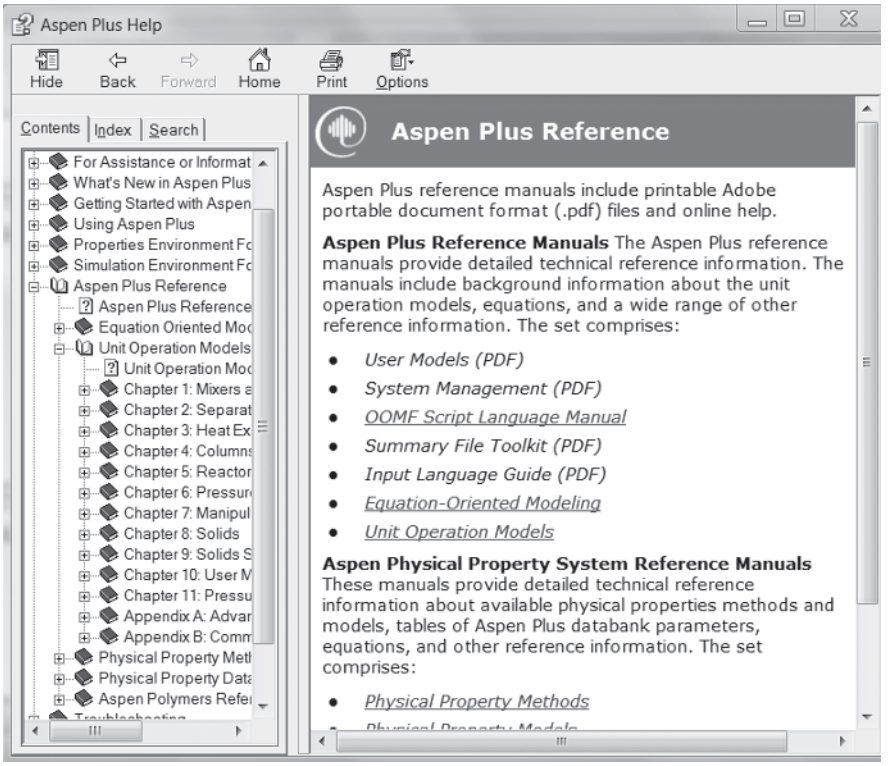


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Figure 1.2. (a) Aspen Plus Reference Manual Release 8.8. (b) Aspen Plus Reference Manual Release 8.x.

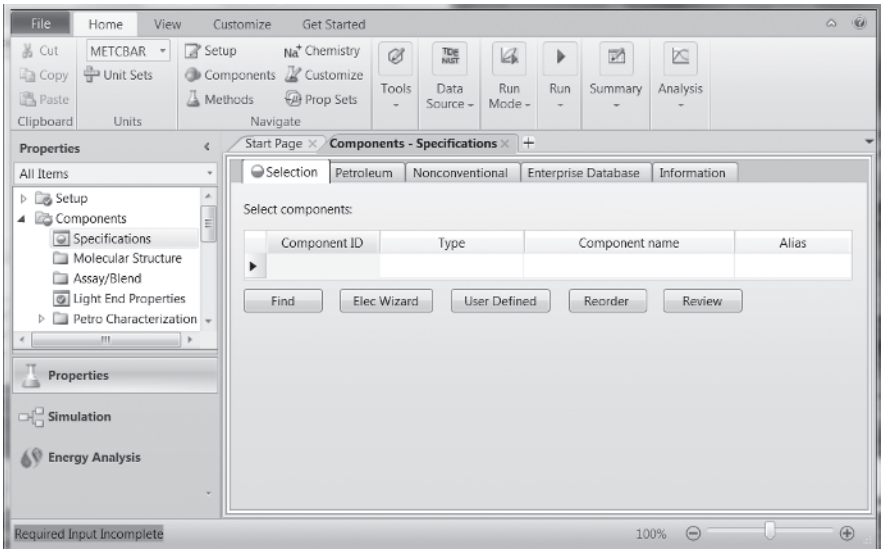

Figure 1.3. The ribbon.

release 8.0–8.6, Figure 1.1b shows the Start Page and Figure 1.2b shows the link to the complete Aspen Plus Reference manual shown in Figure 1.2b.

Access to all Aspen Plus facilities is implemented through the use of a dynamic "ribbon," an example of which is illustrated in Figure 1.3, which appears after a file is opened. Here, the choice of environments is shown in the lower-left corner of the display and the ribbon which has appropriate functions for the "Home" part of the horizontal menu. The contents of the ribbon correspond to the Home selection. Any other selection such as File brings up different functions in the ribbon appropriate for that selection.

Note the list of functions under the Properties title under the left side of the ribbon. These are selections that are available to the user at virtually any time while in the Properties environment or as needed.

The environment Energy Analysis will not be addressed in this book.

1.2 STARTING ASPEN PLUS

When the Aspen Plus User Interface icon on the desktop is clicked or, alternately, the sequence All Programs/Aspen Tech/Process Modeling V8.x/Aspen Plus/Aspen Plus User Interface is selected from the Windows Start menu, the Aspen Plus Startup display, which incorporates the segment shown in Figure 1.1a or Figure 1.1b, appears after selecting File.

If the option New is selected, the user may choose from a list of preconfigured property templates, shown in Figure 1.4, and after a selection is made a display for selecting components, Figure 1.5 is shown. Note the lower-left corner of the display shows the three primary Aspen Plus environments. If any are incomplete they are shown in red. After component selection and all other required property elements are completed, program control may be transferred to other property options or the Simulation environment through the menu shown in Figure 1.6 or manually by selecting the desired item from the Navigation menu.

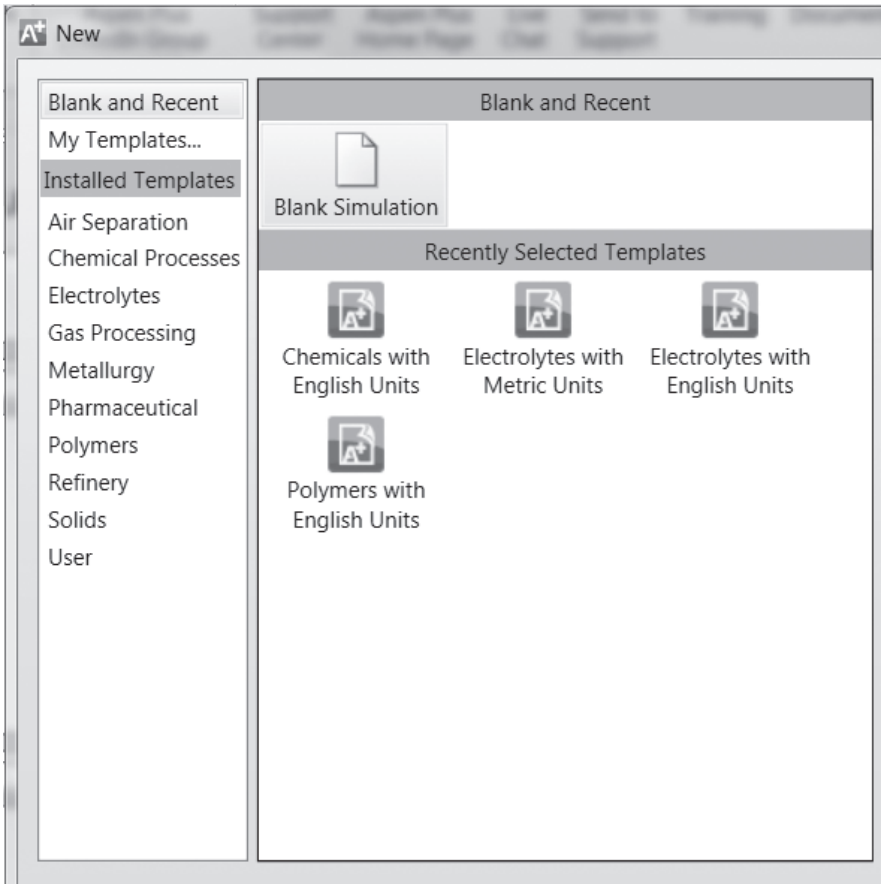

Figure 1.4. Preconfigured property files.

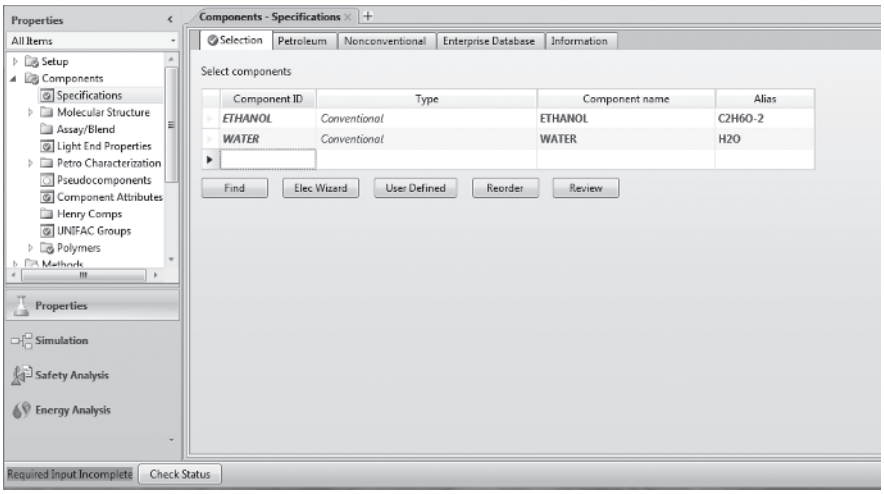

Figure 1.5. Component Specification.

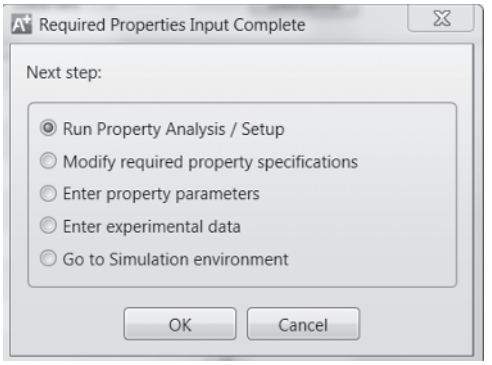

Figure 1.6. Required Properties Input Complete options.

If the option Blank Simulation is chosen, the components and properties for an application can be custom configured by using the Navigation menu at the left of the display. After selecting the required property submenus and providing the required data, one may select a change of environment to Simulation, and a blank workplace that facilitates the graphical user interface (GUI) appears. A selection from a list of existing applications may also be made by selecting Open File.

It is highly desirable to create a personal folder or folders outside the Aspen Plus set of folders, where files can be stored so that one can easily locate the previous work.

1.3 THE NEXT FUNCTION

Aspen Plus provides the user with a mechanism for filling out forms in an orderly fashion. At any point after a property or simulation form has been defined, the user may select the Next function, which appears as the symbol N>, on the ribbon and above the ribbon. The Next function displays the next required input, or the next required form, or shows what is incorrect or missing on the current or next required form. On occasion, after using the Next function, Aspen Plus will prompt the user to select from a choice of actions to be taken. The Next function provides only the minimum required input. For example, when an activity coefficient equation to be used in the simulation is chosen when working in the Property environment, Aspen Plus will use a default data source, such as a specific vapor–liquid equilibrium data set, and will provide binary interaction parameters derived from that set. However, if the simulation involves data not available at the state of the problem, it is the users' responsibility to locate an appropriate data source or estimate it, and regress it in preparation for data entry.

When in the Simulation environment and the Next function is invoked, Aspen Plus will report any flowsheet forms with errors or data that is missing.

1.4 THE NAVIGATION PANE

The Navigation Pane is shown on the left-hand column of most displays in any Aspen Plus environment. For example, when selecting the category menus and submenus that may

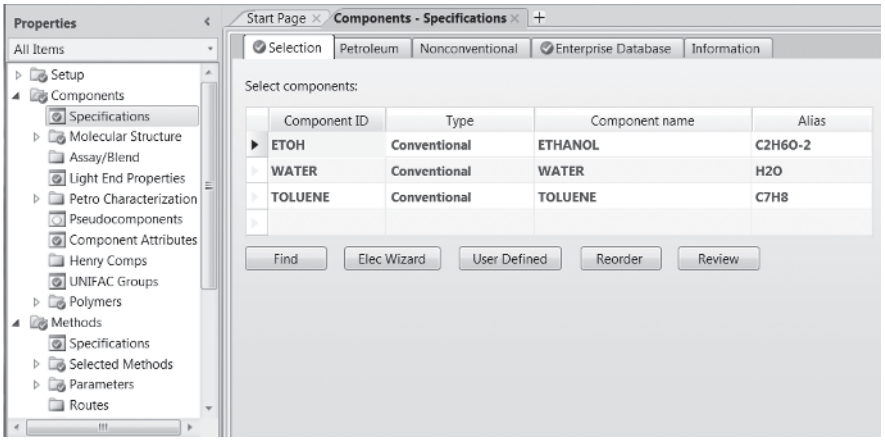

Figure 1.7. Navigation menu.

be used for selecting various options in the Simulation environment, the Navigation Pane will show a list of all possible submenus. An example of the Navigation menu is shown in the left-hand column of Figure 1.7. Additionally, the Model Palette, a list of categorized process models sometimes known as blocks, is shown at the bottom of Figure 1.8. This is used to select and place instances of the generalized models and create connections on a process flowsheet screen. If the model palette does not appear, clicking the View menu/Model Palette will display them. Note that title above the Navigation Pane

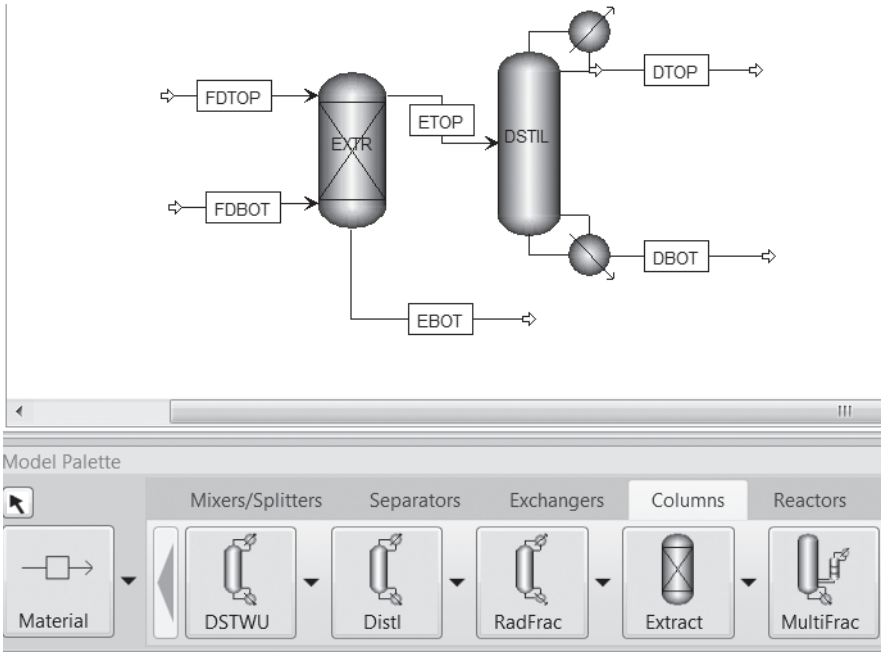

Figure 1.8. The Model Palette.

has changed to Simulation. Also note that the Navigation Panel shows a blue check next to various items in the Navigation Pane. This indicates that the default values are sufficient to proceed with data input; however, this is the minimum required data and the values may need to be modified to meet the requirements of a simulation. If red elements appear on the Navigation Pane, it indicates that user input is incomplete or may have an error. A red element may be deleted by right-clicking on it and selecting delete from the menu that appears if Aspen Plus permits, and alternately by using the Windows Delete key.

1.5 THE PROPERTY ENVIRONMENT

When a new Aspen Plus simulation is initiated, the Property environment is entered and a display, Figure 1.3, for entering components, appears. Components may be entered either by component name or chemical formula. An entry in the box Component ID is a user-provided component short name employed by Aspen Plus for report purposes and in some cases, such as water, is recognized as the component water. Alternately, the user may enter a proper component name or component formula. If either is not recognized as an entry, the user may select the Find button and Aspen Plus will display a set of names or formulas that are alternate names or incorporate part or all of the entry. For example, entering the formula C_7H_8 gives the possibilities shown in Figure 1.9. Upon selection of the component

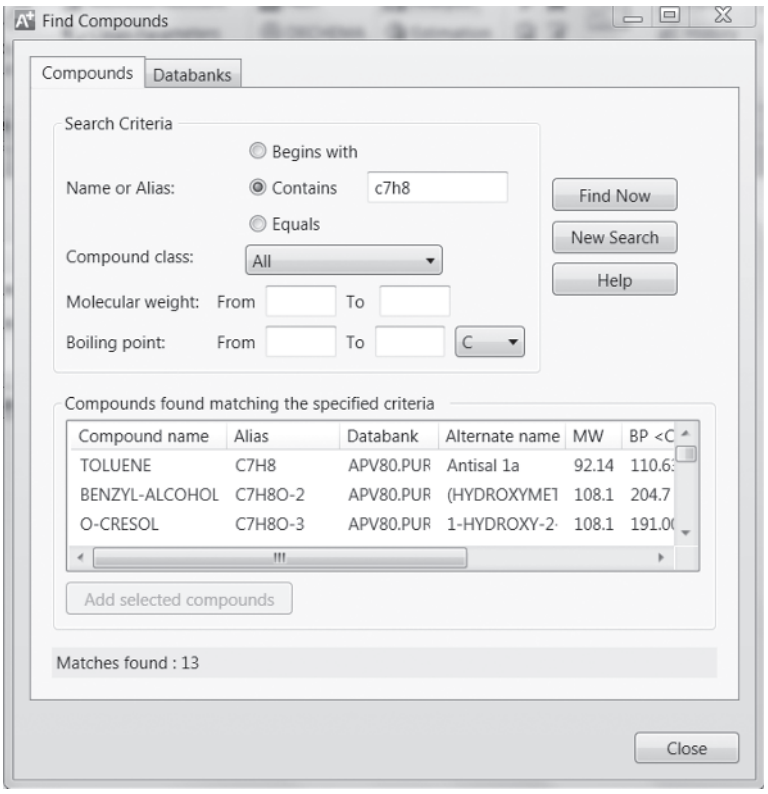

Figure 1.9. Component search.

of interest, pressing the Add Selected Component button enters the component into the component list associated with the current Aspen Plus run.

If a component that does not exist in the Aspen Plus database, choosing User-Defined in Figure 1.3 and the User-Defined Component Wizard shown in Figure 1.10 appears. Note that several properties are required.

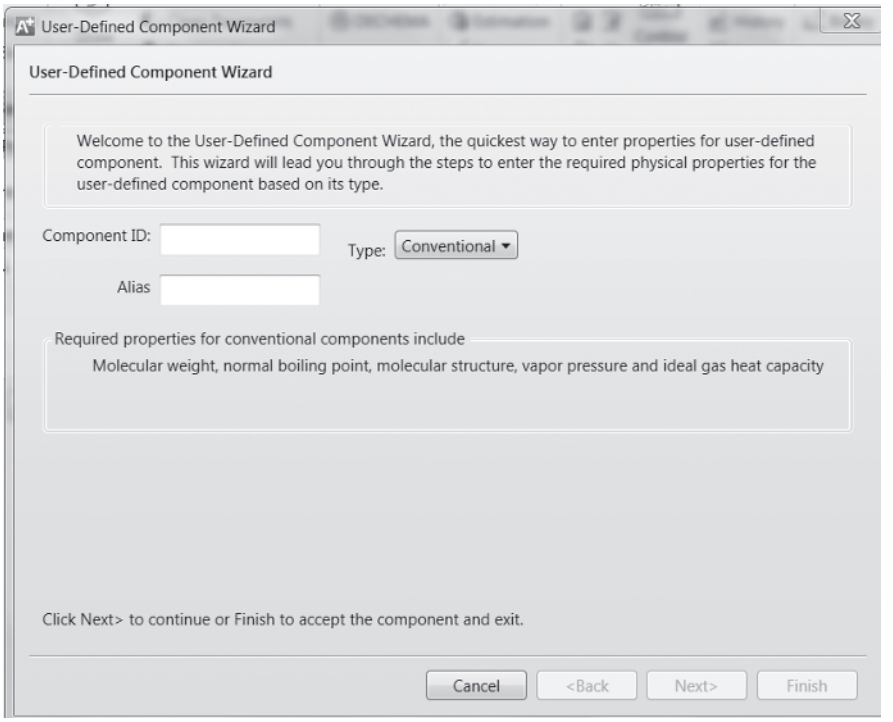

Figure 1.10. User-Defined Component Wizard.

After entering the Component ID and formula, the Basic Data entry display, shown in Figure 1.11 appears. Known experimental data may be entered. If Define molecule by its connectivity is selected, Figure 1.12 appears. Here each nonhydrogen element is assigned a number and the structure is defined by connectivity to adjacent molecules and the type of connecting bond. As the input process proceeds, an option for Aspen Plus to estimate any missing data appears. Chapter Two includes methods for estimating data that may be employed selectively for supplying the missing data above, rather than permit Aspen Plus to provide missing data with default methods.

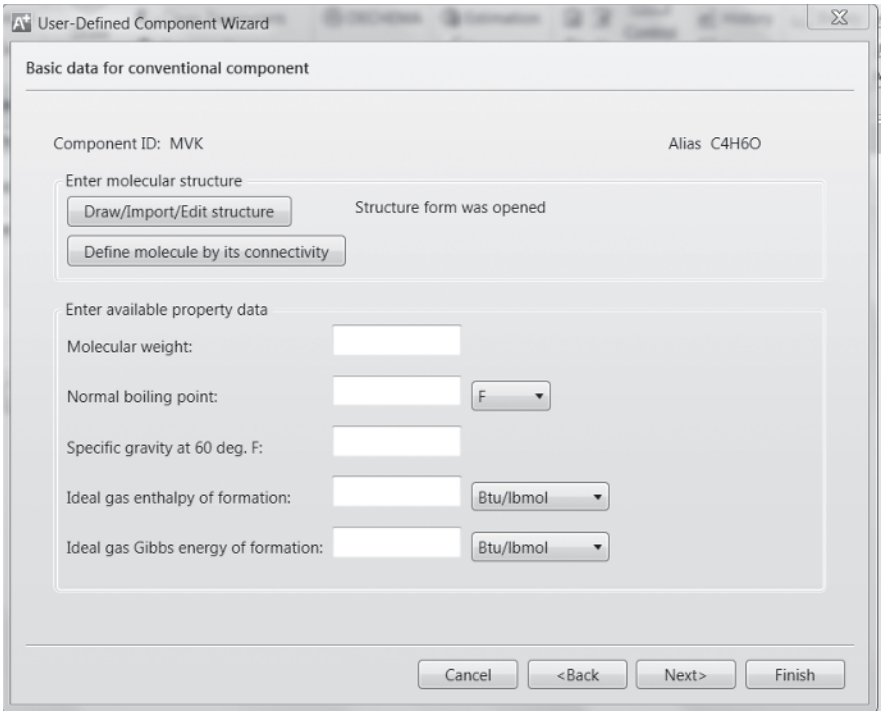

Figure 1.11. User-Defined Component Data and Properties.

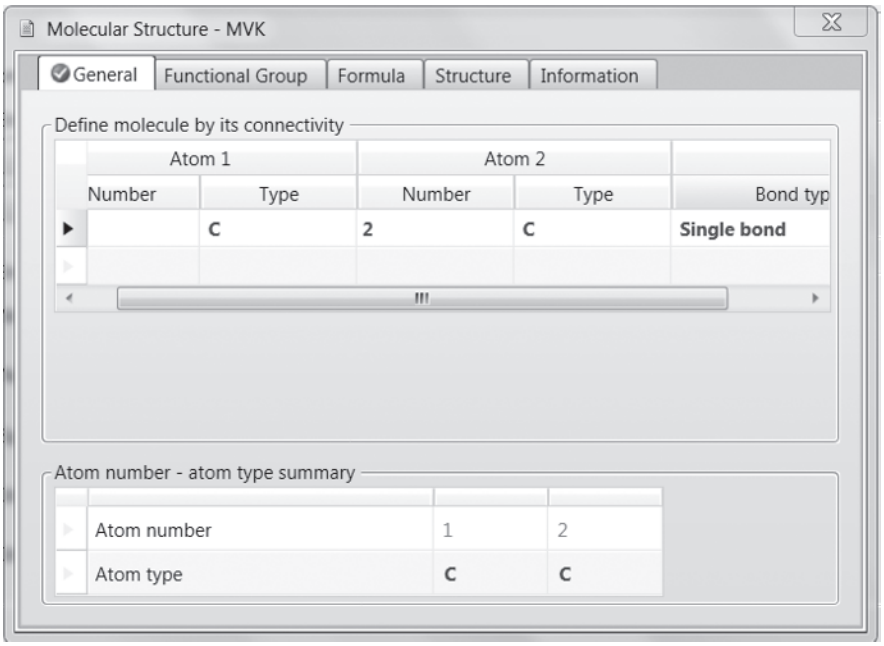

Figure 1.12. Molecular structure by connectivity.

1.6 PROPERTIES FOR SIMULATION

The Simulation environment can be entered by clicking the Simulation environment box on the lower-left corner of most displays. The Properties environment for many simulations should be executed prior to selecting the Simulation environment, so as to establish the properties used for simulation. When selecting properties for a simulation run from within the Properties environment, the choice of a global property method at Methods/Specifications is available. An example that applies to an entire flowsheet is shown in Figure 1.13. If, however, the simulation involves a situation where more than one property method is required, for example, a process involving distillation (vapor–liquid equilibrium) and extraction (liquid–liquid equilibrium), each block in the flowsheet may be defined as part of a unique section when the flowsheet is created. Each section is associated with a particular property method by choosing the Flowsheet Sections tab. A display similar to Figure 1.13 appears and the properties method for each flowsheet section can be identified and the global property method is not used. The display contains the Methods Assistant, which can be used as a guide for selection of a property method for specific applications.

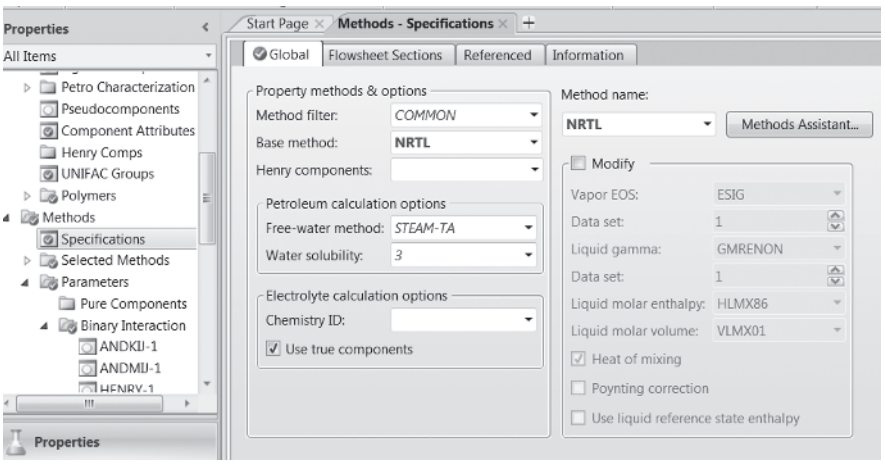

Figure 1.13. Global property method selection.

For example, the file Examples and Workshops/Chapter One/Examples/inputexample.bkp contains process sections S-1 and S-2, which are assigned the property methods Uniquac and UNIQ-2. Aspen Plus sets up the required Uniquac binary parameters for each section. Care must be taken that the appropriate database is accessed for each set of parameters. As an example, if the Navigation Pane topic Methods/Parameters/Binary Interaction is selected and the listing UNIQ-1 is clicked, Figure 1.14 appears. This shows the values of Aspen Plus supplied parameters for each binary pair and the source of the data used in the regression. Note that in Figure 1.14 the source of equilibrium data for each binary pair is identified. A selection of data sources is available by choosing the tab Databanks, which produces Figure 1.15. In the current example, section S-1 contains the extractor, and, therefore, it is important that the data source be liquid–liquid equilibrium data. Section S-2 involves a distillation column, hence the binary parameters source is vapor–liquid equilibrium data.

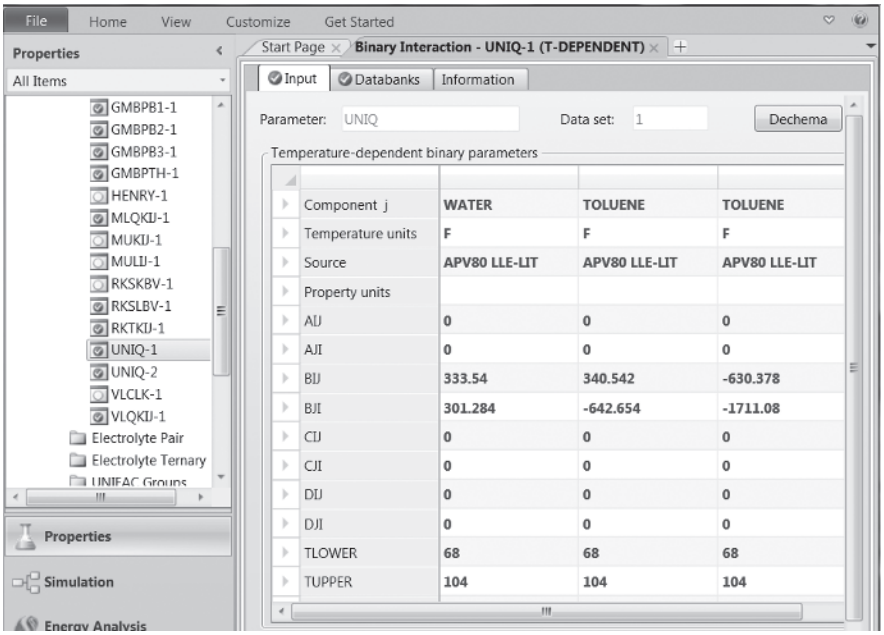

Figure 1.14. UNIQ-1 Binary Interaction Parameters.

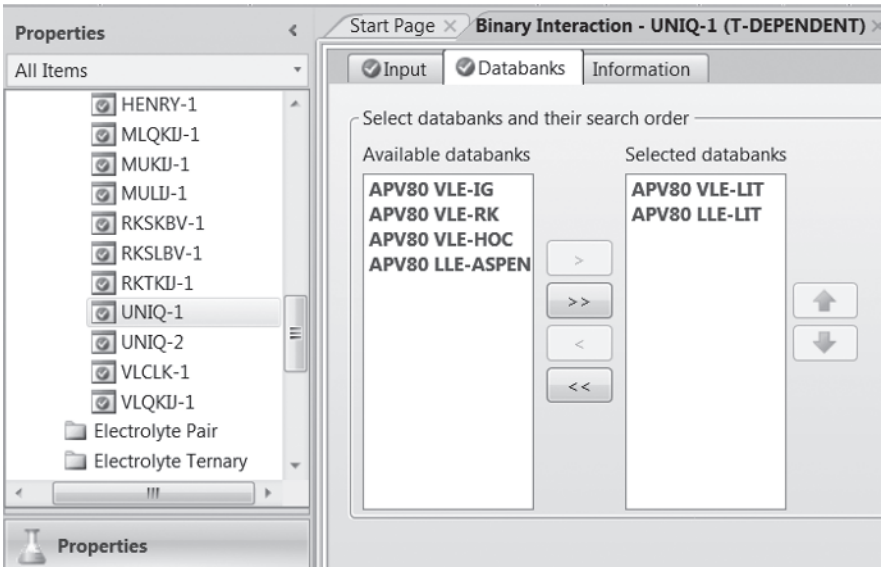

Figure 1.15. Available Databanks.

If data from another source is regressed so as to calculate new values for the binary parameters, they may be entered on the form illustrated by Figure 1.14.

1.7 THE SIMULATION ENVIRONMENT

A GUI is the means by which a simulation flowsheet is defined. The process consists of placing process units (blocks) and streams on the workplace and connecting them. Aspen Plus assigns generic names, such as B1, to the blocks; however, the user may change these names by right-clicking on the element of interest and using the menu that appears. Blocks are selected by choosing a Category tab from the Model Palette, shown at the bottom of Figure 1.8, for example, Columns, and clicking on the icon that represents the desired block. When selecting a block, a movable + sign appears on the open area of the display. After positioning it on the screen, a left click will place the block. The + sign remains and can be moved to insert another instance of the same block. This function ceases when the arrow button at the lower left of the palette is selected. In identical fashion, streams can be placed on the flowsheet. Material, heat, and work streams may be selected. When a stream input is selected and the cursor is moved onto the workplace, the ports to which the streams may be connected are shown and identified. The connection is made by moving the active cursor over an open port and clicking. An example of connecting streams to ports is shown in Figure 1.16, where the bottoms extractor product, EBOT, is disconnected and its connection point is the distillation column feed.

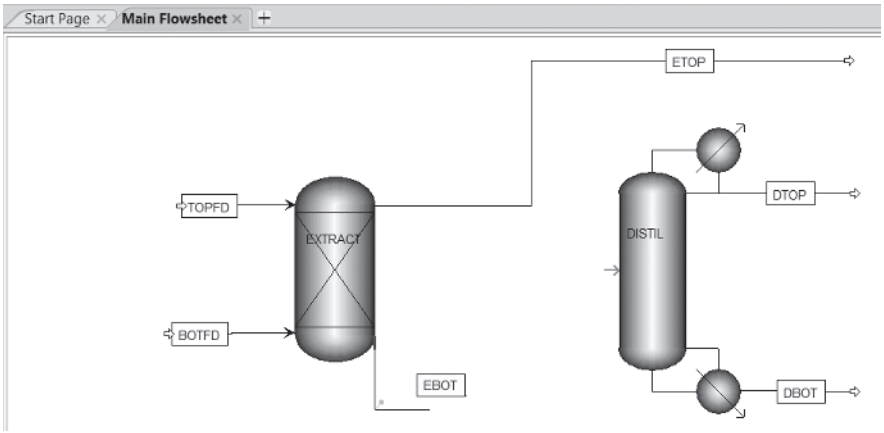

Figure 1.16. Connecting a stream to a block.

All icons, block names, and stream names can be selected, renamed, and moved using standard Windows techniques. Similarly, streams can be moved, rerouted, disconnected, and reconnected. Selecting and right-clicking on any of the objects displays a menu that provides many useful functions for manipulating the graphics. These include changing icons, rotating objects, renaming, deleting, resizing, and aligning the graphics.

1.8 SIMULATION OPTIONS

If the Simulation environment is entered and Calculation Options is chosen from the Navigation Pane, the display shown in Figure 1.17 appears. All of the default values that appear under the various tabs need not be changed except under the tab Calculations, where the

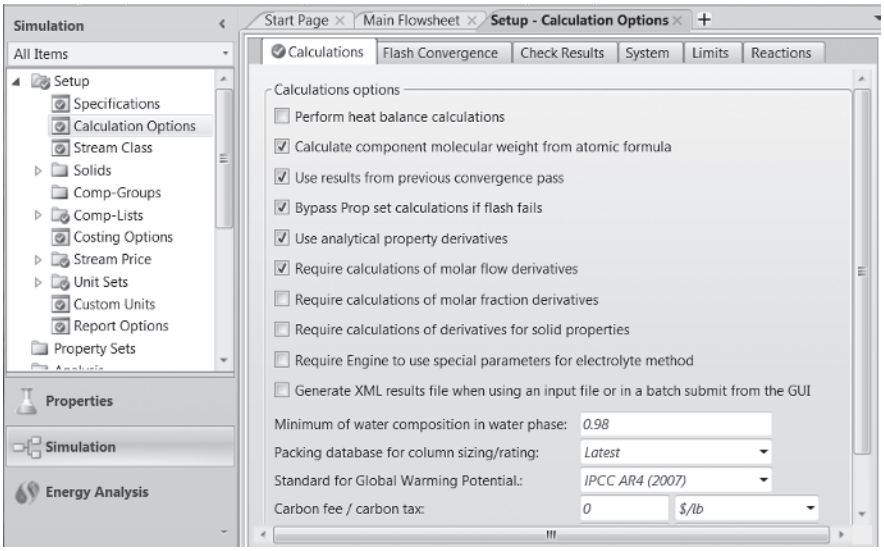

Figure 1.17. Calculations options.

option to use heat balances in the calculations is available, which is important for preliminary calculations. There are many unique simulation options, such as calculations involving solids, electrolytes, and the need for certain derivatives, all of which may optionally be selected by checking the appropriate box.

1.9 UNITS

Aspen Plus provides a user with a choice of units, engineering, metric, metbar, and the international system of units, that is, SI. This is available from the Navigation Pane at Setup/Unit Sets. An important option is the ability to select mixed units, such as the choice of engineering units with mmHg and °C as temperature and pressure, which is not uncommon in some pharmaceutical applications. To accomplish this, at Unit Sets selecting New assigns an Identifier for the new unit set, in this case US-1. The Copy from entry permits the user to select the unit set to be used as a base. Note selection of °C from the temperature drop–down list. Each unit's entry has an appropriate drop–down list that will enable a user to customize units.

Custom units for a specific variable, for example, special composition units, may be defined by selecting the Custom Units entry under the Navigation menu.

Aspen Plus input forms, displays, and specific subject reports are generated using the selected units. Input displays typically have a drop–down list adjacent to input boxes, which permit the user to select the units of the required input data as shown in Figure 1.18.

Selection of the Report Options entry in the Simulation environment in the Navigation Pane/Setup permits customization of the Aspen Plus results displays, which are optionally generated when results are available. The general text Report Options display is shown in Figure 1.19. Additional text reports are available by selecting a tab of interest.

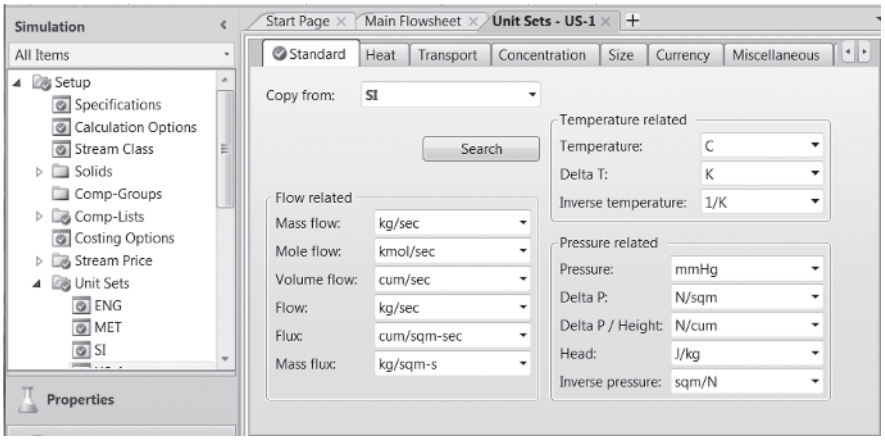

Figure 1.18. Units Selection.

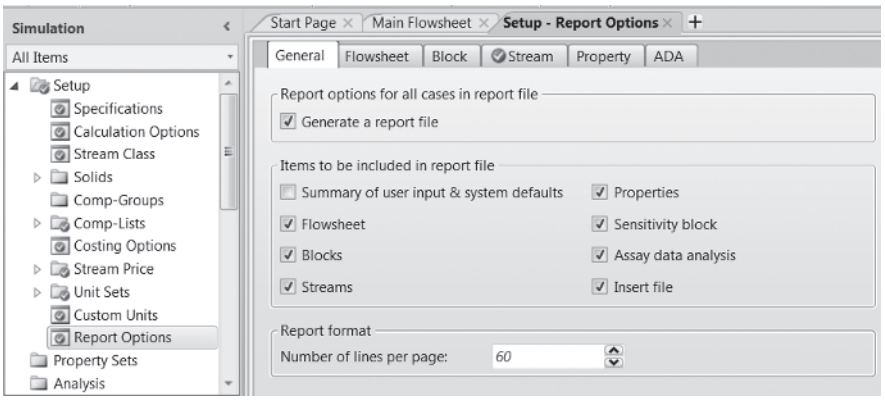

Figure 1.19. Report Options.

1.10 STREAMS

Selecting Next moves the input sequence to the next required input, in this case, stream data. All feed streams are defined using a display such as that given in Figure 1.20. The data entry is very straightforward and provides a user with the possibility for changing the units of both the material flow and the state variables.

For a stream of a single component or several components, the degrees of freedom calculated by the Gibbs Phase Rule applies, namely

$$F = C - P + 2$$

where F is the degrees of freedom, C is the number of components, and P is the number of phases. For a single-phase system with one phase, F equals 2; therefore, two specifications are required. For an n component system, F equals $n + 1$. Since $n - 1$ mole fractions need to be specified and the last calculated by the sum of the mole fractions equal to one, only two additional specifications are required. In both cases, these are usually, but not necessarily, temperature and pressure.

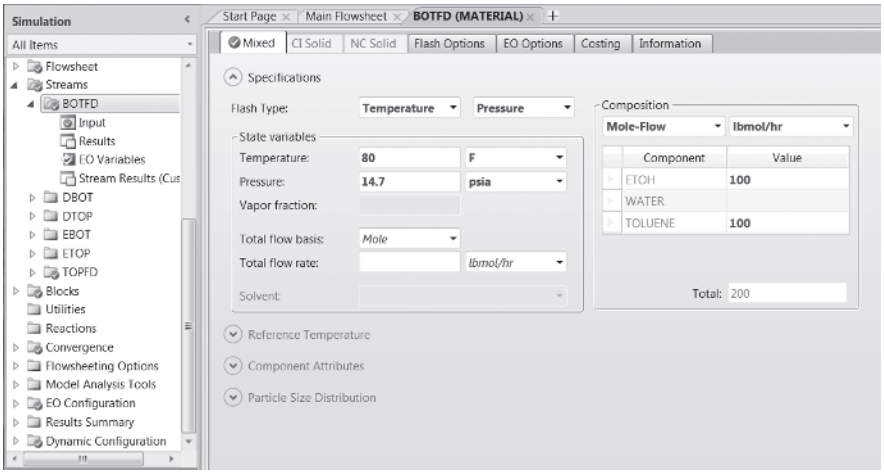

Figure 1.20. Stream Input.

When two phases in equilibrium are involved, only one degree of freedom is available. For example, for a one-component stream, such as a saturated liquid, specification of the temperature fixes the (vapor) pressure. But in such circumstances it is necessary to state the fraction of the mixed stream, which is vapor (or liquid). For a saturated liquid, the V/F specification would be a very small number such as 0.00001. For a multicomponent stream, the situation is identical and it is necessary to specify either temperature or pressure and the vapor or liquid fraction.

If the process contains tear (recycle) streams, they will not be treated as required input and pushing the Next button may not suffice. Typically, Aspen Plus will assign zeros as starting values to the variables that are to be converged, but if a user wishes to provide starting values, the stream name under the streams list in the data browser can be selected and a display analogous to Figure 1.20 will appear.

1.11 BLOCKS

When all stream input has been completed, selecting Next will result in the appearance of the first input form for a block that requires data. Details of block input will be addressed in other chapters. After the data input forms for the first block are completed, selecting Next will produce the forms for the next block in the process until all the block data has been entered.

The Navigation Pane in Figure 1.20 shows some addition topics, which may be appropriate for a user's simulation. These will not appear when Next is selected; however, they may be chosen by clicking on the subject. For example, clicking the Convergence entry permits the selection of the convergence method and parametric default values. These subjects will be addressed in other chapters. When data entry for all blocks and supplementary data entry is completed, selecting the Next button produces a dialog to enable execution. All input can be reviewed, prior or after execution, by selecting the appropriate input form on the Navigation Pane.

1.12 THE OBJECT MANAGER

In certain data input situations, there are specialized setups that involve the specification of material that requires a special set of dialogs to define what is required. Examples are definition of a set of properties to be displayed, regression of a data set to a thermodynamic model, and specification of the value of a block output variable. This type of input is managed through the use of the Object Manager. These situations typically begin with the identification of a function, such as a regression, followed by a series of choices and specifications. An example of the use of the Object Manager for a Calculator block, which is used for in-line calculations, is given in Figure 1.21. The user creates an ID, such as C-1, which is followed by all the required input forms, including association of calculation variables to flowsheet variables and definition, in Fortran, of the calculation details.

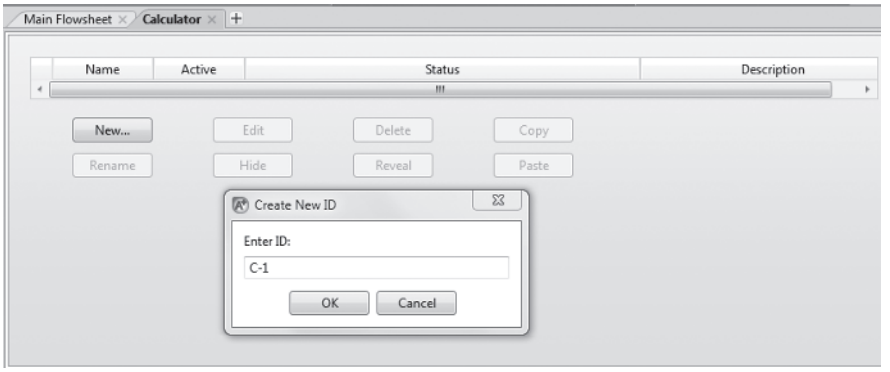

Figure 1.21. Object Manager example.

1.13 MODEL EXECUTION

The mechanisms for controlling Aspen Plus runs and their icons are located on the Home/Run section of the ribbon as shown in Figure 1.22. The symbols from the left represent Next, Run, Step, Stop, Reset (reinitialize) Control Panel, and Reconcile. Moving the cursor over each of the symbols describes its function. Selecting the symbol labeled Control Panel brings up a display that describes all operations during simulation, for example, the convergence of a block, such as a flash, or the successful execution of a complete plant model.

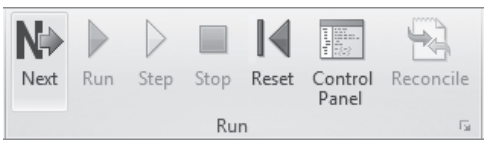

Figure 1.22. Run related icons.

1.14 VIEWING RESULTS

Prior to execution, in preparation of viewing the results, of an Aspen Plus simulation, a user may customize reports by selecting Report Options from the Navigation Pane Setup/Report Options. The General tab displayed in Figure 1.19 shows the variety of options available for configuring the details of information to be displayed in each of the categories displayed. Customization is available under each of the tabs, for example, Figure 1.23 shows options available for stream reports.

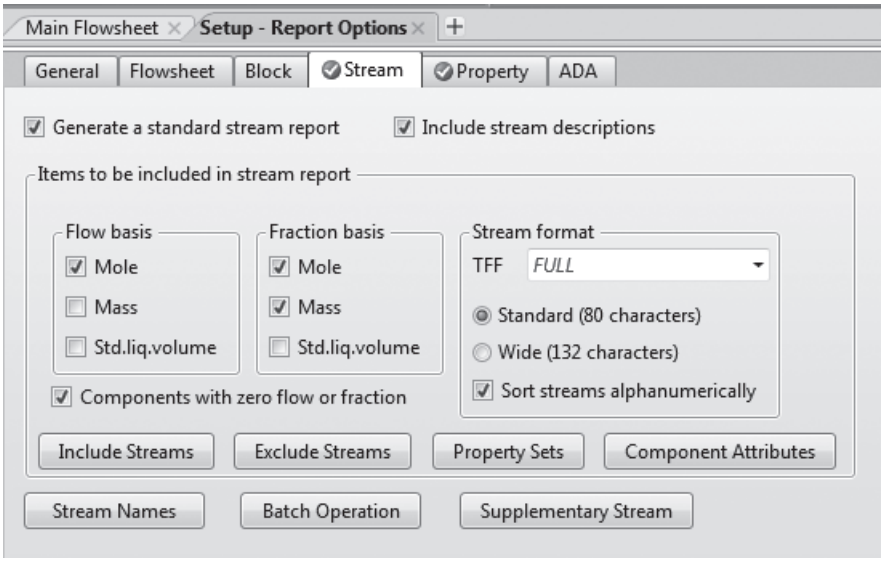

Figure 1.23. Stream Report Options.

At the conclusion of a simulation, the run's Control Panel is usually displayed. If not, it can be viewed from the drop–down list under the main menu item View. This contains a brief summary of the execution of each block and a list of error messages. It is important that users check and correct any errors that might have occurred. When a process contains tear streams, errors that occur during the iterations will be presented. It is not uncommon that errors occur before convergence, but when the process has converged, there should be none. Figure 1.24 displays a segment of the run Control Panel. A summary of the results of the simulation can be viewed by selecting the Results Summary from the Navigation Pane when the simulation run has completed. Detailed on-screen reports of most sections can also be found on the Navigation Pane. For example, at Blocks/*blockname* there are sections labeled Results and others, such as Profiles, which depend on the type of block.

When a simulation has been completed, selection of Report from the main menu item View will produce a .txt report of the complete simulation, in a Notepad window, which can be copied and pasted. An example of this report showing the stream summary is given in Figure 1.25.

The file Chapter One/Examples/inputexample.bkp was used to produce all of the figures in this chapter as well as the inputexample.txt file.

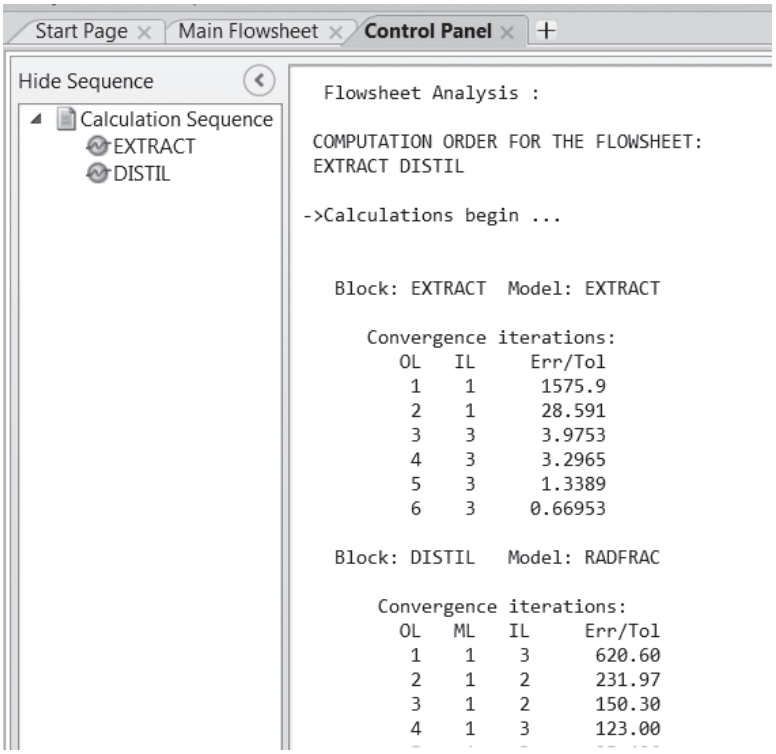

Figure 1.24. Control Panel segment.

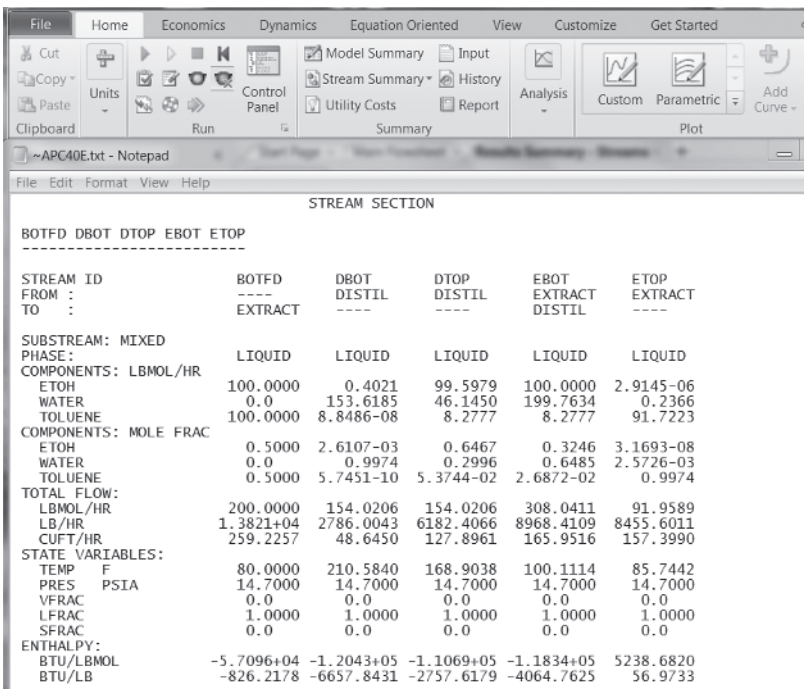

Figure 1.25. The Text Report segment.

1.15 PLOTTING RESULTS

Aspen Plus has a plotting facility that is integrated with the Results selection on a block menu and with other items such as regression results in Chapter Two. The facility provides preconfigured plots or offers the selection of independent and dependent variables manually on the Home/Plot menu on the ribbon. As an example, after obtaining a converged solution to the distillation column, using Examples/input example and selecting Profiles under the DISTIL block menu and the tab TPFQ a series of stage variables appear. Selecting the Temp – Plot produces Figure 1.26, which shows the variation of compositions through the column. For situations where no preconfigured plots are available, but a display in which tabular output is available, such as the results of a sensitivity analysis, details in Chapter Five, one may select a custom plot, where each column of data can be assigned to either the *x* or *y* coordinate. It is also possible to assign two variables to the *y* coordinate. If the scale or title of an axis or the title of a plot is not suitable, one may select it by clicking and a display that offers editing options appears. There is also a selection that permits the data to be formatted in a square plot, and if desired a diagonal line, both of which are suited for vapor–liquid and liquid–liquid equilibrium data.

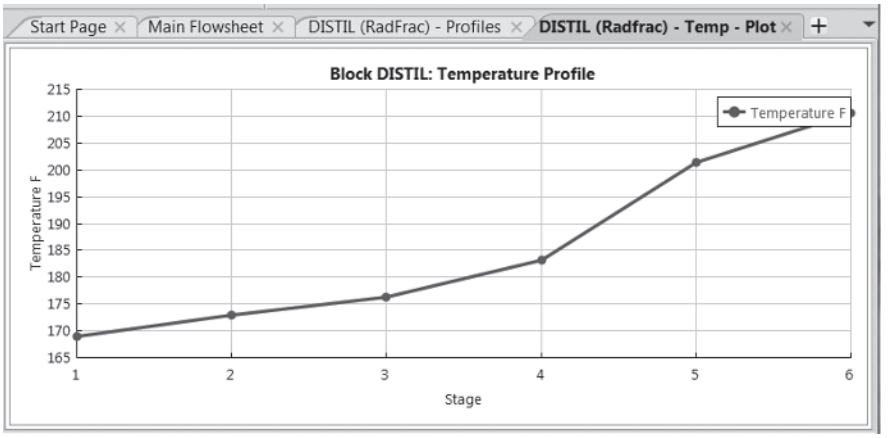

Figure 1.26. Preconfigured plot.

REFERENCES

Aspen Technology Corporation, Aspen Plus On-line Documentation.
Monsanto Corporation, "Flowtran Simulation: An Introduction", Monsanto Corporation (1974).