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**.

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

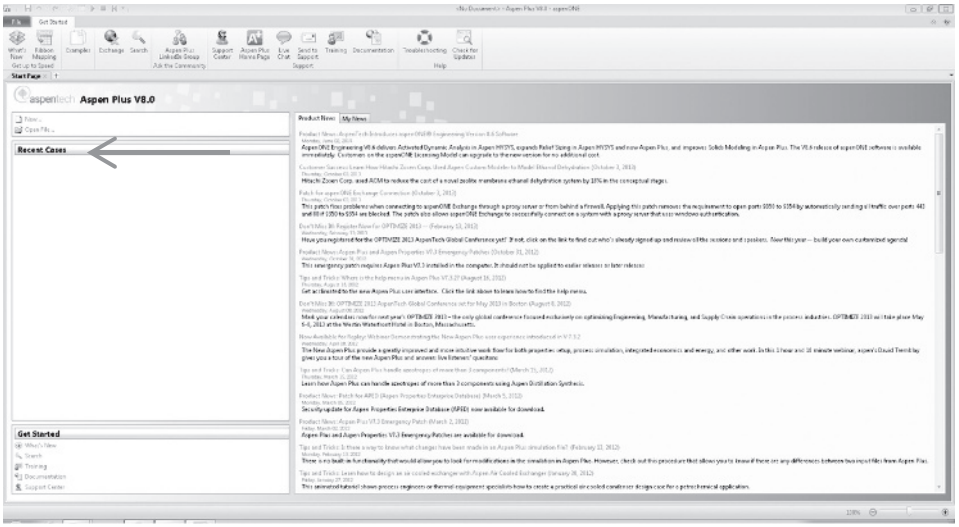

Figure 1-1b Aspen Plus V8.0 Start-up

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.

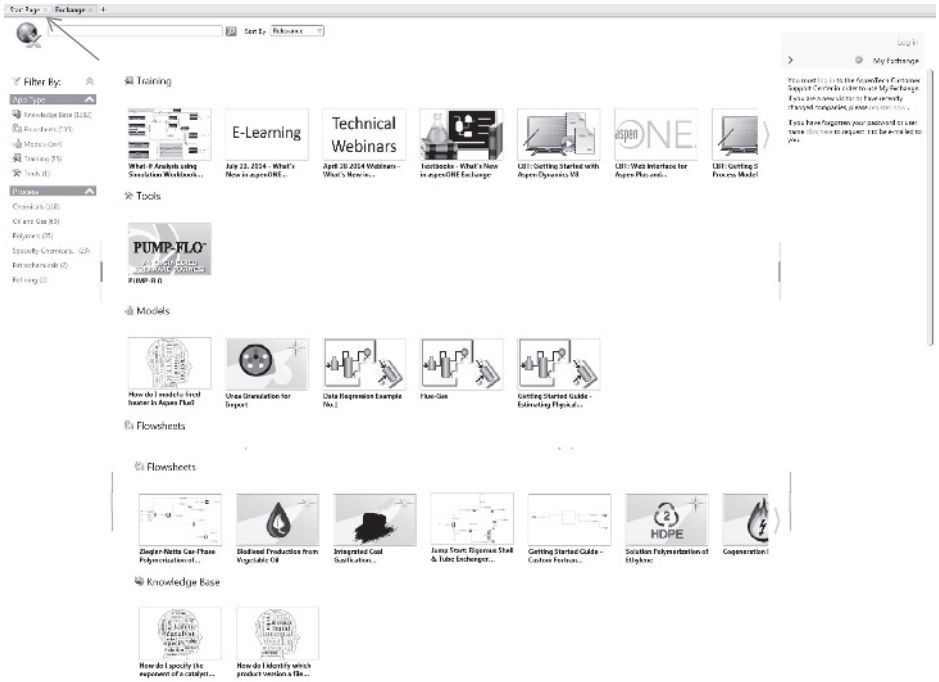

Figure 1-2b

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**.

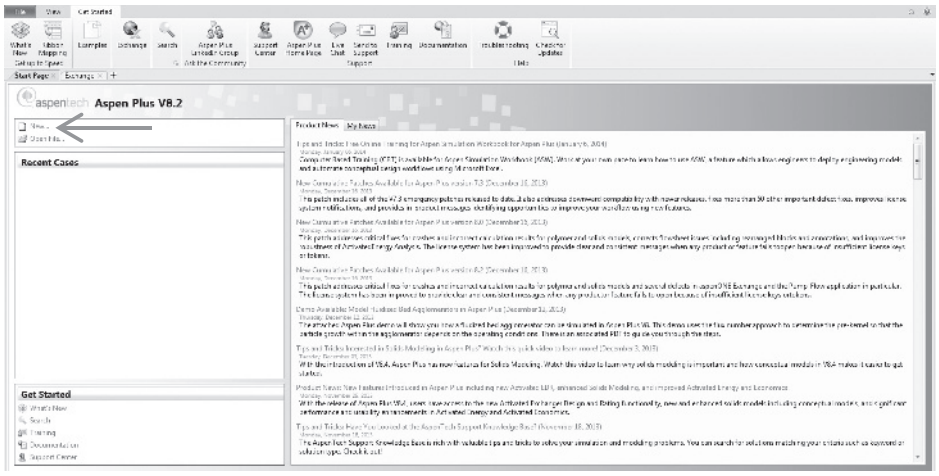

Figure 1-2c

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.

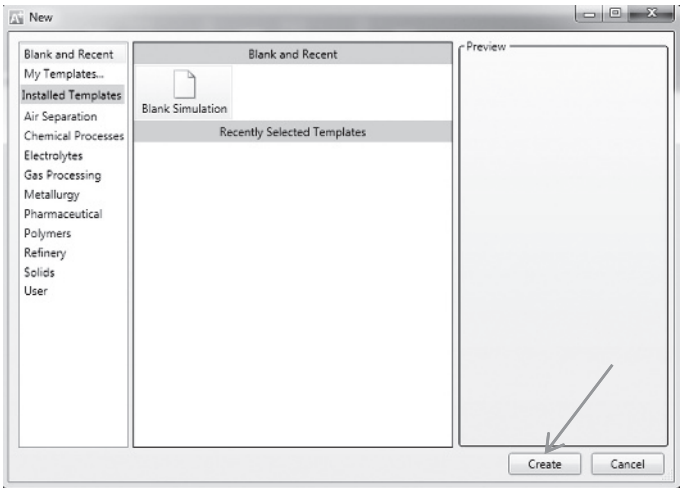

Figure 1-3

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

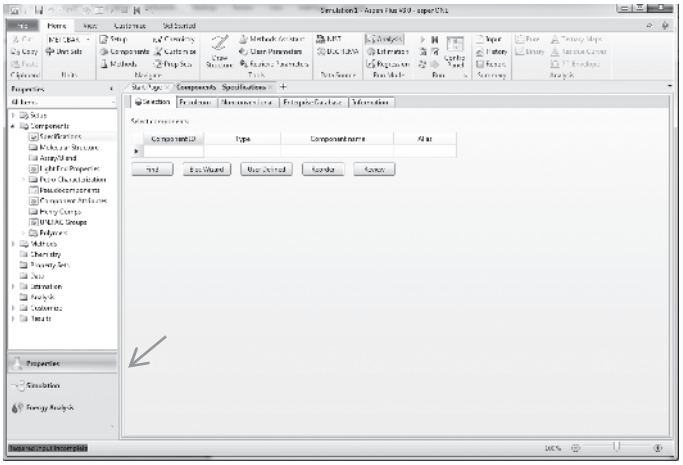

Figure 1-4

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.

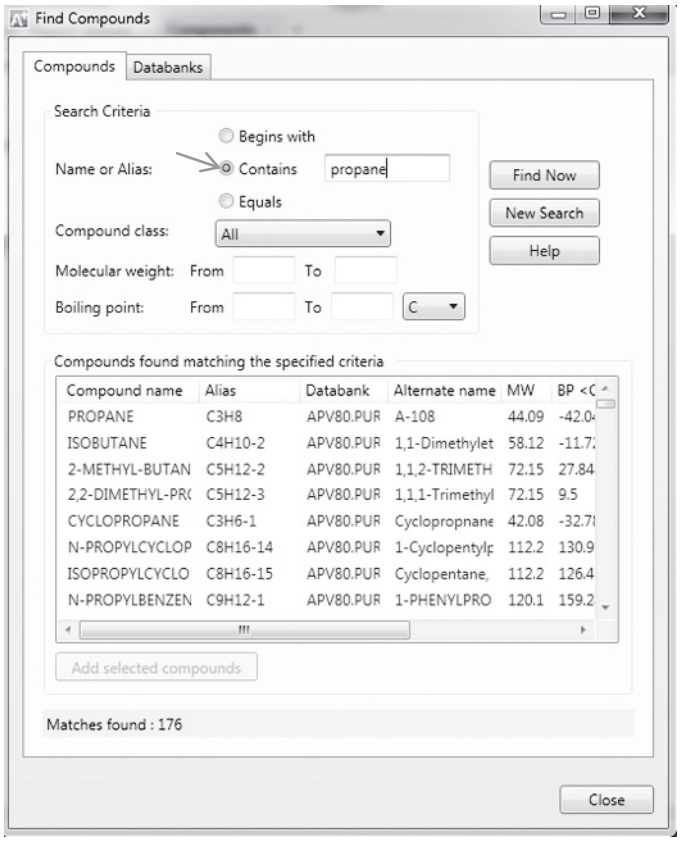

Figure 1-5

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.]

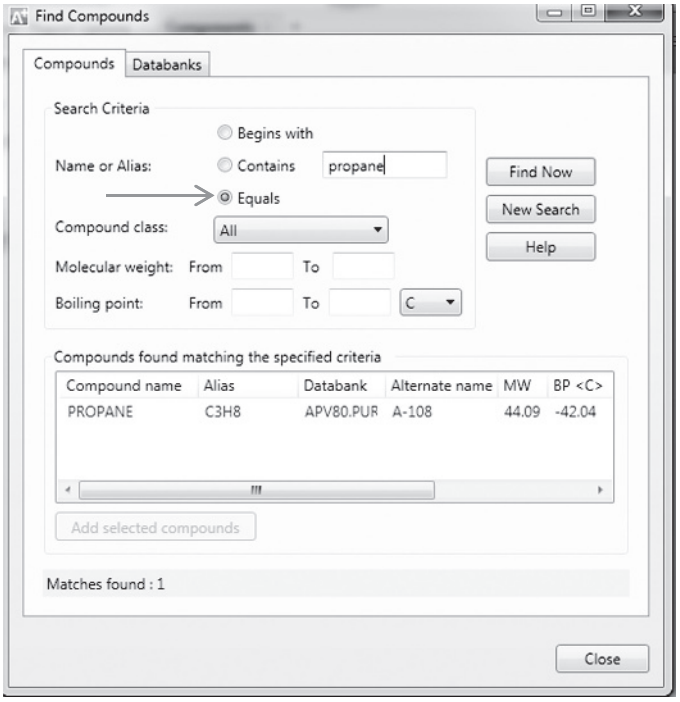

Figure 1-6

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):

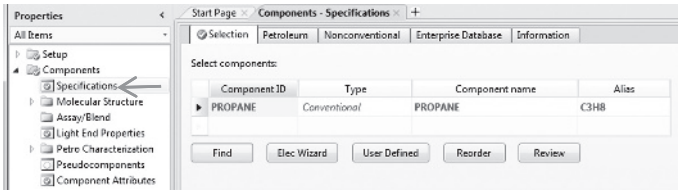

Figure 1-7

[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.

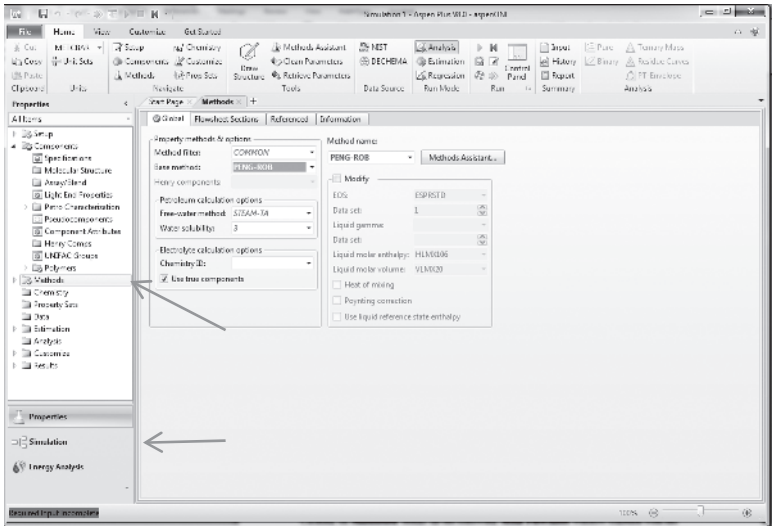

Figure 1-8

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

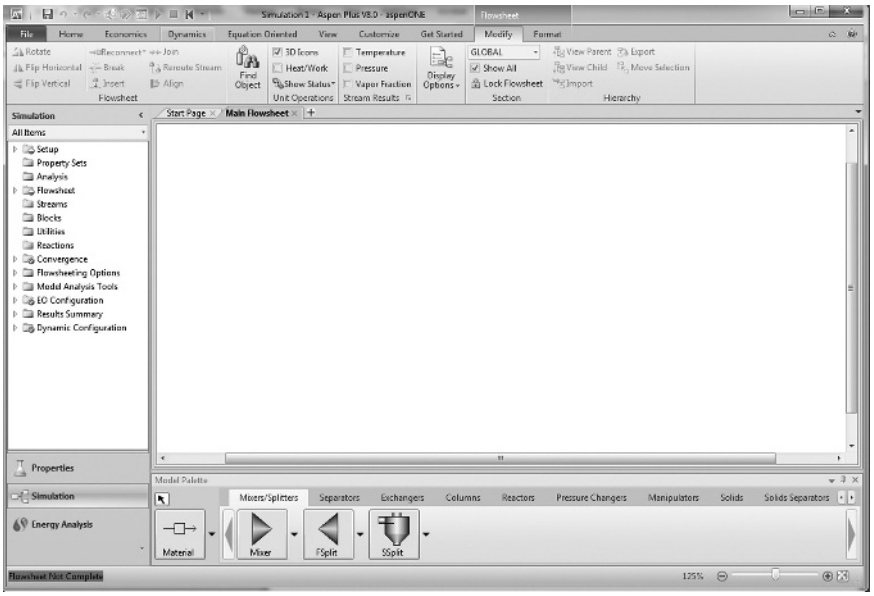

Figure 1-9

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.

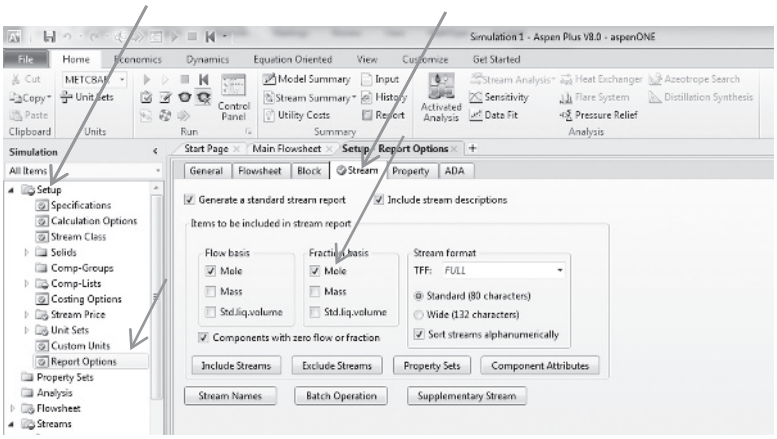

Figure 1-10

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.