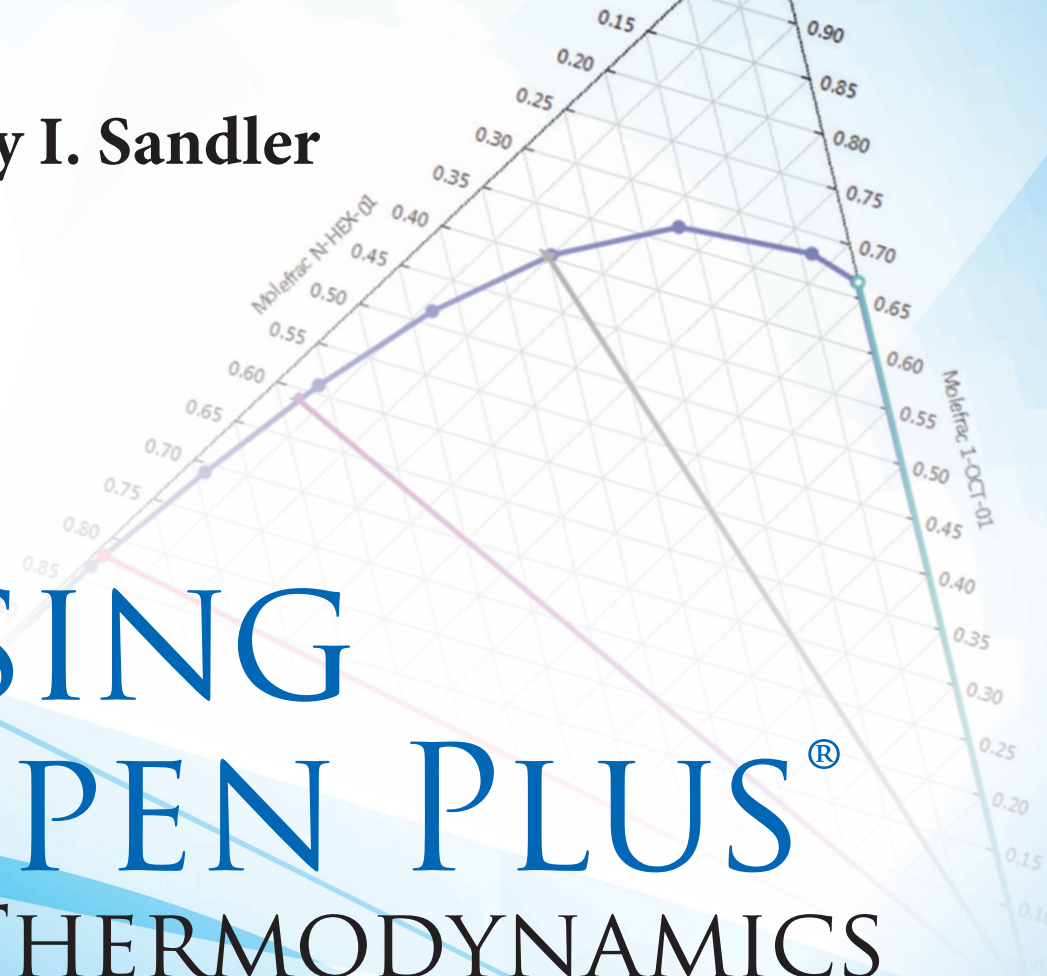
Stanley I. Sandler



Using Aspen Plus® in Thermodynamics Instruction

A Step-by-Step Guide

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A Step-by-Step Guide

Stanley I. Sandler

Department of Chemical and Biomolecular Engineering
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Newark, DE

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Preface

Aspen Plus® is a very powerful process simulator—that is, a tool for modeling chemical processes, including complete chemical and pharmaceutical plants and petroleum refineries. As such, it requires accurate models of thermodynamic properties and phase behavior.

The purpose of this book is to introduce the reader to the use of Aspen Plus in courses in thermodynamics; consequently, very few of the process simulation capabilities are considered here. In undergraduate chemical engineering degree programs, process simulation is heavily used in the capstone design course, and this is where its details and intricacies are generally taught. This book serves as a prelude to instruction in the more complex process simulation and provides a coherent approach to introducing the Aspen Plus simulator in undergraduate thermodynamics courses. I hope it will make such courses more interesting and relevant by allowing calculations of real processes that would otherwise be very tedious. One advantage of doing such calculations by computer is that repetitive calculations with varying parameters are quickly achieved, so that the student gains experience into the ways in which different input parameters affect the output. Such calculations develop engineering insight. Any instructor knows that asking students to do repetitive calculations by hand is met by moans and groans. Doing a calculation for one case is an important learning activity, while doing many cases by hand has much less pedagogical return for the student's time investment.

This book provides the reader with a self-study, step-by-step guide to doing thermodynamic calculations in Aspen Plus. It provides actual screenshots of the Aspen Plus interface to solve example problems of specific types, including vapor–liquid, liquid–liquid, vapor–liquid–liquid and chemical reaction equilibria, and simple applications to liquefaction, distillation, and liquid–liquid extraction. One important feature is that learning occurs by means of illustration. It is not a book of rules but of specific examples, encouraging readers to generalize from those examples and apply what they have observed to a specific problem. Designed for self-study, this book is not meant as an in-class textbook but for out-of-class use. However, there are places in this book where it is useful to refer to fundamental thermodynamic principles. In such cases, for convenience, I provide explicit references to my thermodynamics textbook, *Chemical, Biochemical, and Engineering Thermodynamics*, 4th ed., published by John Wiley & Sons, Inc., in 2006. However, the same material can be found in any standard thermodynamics textbook, so this book can be used with any thermodynamics textbook.

Let me reiterate that although the Aspen Plus program is designed to do process simulation, the purpose of this book is not to emphasize simulation. Examples of using the program for simulation are included, however, because some thermodynamics calculations can only be done in Aspen Plus by using simulation. These include vapor–liquid and vapor–liquid–liquid equilibrium flash calculations, especially an adiabatic flash (i.e., Joule–Thomson expansion) and chemical reaction equilibrium calculations. Please keep in mind that the Aspen Plus program has far greater capabilities than are demonstrated here.

This book is meant to be a step-by-step guide for individual study. As such, the book contains many screen images produced using Aspen Plus®. These screen images of Aspen

Plus® are reprinted with permission of Aspen Technology, Inc. AspenTech®, aspenONE®, Aspen Plus®, and the AspenTech leaf logo are trademarks of Aspen Technology, Inc. All rights reserved.

All suggestions for improvement would be greatly appreciated. Please communicate those to me at sandler@udel.edu.

Finally, I want to acknowledge the assistance provided by Aspen Technology, Inc., that provided an individual license to use Aspen Plus® so that I could work on this manuscript at home while attending to my wife during her final illness. I especially want to thank Chau-Chyun Chen, a former Aspen Technology employee, who made this possible and also provided many helpful comments on an early version of the manuscript. Suphat Watanasiri of Aspen Technology was also helpful in the process.

STANLEY I. SANDLER

January 2015

An Introduction for Students

As you are beginning to see in your courses, thermodynamic calculations for other than ideal gases can be quite time consuming. Also, in class you may have considered a single device, such as a Joule–Thomson valve, or in the case of liquefaction, just a few devices (e.g., a compressor, a heat exchanger, a Joule-Thomson valve and a separator.) Such calculations can require many iterations, both for each unit operation (e.g., equation of state calculations for the compressor) and, if there are recycle streams as in the Linde process, for the overall process as well. You can imagine how difficult and time-consuming such calculations would be for a whole chemical plant or petroleum refinery, with very many different pieces of process equipment and a complex web of many recycle streams. So how are such calculations done in industry, or how will you do them efficiently in your design course, especially if you want to consider many different design options? The answer is by using a complicated computer program known as a process simulator. Such a computer program allows the user to put together a flow sheet of the equipment in the process being considered and to connect all the equipment by the flows of mass (and in the case of heat exchangers and some other equipment by the flows of heat). Then, after the user specifies the components, the feed composition, the conditions, the constraints, and the thermodynamic models to be used, he or she is able to compute the amounts and compositions of all the streams in the process. After seeing the results, the user can easily make changes to the inlet stream and the conditions (e.g., temperature and/or pressure at various points of the process), and rerun the simulation. In this way the engineer acquires an understanding of how the process responds to changes in conditions, allowing the engineer to optimize the process for various metrics: profitability, minimum carbon dioxide or other waste emissions, minimum energy use, etc.

Why introduce process simulation in a course on thermodynamics? Several compelling reasons exist. First, as you progress through your thermodynamics classes you will see that the calculations involved become increasingly more complicated. This alone justifies the use of some type of computer software. Second, a calculation for a single set of process specifications can be tiresome, though doing only one allows the student to understand the basis of the calculation. But this understanding, while important, does not provide the student or engineer with any insight into the way the process will respond to changes in the variables or whether the current set of specifications is optimum. Such knowledge comes only from calculations involving a collection of other operational specifications, and these calculations can be done rapidly with a process simulator, allowing the user to better understand the behavior of the process. In this way he or she can develop engineering intuition that would not come from doing only a single calculation. Third, choosing the correct thermodynamic model(s) is critical to obtaining meaningful results in process simulation, so that thermodynamics and process simulation are linked together in a very important way.

I want to emphasize this last point since it is so important. As an example, suppose the process we want to model contains liquids, but we tell the process simulator to use the ideal gas law to describe the system. What will happen? The process simulator will provide

answers, but the results will be nonsensical. A process simulator will do computations exactly as instructed, but it is unable to determine whether the result obtained is meaningful or not. That is the job of the engineer. In computer lingo there is an acronym, GIGO, which means "garbage in, garbage out." Here it translates to bad thermodynamics, bad results. Unfortunately, in my consulting experience, I have observed another application of GIGO, meaning "garbage in, gospel out." That is, the user of a process simulator accepts the results obtained without critical evaluation. This is often due to the fact that the engineer has had difficulty getting a completely unrelated process simulation calculation to converge (or converge to a reasonable answer) and has tried different thermodynamic models until one yielded a reasonable answer. From then on, the engineer has tended to use that model for all other processes, including the ones for which it is completely inappropriate. This is a serious error of engineering judgment that could prove expensive to rectify or dangerous if a chemical plant were built according to those faulty specifications.

The central point, therefore, is that while using a process simulator can eliminate the tedium of process calculations, the results will only be meaningful if the user has a sufficient understanding of thermodynamics and thermodynamic models to make informed choices. Anyone using a process simulator (or, for that matter, any computer tool for calculations) should carefully check the results against his or her engineering intuition, experience, and knowledge of thermodynamics. For example, in the chapter on chemical reactions, the principle of Le Chatelier and Braun can provide guidance as to how the equilibrium state of a chemically reacting system might shift in response to a pressure change. If the result of a process simulation indicates otherwise, one should make sure that the input and process choices are correct. Similarly, if a change of temperature in a process produces a result that is counterintuitive, further analysis is required. The point is that one should not blindly accept any result derived from a computer. Rather, one must analyze all the factors to see whether they make sense.

While most chemical and petroleum companies initially developed their own in-house process simulators, the expense of maintaining them, of introducing new thermodynamic and equipment models as they became available, and of servicing users became untenable. Consequently, the field of process simulation is now dominated by software from a few commercial vendors and some freeware through the CAPE-OPEN project. A web search will yield a number of available process simulators. Here we will consider only one, Aspen Plus—arguably, the one possessing the largest user base and, in addition, made available to universities at a very affordable price.

The main use of Aspen Plus is for process simulation, and various books and courses are devoted to instructing students in how to employ it. That is not our purpose here; we are interested solely in the way Aspen Plus can be used in undergraduate courses in thermodynamics. Therefore, while Aspen Plus has a wide range of capabilities, we will consider only the following:

1. Basic process simulation
2. Phase equilibria (vapor–liquid, liquid–liquid, and vapor–liquid–liquid)
3. The thermodynamic data regression capabilities
4. **Property analysis** (pure fluids and mixtures)
5. The **NIST TDE** (thermodynamics data engine)
6. The **Property Method Selection Assistant**
7. Simple distillation and extraction

Note: Throughout this text a word or words in **bold** font refer to a specific aspect or function of the Aspen Plus simulator identified as such. Readers of this book when using it to follow an example while using the Aspen Plus simulator, should select, by clicking on it, the relevant text indicated in **bold**.

Chapter 1

Getting Started With Aspen Plus®

Aspen Plus® is a process simulation program that can also be used for many types of thermodynamic calculations, or to retrieve and/or correlate thermodynamic and transport data. In this book it will largely be used for thermodynamic calculations, such as computing phase equilibria and regressing parameters in thermodynamic models, and also for some very simple process simulations, merely to introduce the concept.

To start, open the **Aspen Plus V8.x**, which you may have to locate depending on the setup of your computer. [It may be on your desktop or you may have to follow the path **All Programs>Aspen Tech>Process Modeling V8.x>Aspen Plus>Aspen Plus V8.x**. In doing this you will also see paths to the large collection of specialized Aspen Plus modules that will not be considered here.] The interface is somewhat different for Aspen Plus V8.0 and Aspen Plus V8.2 and higher. For Aspen Plus V8.0 continue here, while for Aspen V8.2 (or higher) go to Fig. 1-2a.

[The screen images shown below and throughout this book were produced using Aspen Plus®. These screen images of Aspen Plus® are reprinted with permission of Aspen Technology, Inc. AspenTech®, aspenONE®, Aspen Plus®, and the AspenTech leaf logo are trademarks of Aspen Technology, Inc. All rights reserved.]

Figure 1-1a Aspen Plus V8.0 Start-up

When you open **Aspen Plus V8.0**, you will briefly see the Aspen logo in Fig. 1-1a. There is then a slight delay while the program connects to the server, and then the **Getting Started** page shown in Fig. 1-1b appears. There you will see a list of **Product News** items (that changes as it updates on a regular basis). From this window you will be able to start a new **Simulation** or open one of your previous simulations that will appear (in the future) in the list under **Recent Cases**.

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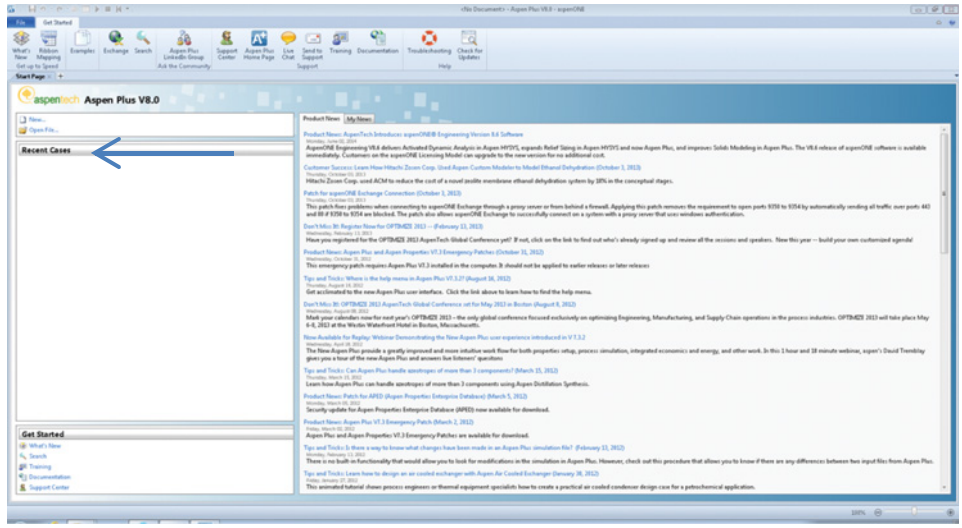

Figure 1-1b Aspen Plus V8.0 Start-up

To proceed, click on **New..**, which brings up the window in Fig. 1-3.

Figure 1-2a Aspen Plus V8.2 Start-up

When you open **Aspen Plus V8.2**, you will briefly see the Aspen logo in Fig. 1-2a. There is then a slight delay while the program connects to the server, and then the **Exchange** window shown in Fig. 1-2b appears.

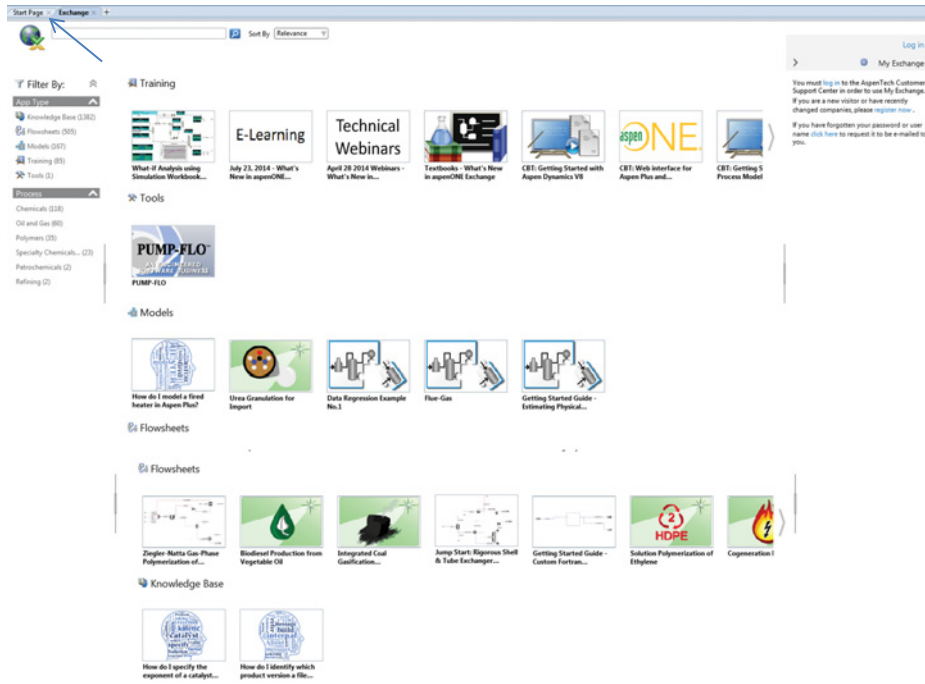

Figure 1-2b

This window contains flow sheets and information about a number of processes, training information, pre-prepared models for specialized unit operations, and other items. These will be ignored here as the emphasis is on thermodynamic modeling. Click on the **Start Page** tab as shown by the arrow in Fig. 1-2b, which will bring up the **Start Page** shown in Fig. 1-2c. There you will see a list of **Product News** items (that changes as it updates on a regular basis). From this window you will be able to start a new **Simulation** or open one of your previous simulations that will appear (in the future) in the list under **Recent Cases**.

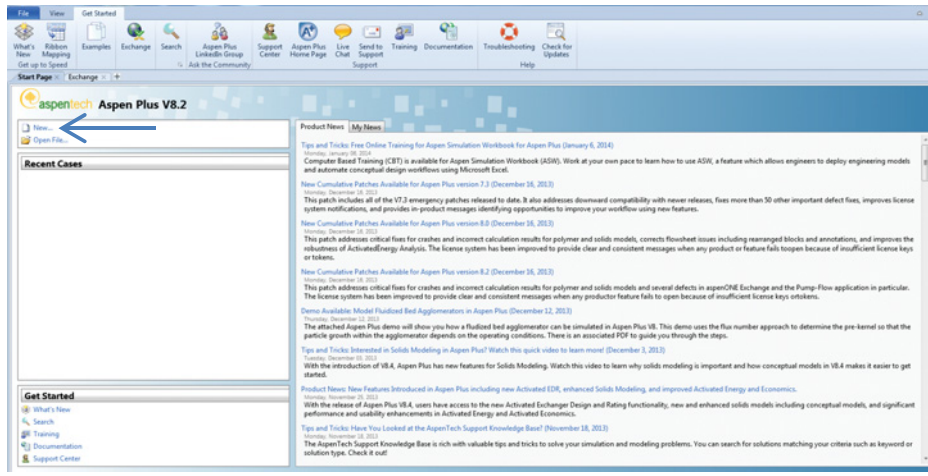

Figure 1-2c

To proceed, click on **New..**, which brings up the window in Fig. 1-3. Continuation for all versions of Aspen Plus V8.0 and higher.

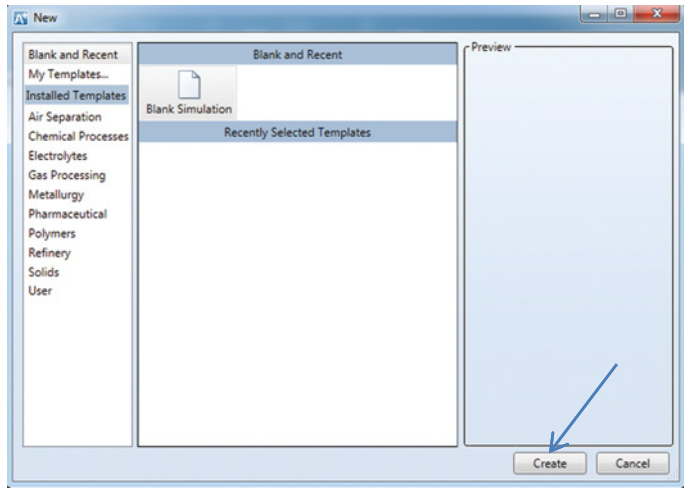

Figure 1-3

Click on **Blank Simulation** and then **Create**. This will bring up Fig. 1-4.

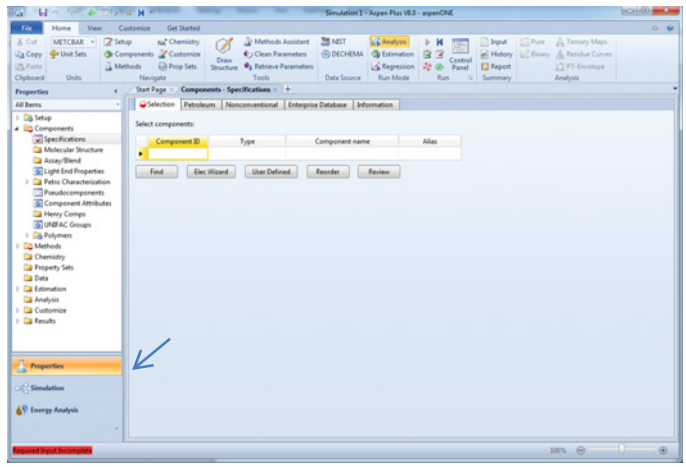

Figure 1-4

On the lower-left-hand corner of this window, there are three choices. The first, which Aspen Plus opens with, is **Properties**; the drop-down menu under **Components>Specifications** is used to specify the component or components for the calculation, and the drop-down menu under **Methods** is used to specify the thermodynamic models and parameters that will be used in the calculation. The second general area is **Simulation** that will take you to a flow sheet window, to be discussed later, and the third is **Energy Analysis** that will not be considered here. The default is to start with **Properties**.

We will proceed by entering the component propane. There are two ways to enter component names. The simplest and most reliable to ensure that you will get the correct component and its properties from the Aspen Plus database is to click on the **Find** box that brings up the **Find Compounds** window and then enter the component name by typing in propane and then clicking on **Find Now**, which produces the window in Fig. 1-5.

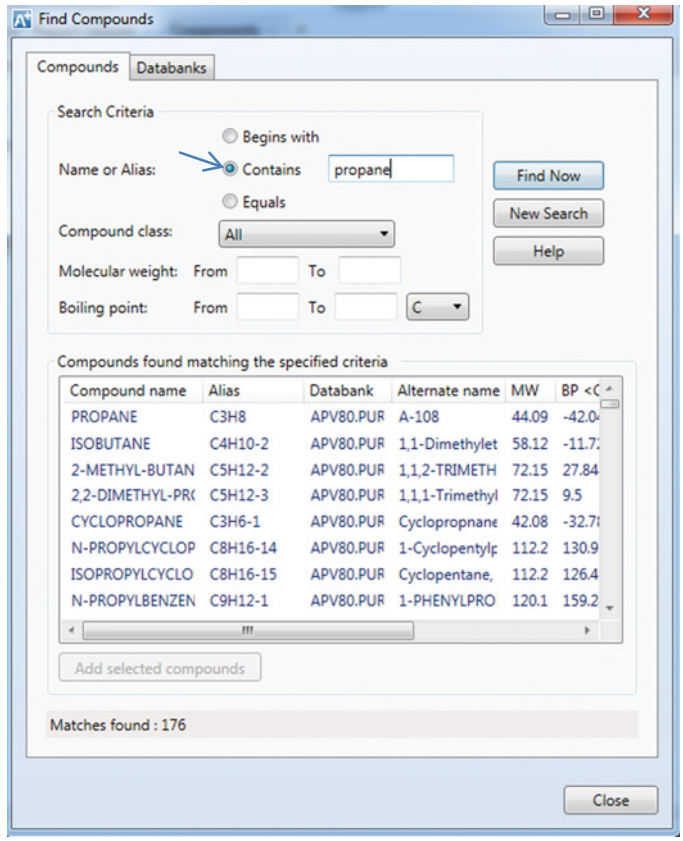

Figure 1-5

A long list of 176 compounds in Fig. 1-5 is generated because the default **Contains** was used in the **Find Compounds** window; as a result every compound in the database that contains propane either in its compound name (e.g., propane, but also cyclopropane) or in its alternate name (e.g., isobutane is also known as 2-methyl propane) appears in the list. The compound we are interested in happens to be first on the list here, but that will not always be the case. Therefore, a better way to proceed in the **Find Compounds** window is to click **Equals** instead of the default **Contains**, and then click **Find Now**, which produces instead a list containing only propane (Fig. 1-6).

[Note that Aspen Plus has a large number of data banks of pure component and mixture thermodynamic and transport properties data. Generally these are called up automatically by the program. Here the pure component names and properties were obtained as shown from the data bank APV80.PURE.x, where 80 indicates the version number of Aspen Plus

(here 8.0) and PURE.x is version x of the pure component properties data bank. Other data banks will be encountered later in this book.]

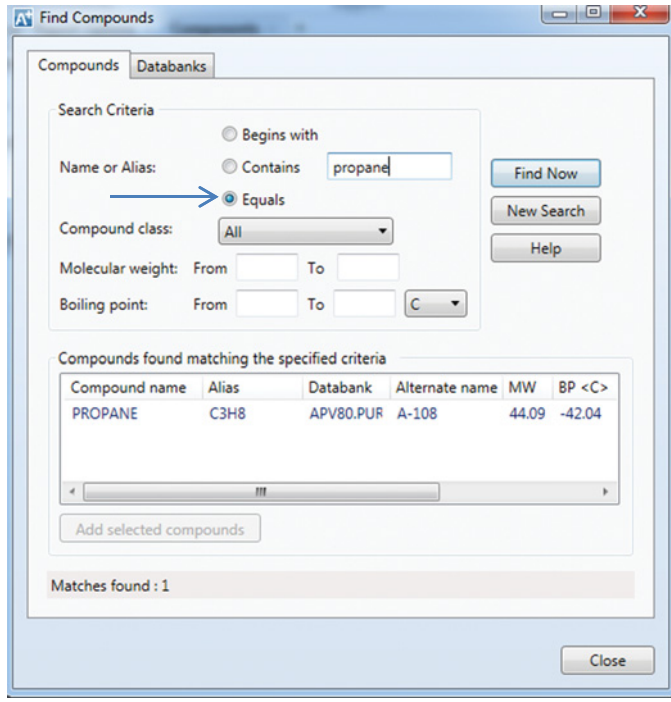

Figure 1-6

Click on **PROPANE** and then **Add selected compounds**, and for this example, then click on **Close**. In cases considered later, several compounds will be sequentially added following this procedure with the exception of not clicking on **Close** after each compound. [Note that the window of Fig. 1-6 provides information on the Aspen Plus data bank used to obtain the data for propane (APV80.PUR here), the molecular weight, boiling point, etc.] You will then see the following (Fig. 1-7):

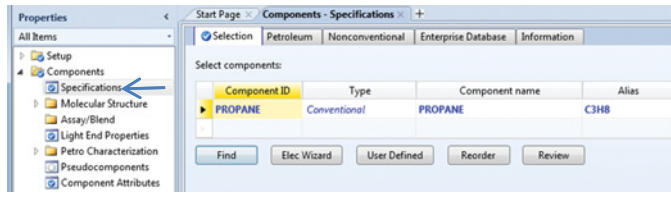

Figure 1-7

[Another alternative is to type in all or part of the name directly in the **Components-Specification** window and see whether Aspen Plus finds the correct name.] Note that propane has now been added to the **Select components** list and that both **Components** and **Specifications** now have check marks indicating that sufficient information has been

provided to proceed to the next step. However, this may not be sufficient information for the problem of interest to the user. If the problem to be solved involves a mixture, one or more additional components may be added following the procedure described above except that the **Close** button in the **Find Compounds** window is used only after all the components have been added.

The next step is to go to **Methods** by clicking on it. The window in Fig. 1-8 appears and here a number of thermodynamic models can be used. For a simple hydrocarbon system at the pressures here, a simple cubic equation of state can be used, for example, the Peng–Robinson or Soave–Redlich–Kwong equation. Here, and frequently throughout this book, the Peng–Robinson (indicated by **PENG-ROB** in Aspen Plus) will be used, though any other equation of state for which parameters are available can be used. Generally, simple equations of state, such as the Peng–Robinson and other cubic equations of state produce results that are not of great accuracy, but they provide adequate descriptions of both the vapor and liquid states, and are adequate for thermodynamic calculations for pure fluids and mixtures that are nonpolar and do not hydrogen bond. The Peng–Robinson equation has been chosen from the drop-down **Base method** menu to calculate the thermodynamic properties of this nonpolar alkane. [Note that if you need help in choosing a thermodynamic model, you can click on **Methods Assistant** … for help. The **Methods Assistant** will be discussed in Chapter 8.] After accepting the Peng–Robinson equation by pressing **Enter**, **Methods** on the left-hand side of Fig. 1-8 will also have a check.

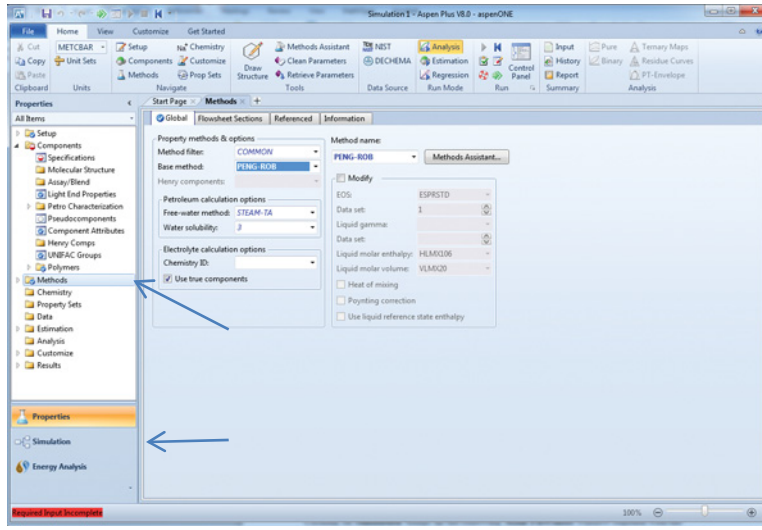

Figure 1-8

Clicking on **Simulation** brings up the **Main Flowsheet** window of Fig. 1-9 together with the **Model Palette** at the bottom of the window.

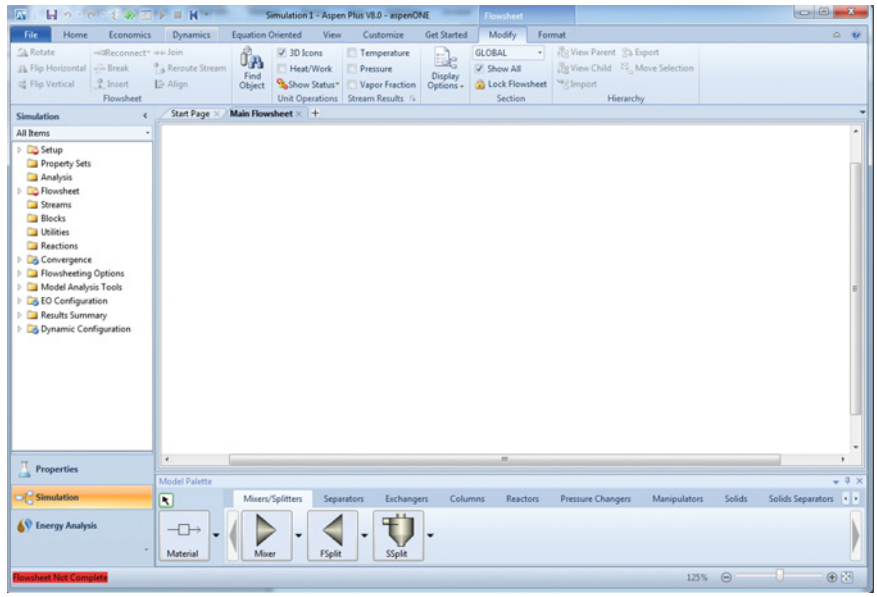

Figure 1-9

It is in this window that a process flow sheet, or even a single process unit such as a vapor–liquid separator or a chemical reactor, will be entered as we will see starting in the next chapter.

However, before ending this chapter, it is useful to note that when doing calculations involving mixtures, the default in **Streams** and **Reports** is mass flow rates and molar flow rates. Sometimes the user may also want to see mole fractions. To ensure that mole fractions appear in the results for the process flow streams in mixture calculations, click on **Setup>Report Options>Streams** and then under **Fraction Basis** click on **Mole** as shown in Fig. 1-10.

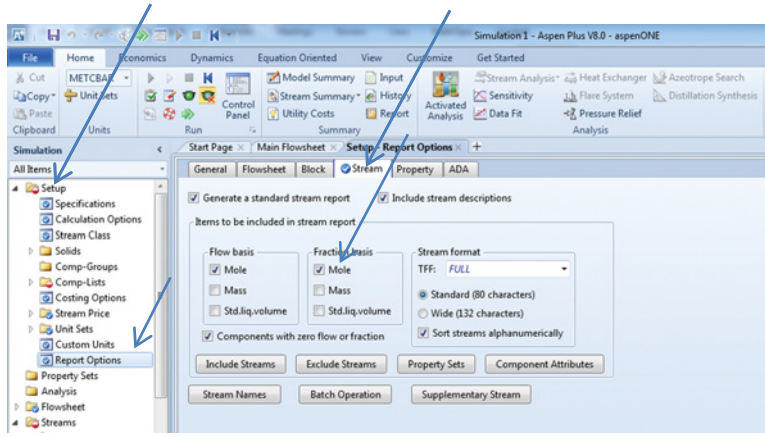

Figure 1-10

What has been described in this chapter needs to be done when starting any new Aspen Plus calculation. In the following chapters it will be assumed that you can successfully navigate through the **Setup**, **Components, and Methods** windows. Therefore, this material is not generally repeated in the chapters that follow.

There is one point to note here when using Aspen Plus. This program is designed for (largely) steady-state process flow calculations, not static calculations. That is, while we may be interested in a thermodynamic calculation for 1 mole of a species, Aspen Plus expects a flow rate. So instead of using the program to solve a problem for a change of state for a fixed amount of material, say 1 mole, in the **Streams** setup one will have to specify a flow rate such as 1 mol/min, 1 mol/hr, 1 kmol/hr. That choice will not affect the equilibrium state or compositions of the streams, but will affect the heat and work flows that are computed in Aspen Plus for the process equipment (referred to as blocks in Aspen Plus) as they depend linearly on the flow rates.

PROBLEMS

1.1. In the Aspen setup choose *n*-pentane as the component and the Soave–Redlich–Kwong equation of state as the base method.

1.2. Set up Aspen to use *n*-pentane and *n*-hexane as the two components in a binary mixture, and the Soave–Redlich–Kwong equation of state as the base method.

1.3. Set up Aspen to use ethanol and water as the two components in a binary mixture, and the NRTL model as the base method.

Chapter 2

Two Simple Simulations

Aspen Plus® was developed as a process simulator. This will be illustrated here for two very simple cases involving pure fluids, merely to provide the student simple examples of the main use of a process simulator. You will use the process simulation capabilities extensively in later courses and especially in the design course. However, in thermodynamics courses it is mostly the thermodynamic and phase equilibrium calculational abilities and the databases that will be used.

As motivation and as an introduction to the use of Aspen Plus as a process simulator, we consider here, as the first of two examples, a simple process for the liquefaction of propane. This process starts with propane vapor at ambient conditions (298 K and 1 bar), which is compressed to 15 bar, cooled back down to 298 K, expanded through an adiabatic (i.e., Joule–Thomson) valve to 1 bar, and then the resulting gaseous and liquid streams are separated. Since propane is not an ideal gas throughout the process because of the conditions (high pressure and the presence of both a gas and a liquid), the Peng–Robinson equation of state will be used as the thermodynamic model, though other equations of state could have been chosen.

Here we start by opening the **Aspen Plus User Interface** as described in the previous chapter. Also, as described in the previous chapter, *n*-propane will be chosen as the single component, and the Peng–Robinson equation of state as the thermodynamic model. Next click on **Simulation**, which brings up a blank **Main Flowsheet** window with the **Model Palette** at the bottom as shown in Fig. 2-1.

We then start constructing the flow sheet. The first piece of process equipment in this liquefaction example is the compressor to adiabatically and reversibly compress the feed propane from 1 bar and 298 K to 15 bar. We place the compressor on the flow sheet by first choosing the **Pressure Changers** tab in the **Model Palette** at the bottom of the screen, which lists six different types of pressure changing devices, choosing the compressor, **Compr**, by first clicking on it, then moving the cursor (now a cross) to the **Main Flowsheet** window, choosing where you want to put the compressor, and then left clicking to produce the window in Fig. 2-1.

Using Aspen Plus® in Thermodynamics Instruction: A Step-by-Step Guide, First Edition. Stanley I. Sandler.
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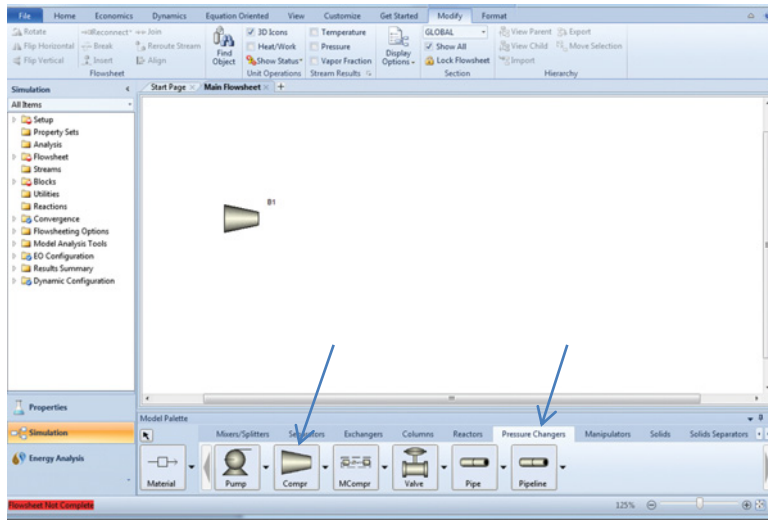

Figure 2-1

Next go to the **Exchangers** tab in the **Model Palette**. Four types of heat exchangers appear; choose the first one, **Heater,** and add it to the flow sheet as shown in Fig. 2-2.

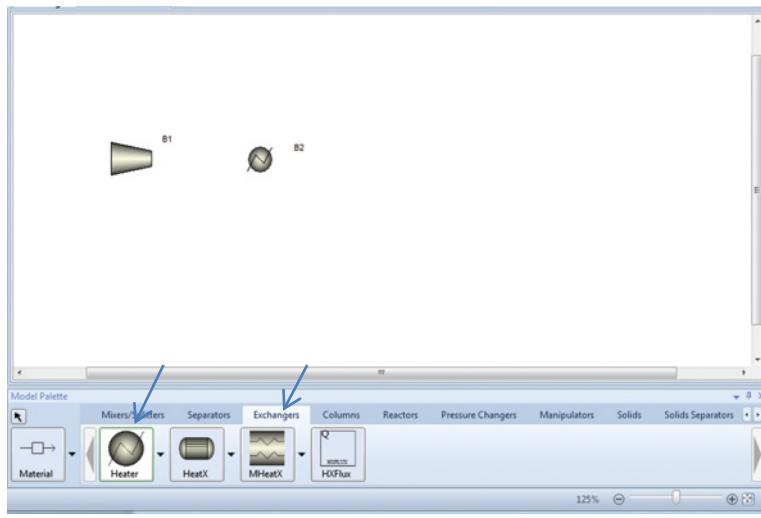

Figure 2-2

Next, go back to **Pressure Changers** and add the **Valve**. Finally, go to the **Separators** tab and add the **Flash2** (two-phase) separator to your flow sheet, which should now look like the window in Fig. 2-3.

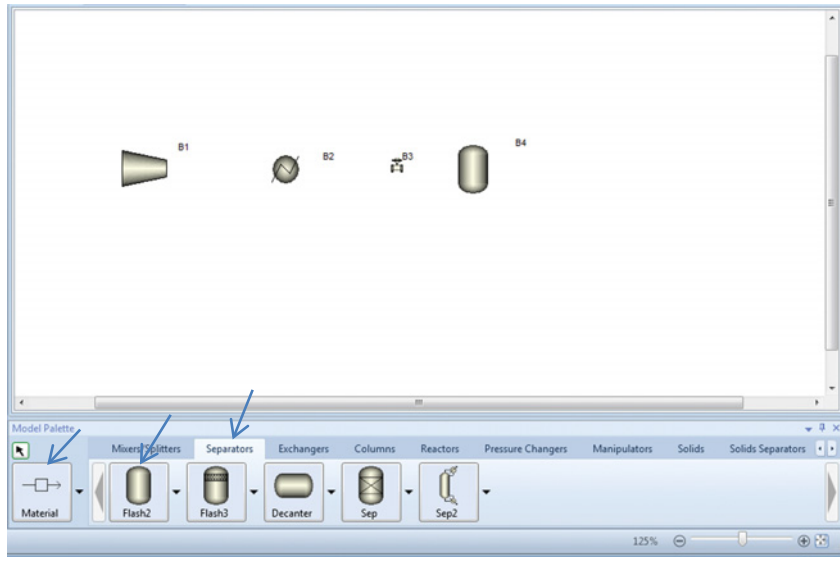

Figure 2-3

Note that in the lower-right-hand corner of the screen, in red, is the statement "Flowsheet Not Complete." Next we have to connect the material flow streams to the process equipment. This is done by clicking on the **Material** icon at the lower-left corner of the **Model Palette**. Start with the feed stream by clicking on the compressor. The window should then be as in Fig. 2-4.

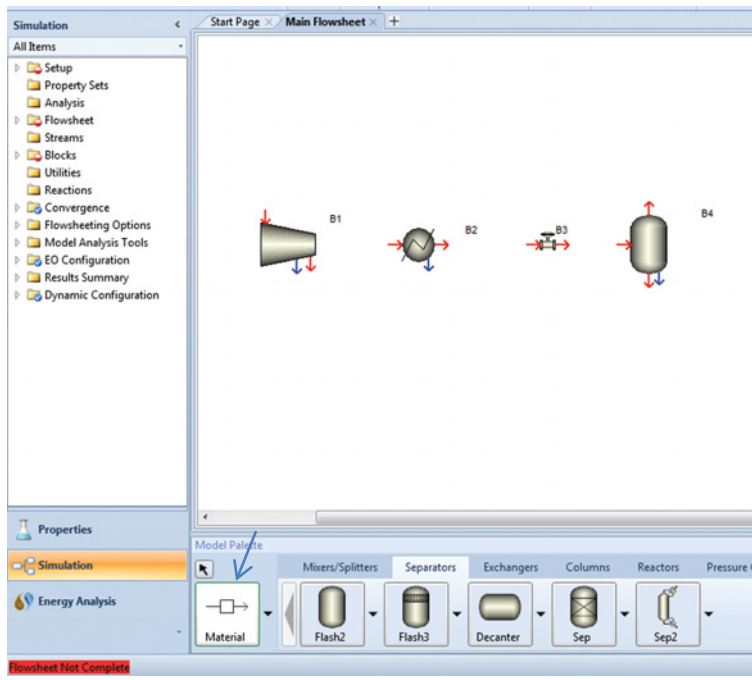

Figure 2-4

Each red arrow indicates a required input or outlet stream for each piece of equipment, while a blue arrow is an optional stream. For the compressor, the red arrow pointing into it is the required feed stream, and there is a required outlet stream (red) and an optional outlet stream (blue), for example, if the outlet contained both gas (red stream) and liquid (blue stream). In this example, all blue streams will be ignored. As the first step in completing the flow sheet, the feed stream will be added to the compressor and the red outlet stream will be connected to the heat exchanger. This is done by clicking and holding on an arrow, moving the cursor to the desired location, and releasing it. Doing this for the inlet (feed) arrow to the compressor, and connecting the outlet from the compressor to the inlet to the heat exchanger produces Fig. 2-5.

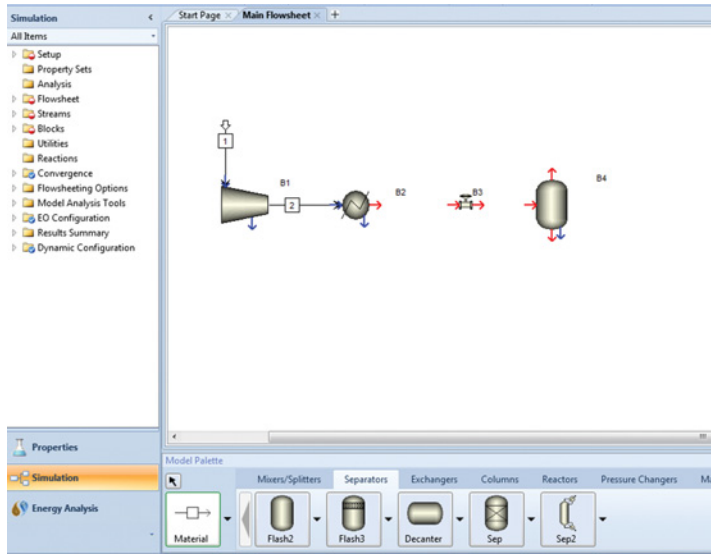

Figure 2-5

The bigger open arrow (above stream 1) pointing inward identifies it as an external inlet stream. A similar arrow pointing outward indicates a stream exiting the process.

Now completing the flow sheet by connecting the remaining streams one obtains Fig. 2-6.

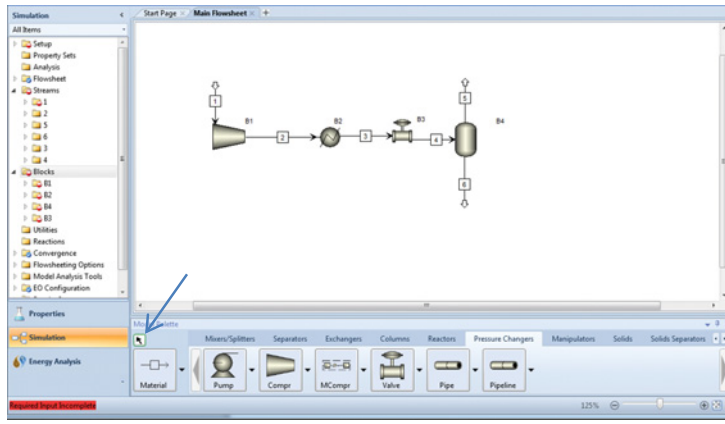

Figure 2-6

To get out of the mode of adding **Material** (streams), click on the arrow above that icon.

Some suggestions for putting together a nice flow sheet:

1. Unless you are very steady with the mouse, the streams are likely to appear jagged. To prettify your flow sheet, you can click on a stream and then on **Align blocks**. I suggest starting at the end of the flow sheet and continuing stepwise backward to the feed; otherwise you may introduce jagged feed streams upstream or downstream.
2. I like to rename the blocks (process units) and streams with names easier to recognize in the output. However, I retain the initial numbers so that the order in the output will be the same as in the flow sheet.

The revised flow sheet based on these suggestions appears in Fig. 2-7.

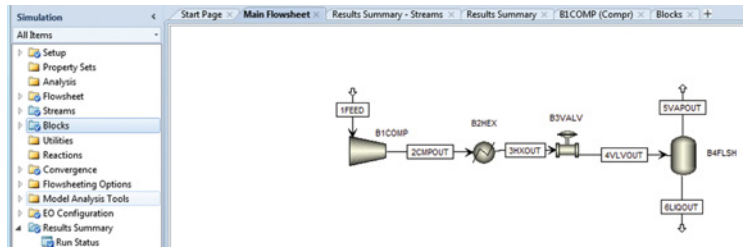

Figure 2-7

To proceed, the user must now provide the specifications for the process, which includes the inlet stream component(s) and conditions, pressures and temperatures where needed, and the type of each process unit or block (e.g., an isentropic compressor, an adiabatic valve) Clicking on **Streams>1** brings up the window in Fig. 2-8, which is completed as in Fig. 2-9. This is the only stream that needs to be specified; the properties of all the other streams will be computed in the simulation calculation once the actions of the **Blocks** are chosen.

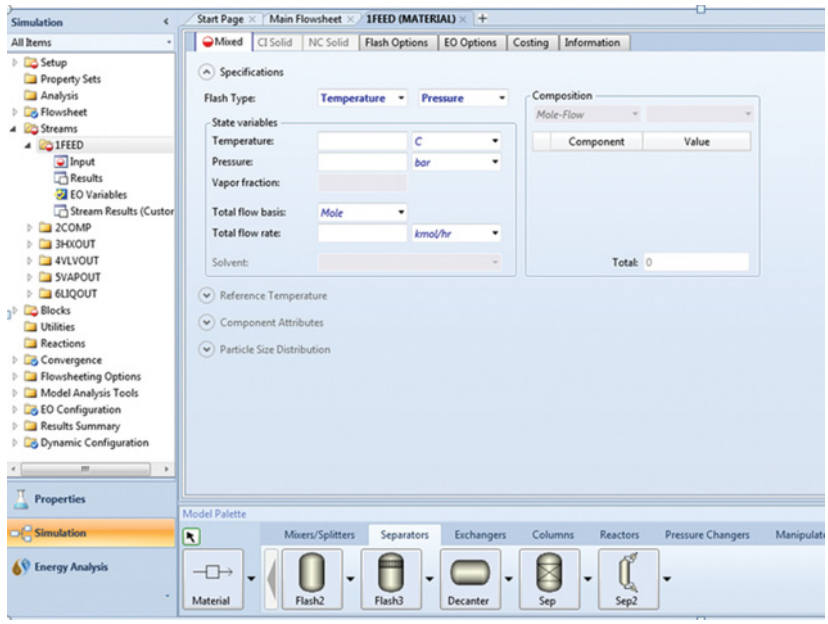

Figure 2-8

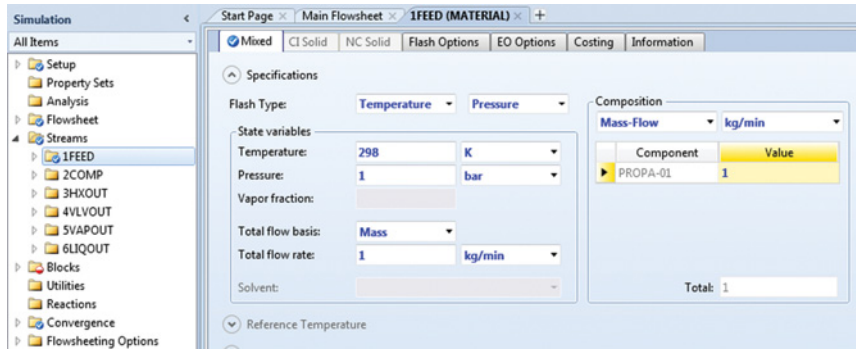

Figure 2-9

We then move on to the specifications for the **Blocks** (process units). Starting at **B1COMP**, the compressor, we specify that it is to be a perfect (all efficiencies equal to 1) isentropic compressor with a discharge pressure of 15 bar; this is shown in Fig. 2-10.

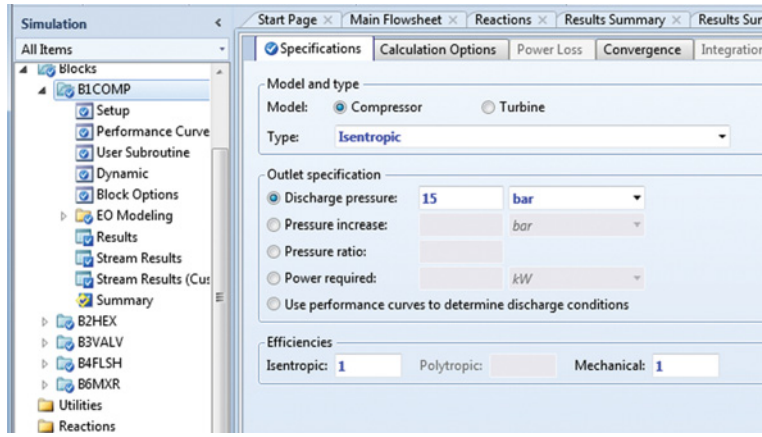

Figure 2-10

Next the heat exchanger, **B2HEX**, in this example is to operate with no pressure loss (15 bar) and an exit temperature of 298 K (see Fig. 2-11.)

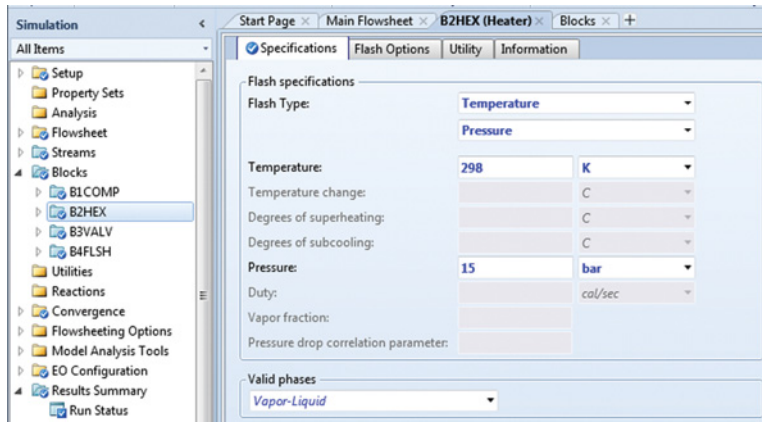

Figure 2-11

The valve, **B3VALV**, is to operate adiabatically with an outlet pressure of 1 bar as shown in the window of Fig. 2-12. [Other entries are the unchanged defaults.]

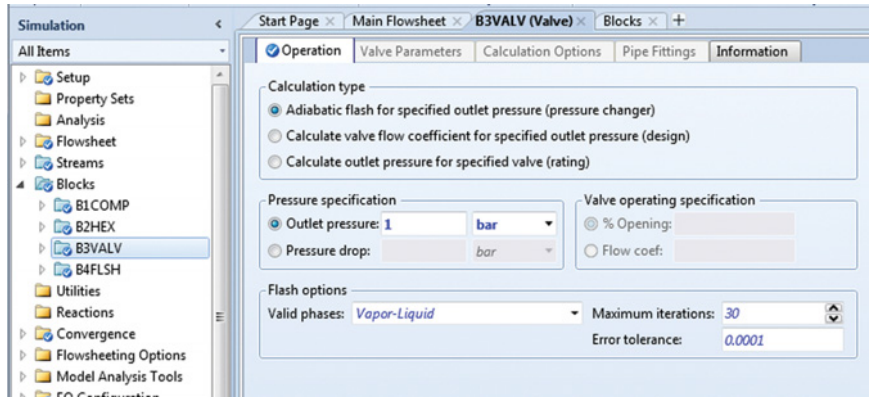

Figure 2-12

Finally, the specifications for the flash unit (Fig. 2-13), **B4FLSH**, are that it operates at 1 bar and adiabatically. The default is that temperature and pressure are fixed, which is not the case in this example. By clicking on the **Temperature**, a drop-down menu appears, and from the choices, **Duty** (meaning heat duty) is selected, and then in the **Duty** drop-down box 0 is entered to specify that the separator operates adiabatically.

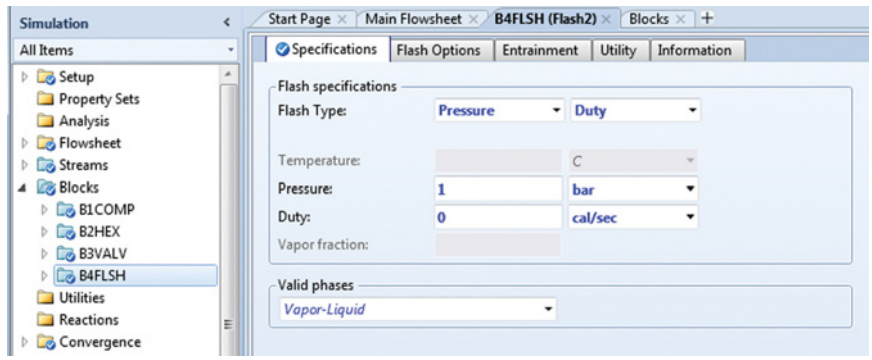

Figure 2-13

Though **Setup** has a check mark as a result of the Aspen Plus defaults, following the instructions in Chapter 1, I chose to click on it and give a title to the simulation and that metric units with temperature in degrees centigrade and pressure in bar (METCBAR) are being used (Fig. 2-14). Now all the necessary boxes are checked, and in the lower-right-hand corner of the window in Fig. 2-14, there is the message "**Required Input Complete**."