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Simulation of Adsorption Processes

This chapter introduces four key concepts inherent to all adsorptive separations, before presenting how these concepts are applied in rigorous simulations. Sections 1.1 and 1.2 provide a high-level overview of adsorption covering the history and driving forces involved. Section 1.3 discusses adsorption equilibrium and summarizes the theoretical assumptions behind the various mathematical models that have been used to describe it. Section 1.4 explains a number of terms and concepts inherent to working with packed beds. Section 1.5 covers the "classic" industrial adsorber configurations, along with commonly used industrial adsorbents. Section 1.6 onward discusses how to apply these concepts in Aspen Adsorption, specifically to pressure swing adsorption (PSA) for oxygen isolation from air (Section 1.7) and hydrogen separation from light hydrocarbons (Sections 1.8 and 1.9), and temperature swing adsorption (TSA) for air drying (Section 1.10). Section 1.11 provides the conclusions of the chapter. Section 1.12 presents practice problems to allow readers to apply the concepts described in this chapter. Section 1.13 includes the nomenclature, and Section 1.14 gives the bibliography.

1.1 Introduction to Gas-phase Adsorption Technologies

Gas-solid separations are incredibly important industrial problems, but have a short history compared to processes such as distillation. The difficulties associated with handling solid adsorbents require both creative process design and detailed understanding of the adsorptive properties of various solids. The investigation of solid-gas absorptivity began in the late 1700s, but it was not until the early 1900s that any industrial application was found. By the end of the 1950s, engineers had already filed patents on the major gas-adsorptive separations we know today, such as hydrogen sulfide removal [1], oxygen/nitrogen separation [2], and some drying applications [3, 4] as well as numerous short-chain hydrocarbon separations [5–7].

Over the years, refinements to these technologies have appeared, and numerous authoritative textbooks have consolidated the scientific knowledge of the subject. It is fair to say that at this point, adsorption technologies are fairly well understood, and there are a variety of resources available for the interested reader.

Design, Simulation, and Optimization of Adsorptive and Chromatographic Separations: A Hands-On Approach, First Edition. Kevin R. Wood, Y. A. Liu, and Yueying Yu.

Rather than rehashing the details of adsorptive separations, this textbook aims to make the reader proficient at software tools that bring all the knowledge contained in those textbooks to bear on adsorptive problems. Toward that end, the bulk of this chapter will consist of workshops on Aspen Adsorption. This approach systematically introduces the reader to all the relevant adsorption concepts by their implementation through the software tools.

In this chapter, we learn about both the theory of adsorptive separations as well as their implementation in Aspen Adsorption.

1.2 Core Concepts in Gas Adsorption

Gas adsorption occurs when gas molecules interact with and become retained by a solid material. The reasons for this adhesion are numerous, and may include charge differences, chemical reactions, and size or shape effects. These interactions frequently differ between gas molecules, and therefore serve as a useful basis for their separation.

Continuous adsorptive separation processes, which manipulate these effects, must always involve at least two steps:

1) The *adsorption* step, during which the adsorbent selectively retains the adsorbed species from the feed.
2) The *regeneration* or *desorption* step, during which the adsorbent releases the retained species, thus regenerating the adsorbent for use in the next cycle.

As there are only a limited number of methods that accomplish the release in the regeneration phase, these methods characterize gas adsorption technologies. When regeneration is accomplished by changing the pressure, the process is called PSA. The alternative, which is accomplishing the regeneration through temperature change, is called TSA. Of course, these approaches can be combined, and there are some subtypes of each; for example, when a PSA process involves a vacuum, it is referred to as a vacuum pressure swing adsorption, or a VPSA, process.

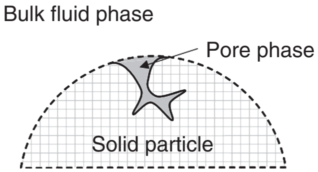
1.2.1 The Adsorption Process

Adsorption is a multistep process by which a molecule moves from the bulk liquid phase and becomes attached to the surface of a solid particle. For our purpose, we treat this process as involving three distinct regions, as shown in Figure 1.1. Specifically, the adsorption involves:

1) the diffusion of a component from the bulk fluid into the pores of a solid particle;
2) the binding of that component to the solid surface inside a pore.

The driving force for the migration of the chemical species into the pore phase is the difference in concentration. This is a very intuitive concept. If the pore phase is poor in a component that the bulk phase is rich in, then that component will be driven to diffuse into the pores.

Figure 1.1 The phases involved in the adsorption process.



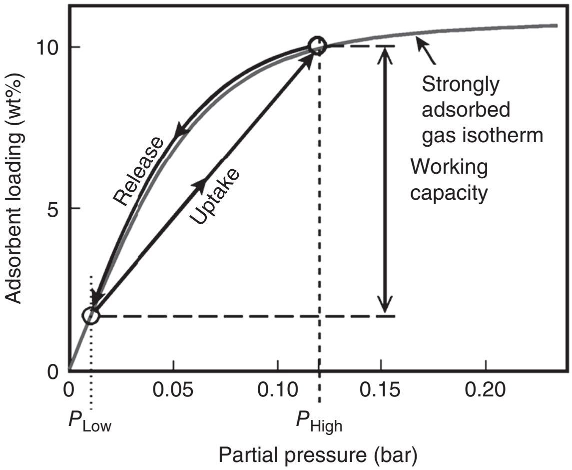
More detailed models of this process distinguish between the bulk phase and the laminar boundary layer surrounding the solid particle, and may also attempt to characterize the concentration gradients that form inside the pores. We could also attempt to describe the motion of the adsorbed components once they have been adsorbed onto the solid surface. That much detail, however, is not usually needed for the purpose of modeling the adsorptive unit operations we are interested in.

1.2.2 How the Driving Forces Achieve Separation

Figure 1.2 shows schematically how changing the pressure allows us to accomplish the regeneration, and therefore the separation. In this figure, the solid adsorbent is able to hold more of the retained component at high pressure. Therefore, when a bed containing this adsorbent is pressurized with the feed gas, the solid will be “loaded” with the adsorbed component along the line labeled “Uptake.” Once the pressure is allowed to drop, the adsorbed molecules will be released along the curve labeled “Release.” The curve labeled “strongly adsorbed gas isotherm” describes the maximum capacity of the solid for each pressure. The name isotherm comes from the fact that this entire cycle occurs at roughly constant temperature.

The “working capacity” of the adsorbent loading is defined as the difference between the isotherm point at P_{low} and the isotherm point at P_{High} in the figure. Since the y axis is loading, given by (mass adsorbed component)/(mass adsorbent), the difference represents the maximum mass of the adsorbed gas that can be recovered, per cycle, per mass of adsorbent.

Figure 1.2 The basic schematic isotherms in a PSA operation for an adsorption process.



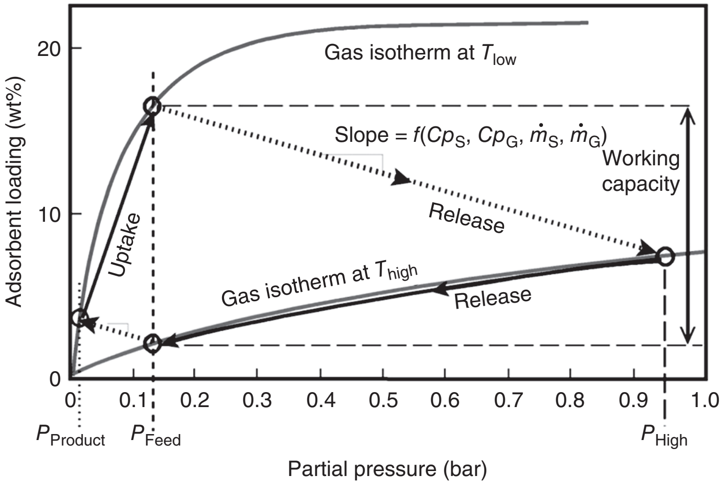


Figure 1.3 The basic schematic isotherms in a TSA operation for an adsorption process.

Temperature swing technology works in much the same way. Instead of simply alternating between high and low pressures, the bed also alternates between high and low temperatures. A higher temperature stream typically consisting of steam typically drives the temperature rise, although other methods such as microwave radiation are sometimes used. Figure 1.3 shows the analogous cycle for a process that cycles temperature and pressure. Notice the difference between the two gas isotherms; they represent isotherms at different temperatures. At higher temperatures, the solid phase typically has lower capacity, which is analogous to gas–liquid systems.

In Figure 1.3, we see that the cycle for pressure and temperature swing appears much more complex than that for PSA. The important distinction to be made is that the heating and cooling steps also change the pressure (dashed lines). The slope of these lines is a function of the heat capacities of the adsorbent and gas phases (Cp_s, Cp_g), along with the masses of the solid and adsorbent (m_s, m_g). Once again, we define a working capacity as the difference between the highest and lowest loading in the cycle.

PSA is, overall, more common than TSA. The significant reason for this difference is that the pressure swing can be accomplished much more quickly than the temperature swing. TSA is beneficial when the adsorbed component is very strongly adsorbed. In such a situation, the increase in temperature allows a much more effective regeneration step, since the pressure swing alone would be unable to release sufficient quantities of the adsorbed components.

1.3 Isotherms

In Section 1.2.2, we discussed how isotherms define a working capacity for an adsorption system. Here, we look at some specific isotherms and discuss what the different isotherms assume about the physical properties of the system.

Isotherms generally have a form as shown in Eq. (1.1). The total amount of a gaseous species (the adsorbate) adsorbed by the solid adsorbent is given as a function of the partial pressures of all the species in the gaseous phase (the nomenclature for this chapter appears in Section 1.13).

$$\frac{\text{mass adsorbate}}{\text{mass adsorbent}} = f(p_1, p_2, \dots, p_n). \tag{1.1}$$

A large number of equations can provide this relationship between the fluid-phase concentration and the adsorption capacity on the solid surface. Many of these relationships are essentially empirical; the equations were originally derived as convenient best-fits of experimental data. Some, most notably the Langmuir isotherm, are backed by physical models for describing how molecules transition from a solvated state to an adsorbed state. Not surprisingly, the model used to derive the Langmuir isotherm is called the Langmuir Adsorption Model, and serves as the basis for several isotherm variants.

1.3.1 The Langmuir Isotherm [8] (1918)

The Langmuir isotherm, Eq. (1.4), is the most popular isotherm in simulated moving bed applications. Although it was originally derived for ideal gasses (and, in fact, has the ideal gas behavior as an assumption), it turns out that it works well with liquid adsorption. There are a handful of Langmuir variations that are also used; for example, the “Dual Site” or “Bi-” Langmuir isotherms consist of two basic Langmuir equations summed together, see Eq. (1.3) (the nomenclature for this chapter appears in Section 1.12).

$$q_i = \frac{a_i c_i}{1 + \sum_{j=1}^{\mathrm{NC}} b_j c_j} \tag{1.2}$$

$$q_i = \frac{a_i c_i}{1 + \sum_{j=1}^{\mathrm{NC}} b_j c_j} + \frac{\alpha_i c_i}{1 + \sum_{j=1}^{\mathrm{NC}} \beta_j c_j} \tag{1.3}$$

1.3.2 The Linear Isotherm

The linear isotherm is essentially a Henry’s law model. It is considered useful in cases of low concentrations and loadings.

$$q_i = H_i c_i \tag{1.4}$$

1.3.3 The Brunauer–Emmett–Teller (BET) Isotherm [9] (1938)

This isotherm extends the Langmuir model to work in cases where adsorbed molecules can form layers on the surface of the adsorbent [2]. Relatively recent work finds that the appropriate form of the Brunauer–Emmett–Teller (BET) equation for use in liquid systems is given by

$$q_i = \frac{q_{\mathrm{m}} K_i^{\mathrm{S}} c_i^{\mathrm{eq}}}{(1 - K_{\mathrm{L}} c_i^{\mathrm{eq}})(1 - K_{\mathrm{L}} c_i^{\mathrm{eq}} + K_i^{\mathrm{S}} c_i^{\mathrm{eq}})} \tag{1.5}$$

1.3.4 The Freundlich Isotherm [10] (1906)

This empirical equation was originally used on gasses, Eq. (1.6). It has applications in protein and other bioseparations. The model is almost entirely empirical.

$$q_i = h_i c_i^{1/n} \tag{1.6}$$

1.3.5 The Sips (Langmuir–Freundlich) Isotherm [11] (1948)

This model is an attempt to put the Freundlich isotherm into a more physically meaningful form. At low concentrations, it mimics the Freundlich behavior, while at high concentrations, it predicts a monolayer that is similar to the Langmuir isotherm.

$$q_i = \frac{a_i c_i^n}{1 + \sum_{j=1}^{\mathrm{NC}} b_j c_j^n} \tag{1.7}$$

1.3.6 The Toth Isotherm [12] (1971)

This empirical isotherm is primarily used in gas-phase adsorption, and is similar in form to the Sips equation.

$$q_i = \frac{h_i c_i}{(a_i + c_i)^{1/t}} \tag{1.8}$$

1.3.7 Summary

Figure 1.4 shows what these isotherms look like in the single-component case.

1.4 The Properties of Packed Beds

In Section 1.3 on isotherms, notice that the sample plots in Figure 1.4 show the relationship between fluid phase concentration and *adsorbent volume* rather than adsorbent mass. Of course, we can convert between mass and volume with information about the adsorbent density; but in packed beds, the concept of “density” is less well defined than in the case of gases and liquids.

In order to describe any adsorptive separation, it is important to think clearly about how to characterize the particles and voids within the adsorbent bed. As with most systems involving solid particles, the terms and conventions can be confusing or misleading because many different disciplines have developed their own partially overlapping naming schemes.

In adsorptive separations, the questions that we typically ask ourselves about the solid phase is essentially this: “Given some bed that is filled with both fluid and solid particles, what volume of the bed can be said to belong to the solid phase and what volume to the liquid phase?” It turns out that we can answer that question in several different ways, and which answer is “correct” depends on the details of the system. However, despite the variety of possible answers, the answer always involves reference to two physical properties: density and void fraction.

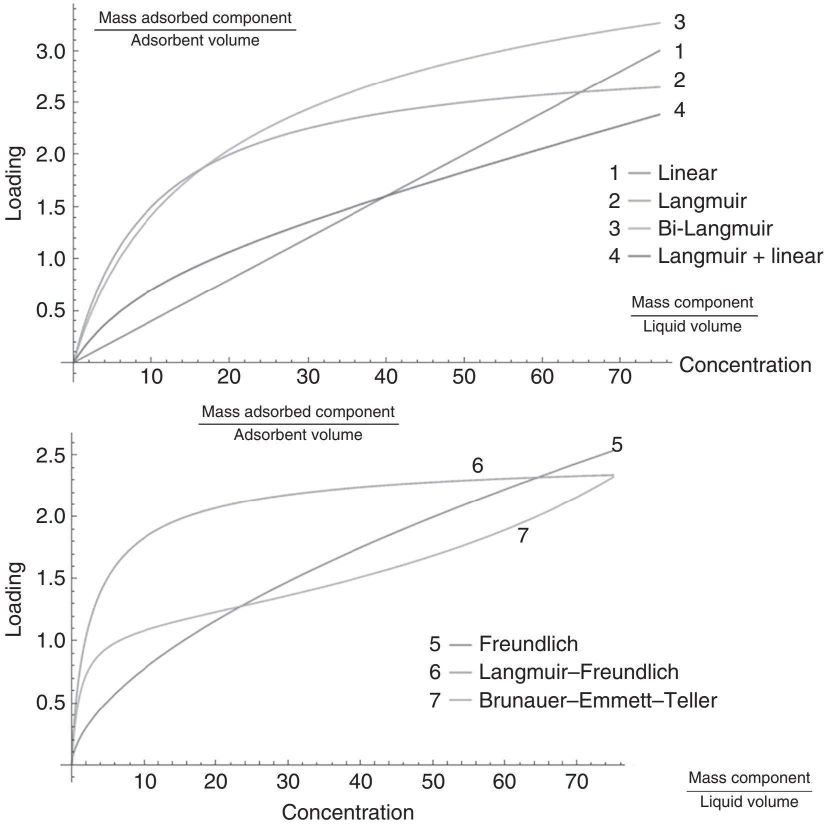


Figure 1.4 Sample isotherm curves.

1.4.1 Void Fractions

The first set of important parameters, which are intimately tied to density, are the void fractions (or porosities) of a packed bed. Figure 1.5 depicts the three voids that are most relevant to adsorptive separations. Of course, the drawings in Figure 1.5 represent the voids themselves, but we want to know about the void fractions, that is the size of the voids relative to some reference volume.

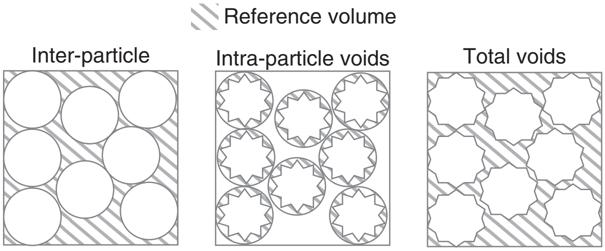


Figure 1.5 The locations of the various reference volumes.

1.4.2 External Voids

The first and most intuitive void fraction is the ratio of the volume of space *not* occupied by particles in the bed, to the total bed volume. We refer to this ratio as the **interparticle, external,** or **interstitial** void fraction. While this seems simple at first, it is somewhat difficult to exactly determine what space is "inside" a particle and what space is "outside." Particles can have very irregular geometry, which can make the boundaries very fuzzy for both theoretical definition and practical measurement.

1.4.3 Internal Voids

The second void fraction follows naturally from the first; since the external porosity defines the volume *outside* the particles, it is natural to want a ratio to describe the voids *inside* a particle. Unfortunately, toward this end, two conventions have arisen. *In chromatographic practice*, it is common to define the **internal** or **intraparticle** void fraction as the ratio of voids in the particles to the total column volume. However, *in chemical engineering circles*, it is more common to use **internal** or **intraparticle** void fraction to refer to the ratio of voids in the particles to the total volume of *particles* instead of the *column*. To see this in mathematical terms, refer Table 1.1.

The final void fraction is simply derived from the sum of both internal and external voids. The **total** void fraction is therefore the ratio of all voids in the system, to the total system volume.

1.4.4 Densities

Density is simply characterized by dividing a mass of particles by a reference volume, and as you might have guessed, there are several meaningful ways to characterize the density of a group of particles. Figure 1.6 illustrates the different ways that can be used to create reference volumes to divide our particle mass.

1.4.4.1 Bulk Density

The simplest and most intuitive is the density of many particles in aggregate. This is the density found by pouring the particles in a beaker and measuring their mass and volume. It is commonly referred to as the **bulk** density.

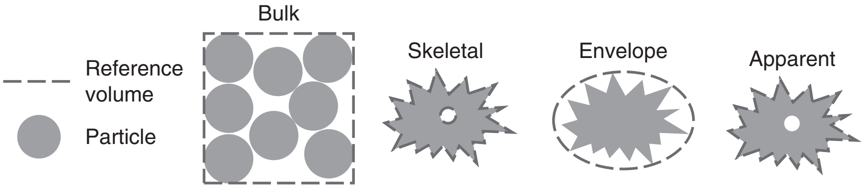


Figure 1.6 Illustration of bulk, skeletal, envelope, and apparent volumes.

Table 1.1 Definitions of different voids, densities, and porosities.

Quantity	Symbol	Units	Example relationships
Total system volume	V_T	Volume	For example, in a cylindrical column $V_T = \pi R^2 L$
External void volume	V_X	Volume	$V_X = \varepsilon_i V_T$
Internal void volume (pore volume)	V_P	Volume	Chromatographic convention: $V_P = \varepsilon_p V_T$ Chemical engineering convention: $V_P = \varepsilon_p (1 - \varepsilon_i) V_T$
Bulk density	ρ_b	$\frac{\text{Mass}}{\text{Volume}}$	$\rho_b = \frac{M_{\text{particles}}}{V_T} = (1 - \varepsilon_i)\rho_e = (1 - \varepsilon_t)\rho_s$
Skeletal or solid density	ρ_s	$\frac{\text{Mass}}{\text{Volume}}$	$\rho_s = \frac{M_{\text{particles}}}{V_T - V_X - V_P} = \frac{\rho_b}{1 - \varepsilon_t}$
Envelope density	ρ_e	$\frac{\text{Mass}}{\text{Volume}}$	$\rho_e = \frac{M_{\text{particles}}}{V_T - V_X} = \frac{\rho_b}{1 - \varepsilon_i}$
External or interparticle porosity	ε_i	$\frac{\text{Volume}}{\text{Volume}}$	$\varepsilon_i = \frac{V_X}{V_T} = 1 - \frac{\rho_b}{\rho_e}$
Internal or intraparticle porosity	ε_p	$\frac{\text{Volume}}{\text{Volume}}$	Chromatographic convention: $\varepsilon_p = \frac{V_P}{V_T} = (1 - \varepsilon_i) - \frac{\rho_b}{\rho_s}$ Chemical engineering convention: $\varepsilon_P = \frac{V_P}{V_T - V_X} = 1 - \frac{\rho_b}{\rho_s}$ Conversion: $\varepsilon_{p,\text{ eng}} = \varepsilon_{p,\text{ cro}} + \varepsilon_i$
Total porosity	ε_t	$\frac{\text{Volume}}{\text{Volume}}$	$\varepsilon_t = \frac{V_P + V_X}{V_T}$ Chromatographic convention: $\varepsilon_t = \varepsilon_i + \varepsilon_p$ Chemical engineering convention: $\varepsilon_t = \varepsilon_i + \varepsilon_p (1 - \varepsilon_i)$

1.4.4.2 Skeletal or Solid Density

The next relevant density is that of the pure solid. This is the density you would get if there were a perfect cube of a solid (i.e. with no holes or voids) and its mass was divided by the volume of the cube. Since it is impractical to make such a perfect solid, this density is often measured by forcing gas into all the pores of the particles. When the volume of the gas is known, and the volume of the gas-particles mix is known, the volume of the pure solid "skeleton" is simply their difference. The density is therefore the mass of the particles divided by the "skeleton" volume. This density is referred to as the **skeletal** or **solid** density.

The skeletal density is very similar to another density, which includes a particle's internal voids. When the reference volume includes internal voids, the density is referred to as the **apparent** density.

1.4.4.3 Envelope or Particle Density

The final density is less intuitive and falls between the bulk and skeletal densities. This density is found by defining a hypothetical "envelope" around each particle; the envelope contains both the solid mass as well as the particle's internal and external pores. The density is then found by dividing the mass of the particles by the volume of their envelopes. However, arriving this density value is difficult thanks to the difficulty in selecting and measuring an appropriate envelope; what constitutes appropriate frequently depends on the application. There are some techniques, such as mercury porosimetry, which allow measurement of envelope volumes. The density thus obtained is usually referred to as the **envelope** or **particle** density.

1.4.4.4 Caveats

Some authors use **true** density to mean **skeletal** density, while others use it to refer to **apparent** density. Some authors use **apparent** density to refer to **bulk** density, while others use it to refer to **envelope** density. When gathering data from the literature, vendors, or even your own experiments, you should be careful to ensure that you know exactly what your density is referring to.

1.4.5 Relationships

As might be expected, all these parameters are related to each other. We summarize their relationships in Table 1.1. This text will exclusively use *the chemical engineering convention,* but the chromatographic convention is presented here for completeness. The source of the difference between the engineering and chromatographic conventions is the definition of ε_{p}, where the engineering convention defines the fraction in terms of **the solid volume**, while the chromatographic convention defines it in terms of **the total system volume**.

1.4.6 Gas-phase Behavior

The behavior of gasses in packed beds is the final piece of the puzzle we need before we can begin to discuss actual absorber configurations, and construction of Aspen models. As a gas flows through a packed bed, its properties change, even in the absence of adsorption.

1.4.6.1 Pressure Drop

Gas flowing through a packed bed suffers a decrease in pressure. In an empty tube, the no-slip boundary condition at the walls represents the only frictional force; but in a packed bed, each particle represents a source of additional friction. Just like flow through a pipe, this frictional force depends on whether or not the flow is laminar, as well as on some properties of the gas.

The simplest packed-bed pressure drop equation is the Carman–Kozeny equation (1.9), which dates back to 1927 [13]. This equation calculates pressure drop by assuming that the space between the particles behaves like many small pipes governed by Poiseuille's law [14]. As such, this equation is only valid for laminar flow.

$$\frac{\partial P}{\partial z} = -1.5^{*}10^{-3}\frac{\mu(1-\varepsilon_{\mathrm{i}})^2}{(2r_{\mathrm{p}}\psi)^2\varepsilon_{\mathrm{i}}^3}v_{\mathrm{g}} \tag{1.9}$$

Here, ψ is a *shape factor* that describes how spherical the particles are, and v_{g} is the interstitial velocity of the gas phase. Refer to Section 1.13 for nomenclature used throughout this chapter.

The Burke–Plummer equation (1.10) describes the pressure drop in the case of turbulent flow (Re > 2000) [15]. MW in this equation refers to the molecular weight of the gas.

$$\frac{\partial P}{\partial z} = -1.75^{*}10^{-3}\frac{\rho_{\mathrm{g}}\,\mathrm{MW}\,(1-\varepsilon_{\mathrm{i}})}{2r_{\mathrm{p}}\psi\varepsilon_{\mathrm{i}}^3}v_{\mathrm{g}}^2 \tag{1.10}$$

The most commonly used equation, the Ergun equation [16], is able to handle both turbulent and laminar flows. It does this by combining the Carman–Kozeny and the Burke–Plummer equations.

$$\frac{\partial P}{\partial z} = -\left(1.5^{*}10^{-3}\frac{\mu(1-\varepsilon_{\mathrm{i}})^2}{(2r_{\mathrm{p}}\psi)^2\varepsilon_{\mathrm{i}}^3}v_{\mathrm{g}} + 1.75^{*}10^{-3}\frac{\rho_{\mathrm{g}}\mathrm{MW}\,(1-\varepsilon_{\mathrm{i}})}{2r_{\mathrm{p}}\psi\varepsilon_{\mathrm{i}}^3}v_{\mathrm{g}}^2\right) \tag{1.11}$$

1.4.6.2 Compressibility

As a gas flows through the pressure gradients in a packed bed, it changes volume. This volume change affects the gas velocity and temperature, which in turn influences the pressure drop. Therefore, it is important to be able to select the correct thermodynamic model of the gas phase, so that our calculations generate correct volumetric flow rates. It is also important for nonisothermal systems.

There are a large number of options when it comes to selecting these thermodynamic models. The simplest and most idealized is simply to use the ideal gas law. While this works reasonably well for low-pressure systems (less than a few bar), higher pressure systems require better models.

One such model is the **Redlich–Kwong–Soave (RK–Soave)** [17] equation of state. It is a cubic equation of state that works well for most vapor systems up to around 10 bar. It was designed for use with hydrocarbons, and works well.

A second detailed model is the **Peng–Robinson** [17] equation of state, which works well with moderately nonideal gas phases over a slightly wider range of pressures than RK–Soave. It works very well with gas phases containing CO, CO_2, H_2 and O_2, and is commonly used in refinery processes.

1.5 PSA and TSA Implementation Details

1.5.1 Common Adsorbent Characteristics

The most common adsorbent for PSA systems are zeolites, because they are selective for a number of industrially important molecules. Table 1.2 [18] shows several common zeolite types, along with a molecular diameter that describes the kinds of molecules such an adsorbent would be able to separate.

Another common feature of PSA systems is the use of two adsorbent beds. While it is possible to operate a PSA separation with one bed, some separations use six or more. The two-bed configuration allows for important energy-saving schemes that easily outperform the one-bed process, while the additional complexity of more beds is typically only worthwhile for larger-scale separations. We discuss the energy-saving schemes in the first workshop in Section 1.7.

1.5.2 Common Process Configurations

The classic two-bed PSA process was patented in the 1960s by Charles Skarstrom [5], and has come to be known as *the Skarstrom cycle*. The basic Skarstrom cycle utilizes two packed adsorbent beds, as shown schematically in Figure 1.7. The "core" cycle consists of four steps: ***pressurization, adsorption, countercurrent blowdown, and countercurrent purge***. It is possible to add an additional **pressure equilibration** step that allows to save energy. In step 1, feed flows into bed 1, and raises its pressure, while the fully loaded second bed is connected to the extract product. Once the desired pressure has been reached, the system enters step 2, where the more strongly adsorbed component is retained in bed 2 and the gas outlet stream is enriched in the less strongly adsorbed component. A portion of the raffinate product is diverted to the second bed, to help fully regenerate it. Once the first bed has been loaded, and the second bed regenerated, a pressure equalization step may take place. This allows for energy saving by reducing the quantity of gas that needs to be compressed. After the equilibration step, the process repeats, but with the roles of the two beds reversed.

Figure 1.7 shows a common PSA scheme. This is only one possible configuration; Table 1.3 lists several additional options for each step, as well as the rationale behind them.

Table 1.2 Zeolites and their adsorptive properties.

Molecular sieve zeolite	Effective molecular diameter cut-off (molecules smaller than this will be adsorbed; larger molecules will be rejected) (Å)
3A	3
4A	4
5A	5
10X	8
13X	10

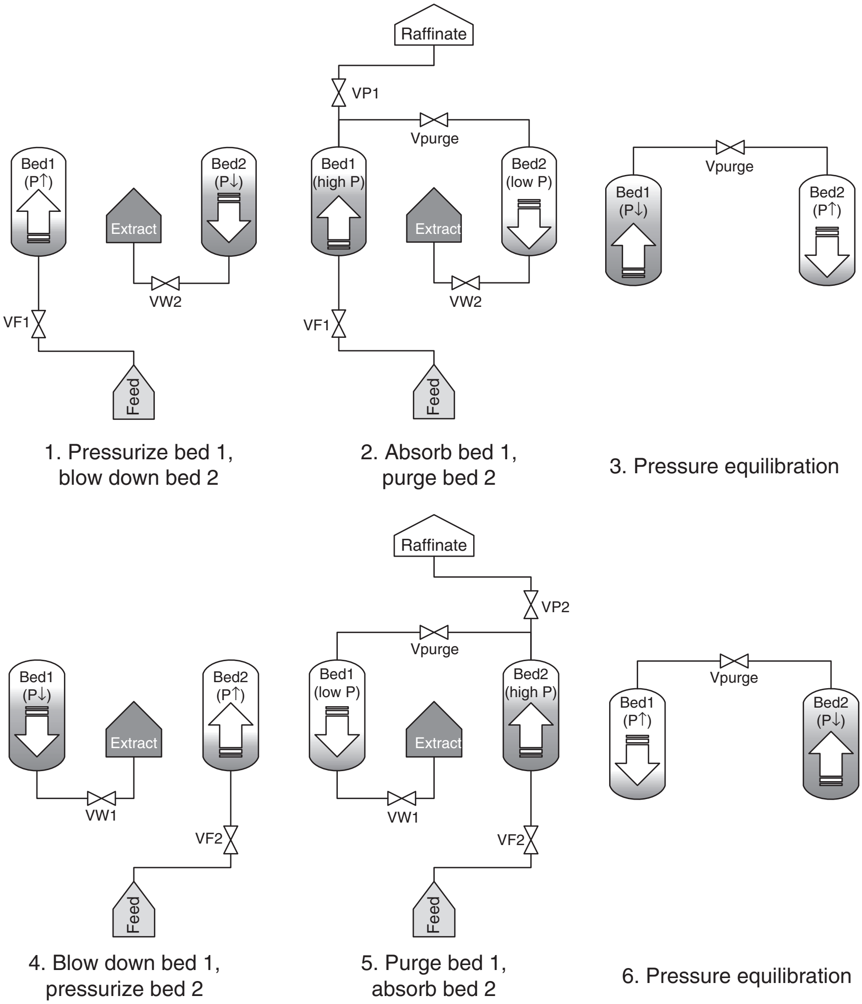


Figure 1.7 The basic principle of the Skarstrom cycle in the PSA process.

1.6 Introduction to Aspen Adsorption

Given the above introduction to the basics of TSA/PSA systems, we learn the details of their design through a hands-on workshop using Aspen Technology's software, Aspen Adsorption.

Aspen Adsorption is a comprehensive flowsheet simulator for the optimal analysis, design, simulation, and optimization of industrial gas- and liquid-adsorption processes. This software simulates gas processes with adsorption only, or reactive gas adsorption processes where both reaction and adsorption occur simultaneously.

For gas processes, Aspen is capable of handing the following conditions "out of the box":

- Isothermal or nonisothermal operation.

Table 1.3 Common steps used in PSA.

Step name	Description	Motivation
Pressurization	In this step, the bed is pressurized, typically with material from the feed stream	This step forces any enriched gas still present in the bed toward the product stream, while raising the bed pressure in preparation for the adsorption step
Adsorption	This step is operated at high pressure; the gas and solid interact to extract the strongly adsorbed component. The raffinate is collected during this step, and its withdrawal may or may not lower the bed pressure.	Allow maximum extract adsorption and recovery of the less-adsorbed component
Blowdown	One end of the bed is connected to a low-pressure sink. If the blowdown is counter-current, the raffinate will have higher purity. Co-current blowdown is sometimes used to improve extract purity (see also: equilibration)	Purge the bed of the remaining raffinate gas and prepare the bed for low pressure desorption
Desorption	The solid phase is allowed to release the adsorbed component, and the gas is collected as the extract. May be done as in vacuum, and with or without a purge	Regenerate the solid for the next Adsorption cycle. The use of a purge may involve a trade-off between the extract purity and raffinate recovery
Equilibration/ equalization	The high pressure bed is connected to the low pressure bed, typically at the raffinate end	Lower energy consumption (less pressurization required)

- Plug flow or plug flow with axial dispersion.
- The system may or may not be well-mixed in the radial direction.
- The gas phase is ideal or nonideal.
- Gas-phase pressure may be constant, or the pressure may vary according to momentum balances.
- Mass transfer is described using a lumped overall resistance, or by a model that accounts separately for micro- and macropore effects. The driving force is based on a liquid or solid film, and is either linear, quadratic, or user-specified. Mass-transfer coefficients are either constant, or vary with local conditions.
- Adsorption isotherms are available for single or competitive multicomponent adsorption.
- Reactions may occur at any point.

We cover the details of these conditions as we encounter them in our workshops.

1.7 PSA Workshop: Aspen Adsorption Modeling for Air Separation

Having briefly introduced the concept of PSA for gas-phase separation, we now cover the details required to specify a complete PSA operation, specifically the use of PSA for air separation. Since we have already established that the Skarstrom process is considered to be the classic PSA implementation, and because the original Skarstrom patent dealt with oxygen isolation [5], this is the process we now model in Aspen Adsorption.

The Skarstrom process for oxygen purification has been commercialized at scales ranging from a few liters per minutes for small-scale units to tens of tons per day for industrial systems. The processes originally used a zeolite adsorbent, generally 5A or 13X, while modern processes employ a LiLSX adsorbent [19,20]. Most small-scale units use a two-bed system, sometimes with the addition of pressure equalization steps. For this model, we assume a binary air separation system of 79% N_2 and 21% O_2 using a 5A zeolite as the adsorbent.

In this PSA system, the zeolite preferentially adsorbs O_2 at higher pressure in the adsorption step, and releases O_2 when lthe pressure during the desorption step is lowered. We can find the information required to describe this adsorption in the literature [2,5,19,21–23].

Figure 1.8 shows the cyclic PSA unit we build with two beds for a binary separation. The process is inherently cyclic, because the beds will alternate

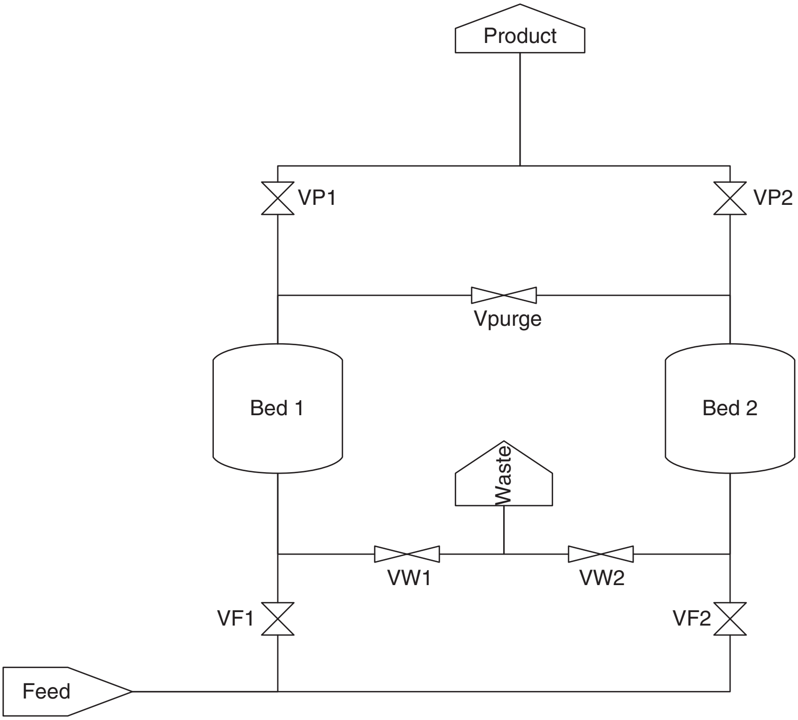


Figure 1.8 Diagram of a basic two-bed pressure swing adsorption separator.

between adsorption and desorption. While bed 1 is in the adsorption stage, bed 2 is in the desorption stage. During the adsorption stage, at a relatively high pressure, the solid adsorbent in the bed will selectively adsorb the oxygen from the binary gas mixture. The leftover nitrogen produced in this step is referred to as the **raffinate**, since it has been refined by having the oxygen removed. Since this product is less strongly adsorbed, and is removed from the top of the column, it is sometimes referred to as **the light product (LP)**. In the following desorption step, by lowering the gas-phase partial pressure inside the bed, the adsorbent releases the adsorbed components, in this case oxygen, to produce a gas stream called the **extract** (because it was *extracted* from the main gas stream.) Some sources refer to this as **the heavy product (HP)** because it is enriched in the more strongly adsorbed components. From here, the cycle repeats.

To accomplish this kind of switching, we need to carefully schedule when to open and close the valves. To do this, we construct a diagram like the one shown in Figure 1.8, which shows the four steps required to cycle between adsorption and desorption. The steps for bed 1 are specifically as follows:

1) Under high pressure, the feed gas is fed into the bed, and adsorption takes place.
2) Once the bed is adequately pressurized, we begin collecting the least adsorbed component in the raffinate, while the bed is being loaded. We take a portion of the raffinate and feed it into the second bed to help drive out the more strongly adsorbed component.
3) When the bed is fully loaded, we depressurize it in the "blow down" step. The bed is connected.
4) Once the bed has been completely cleared of the HP, the LP is used to repressurize the bed for the feed stream.

If we look carefully at the schedule, as well as the valve layout described in Figure 1.8, we can easily come up with the schedule for valve opening and closing listed in Table 1.4. Table 1.5 explains the valve specification numbers 0, 1, 2, and 3 appearing in Table 1.4.

Now that we have an idea of the layout of our system, as well as the system behavior, let us begin creating the flowsheet in Aspen Adsorption.

Table 1.4 Valve schedule for a two-bed four-step process.

Step	Function	VF1	VF2	VW1	VW2	VP1	VP2	VPurge
Step 1	Adsorb bed 1, purge bed 2	1	0	0	1	1	0	2
Step 2	Blowdown bed 1, pressurize bed 2	0	1	1	0	0	1	0
Step 3	Purge bed 1, adsorb bed 2	0	1	1	0	0	1	2
Step 4	Pressurize bed 1, blowdown bed 2	1	0	0	1	1	0	0

Table 1.5 Valve specification meanings.

0	The valve is fully closed (the flow rate through the valve always be zero)
1	The valve is fully open (the flow rate through the valve will be determined by mass balance)
2	The valve's flow rate will have a linear relationship with pressure drop
3	The valve will have a fixed flow rate

1.7.1 Adding Components to an Aspen Adsorption Simulation

Step 1: If you already have Aspen Adsorption open, select "new" from the file menu to create a new blank simulation (Figure 1.9)

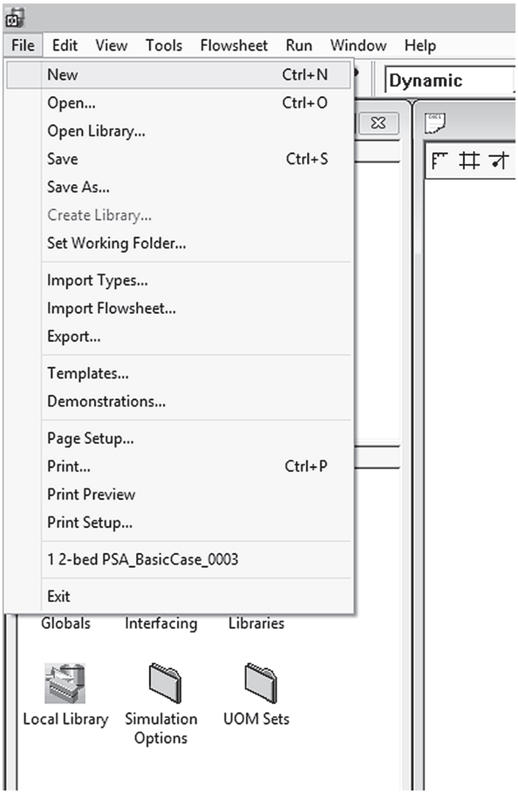


Figure 1.9 A new file in Aspen Adsorption.

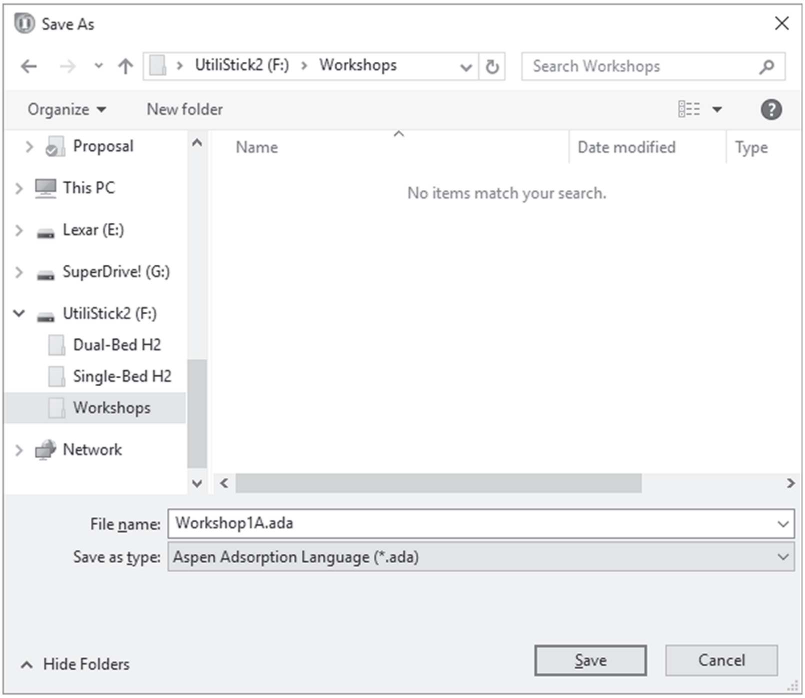
Step 2: It is important to save Aspen simulations frequently

Saving guards against two undesirable outcomes:

- Computer crashes
- Irreversible changes to the Aspen flowsheet.

The numeric solvers Aspen Adsorption uses frequently store temporary, initial, and intermediate values while you are creating and running simulations. When the values the solvers have stored correspond well to your simulation, it can make your simulation run faster. However, making certain changes to the flowsheet can cause these values to become unhelpful, and your simulation might not run at all; in some cases, the simulation may continue to fail even after you ostensibly revert the simulation to a state that previously worked. In such a scenario, the best thing to do is to open a saved file from before you made the changes.

Save the simulation as **Workshop1A.ada** (Figure 1.10)



No items match your search.

File name: Workshop1A.ada

Save as type: Aspen Adsorption Language (*.ada)

Figure 1.10 Saving the PSA process with four steps for air separation.

Step 3: Add chemical components to Aspen's component list

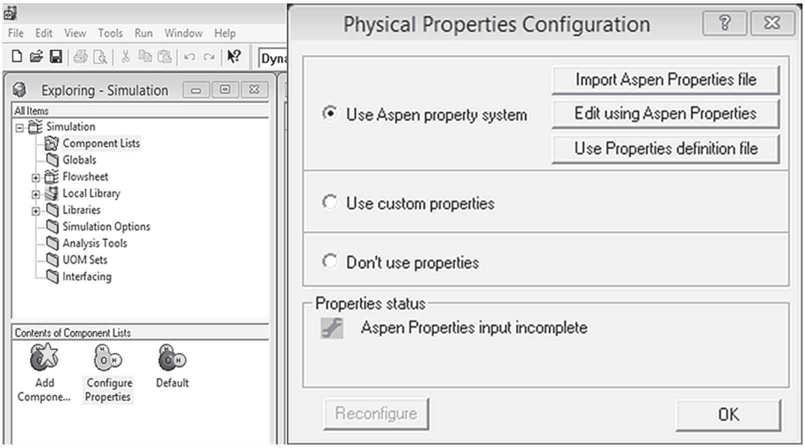
There are two methods of adding chemical components into the model: component list and component set.

A Component List is the simplest way to add components. All that is required is a list of chemical names. However, a component list contains no information about the physical properties of these chemical components, and so all required properties must be provided by the user.

On the other hand, a Component Set allows for much more detailed simulations because each component is associated with a list of optional parameters and their values. These values provide the information required for the Aspen property system to calculate the component's physical properties automatically, without any additional input from the user. When we have access to a nice collection of physical property data (as we do in Aspen Properties) using a component set is the natural choice.

When we use Aspen Properties for physical properties, we can invoke the Aspen Properties user interface directly if we have it installed. In order to edit physical property options, we need to follow the steps in Figure 1.11:

1) In the Simulation Explorer, click "**Component Lists**".
2) In the **Explorer of the Component Lists folder**, double-click the "**Configure Properties**" **node**.
3) In the **Physical Properties Configuration** dialog box, choose "Use Aspen property system" option, and then click "**Edit using Aspen Properties**" **button to launch the user interface**.



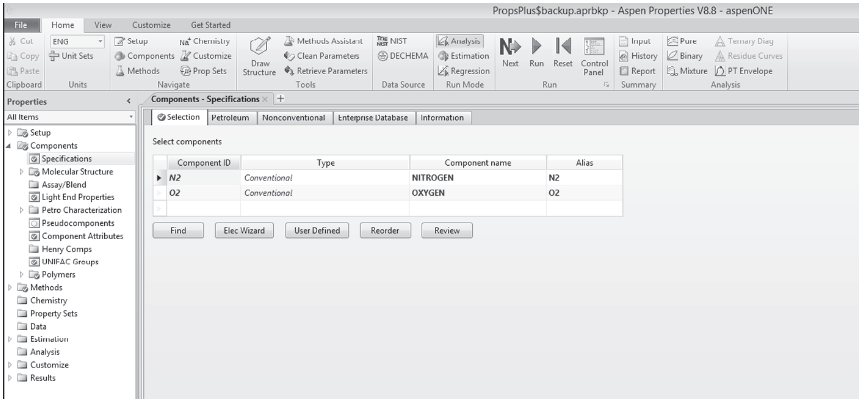
● Use Aspen property system
○ Use custom properties
○ Don't use properties

Properties status
Aspen Properties input incomplete

Figure 1.11 The physical properties configuration pane.

Step 4: Add component names in Aspen Properties

Once "**Edit using Aspen Properties"** in the **Physical Properties Configuration** pane is clicked, it automatically opens the Aspen Properties for us to add component names and edit their physical and chemical properties. Figure 1.12 displays that we are trying to separate nitrogen from the nitrogen and oxygen mixture.



Select components

Component ID	Type	Component name	Alias
N2	Conventional	NITROGEN	N2
O2	Conventional	OXYGEN	O2

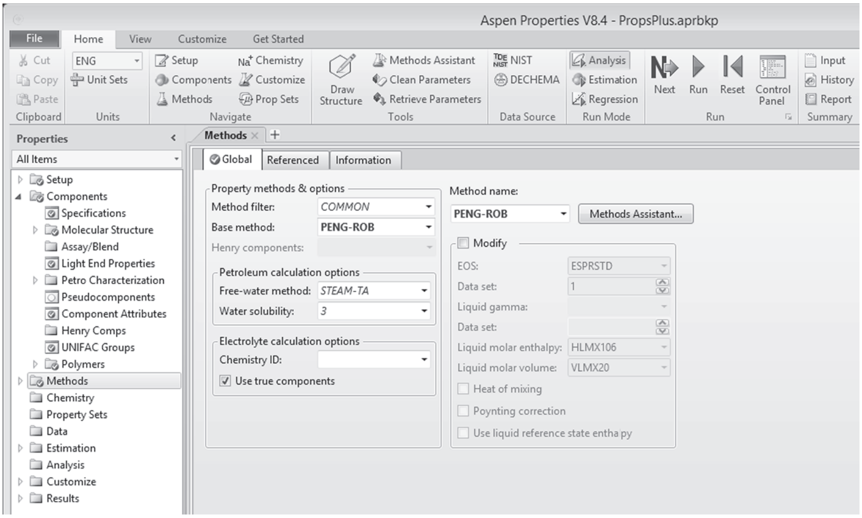
Figure 1.12 The Aspen Properties interface.

Step 5: Select the Appropriate Property Method

In this step, we specify the methods that calculate the thermodynamic properties for our simulation. The “Base-method” and “Method name” drop-down menus in Figure 1.13 are essentially redundant, although the “Base method” option allows you to filter the long list of methods by application. For example, PENG-ROB shows up when the method-filter is set to COMMON; however, specialized variants of the Peng–Robinson method (such as PR-BM, the Peng–Robinson model with Boston–Mathias alpha-function) do not show up unless the filter is set to “GasProc”

To edit the components’ physical properties in Aspen Properties, we follow the steps in Figure 1.13:

1) In the “All Items” pane of the “Properties”, click “Specification” in the “Methods” folder.
2) Select “PENG-ROB” as the base method.
3) In the pane of “Home”, click the “Run” button (Figure 1.14).
4) Save the file until the run is completed in the Control Panel. See Figure 1.14.



Property methods & options

Method filter: COMMON

Base method: PENG-ROB

Henry components:

Petroleum calculation options

Free-water method: STEAM-TA

Water solubility: 3

Electrolyte calculation options

Chemistry ID:

☑ Use true components

Method name: PENG-ROB

☐ Modify

EOS: ESPRSTD

Data set: 1

Liquid gamma:

Data set:

Liquid molar enthalpy: HLMX106

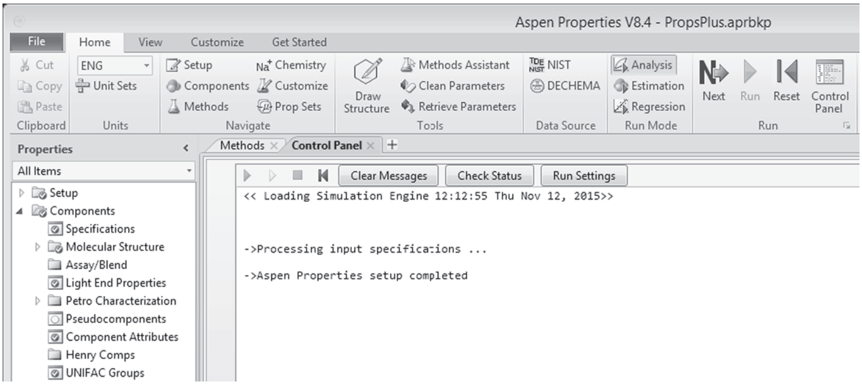
Liquid molar volume: VLMX20

☐ Heat of mixing

☐ Poynting correction

☐ Use liquid reference state enthalpy

Figure 1.13 The specification of the components in Aspen Properties.

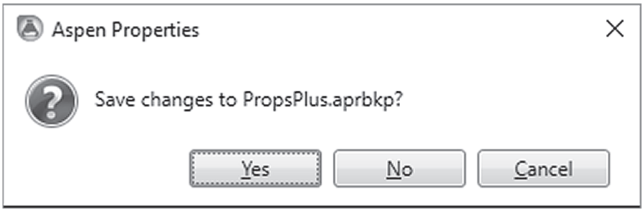


```
<< Loading Simulation Engine 12:12:55 Thu Nov 12, 2015>>


->Processing input specifications ...

->Aspen Properties setup completed
```

Figure 1.14 The completion in control panel in Aspen Properties.

Step 6: Tell Aspen Adsorption to use the Aspen Properties file that is created

Once the Aspen Property file completes the run, you may close Aspen Properties. Make sure that you choose "yes" to save the document as **PropsPlus.aprbkp** while closing! (Figure 1.15)

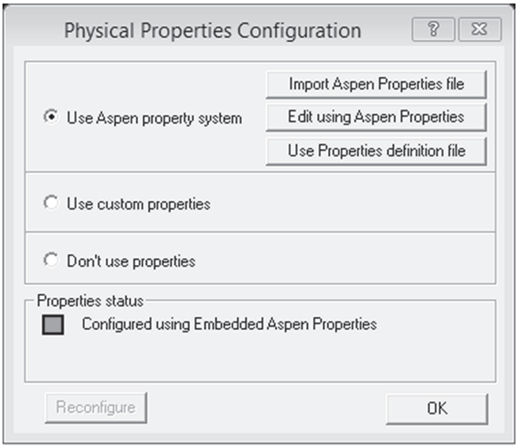


Save changes to PropsPlus.aprbkp?

Figure 1.15 Ensure the properties document is saved.

The saved properties document will be included in our Aspen flowsheet automatically. We can tell that the properties are successfully configured by looking for a green square next to "**Configured using Embedded Aspen Properties**" in the properties configuration form (Figure 1.16).

Figure 1.16 The completion of the physical properties configuration.



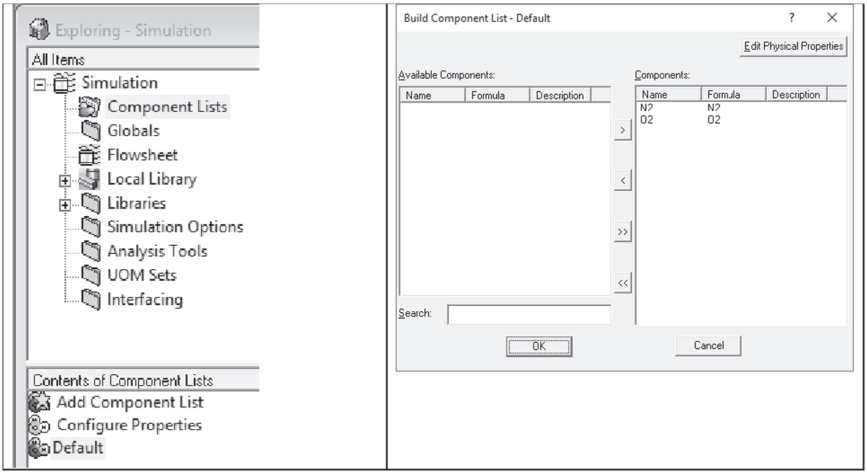
● Use Aspen property system
○ Use custom properties
○ Don't use properties

Properties status
▨ Configured using Embedded Aspen Properties

Once we press "OK" on this form, we must add the components we choose in Aspen Properties to our flowsheet. To do this, double-click on "Default" in the Explorer to open up the component list builder. Move components N2 and O2 from Available Components on the left to Components on the right (Figure 1.17).

This distinction between the components available in Aspen Properties and those available in the flowsheet is useful in situations where we are building a chemically complex model, but want to start with only a few components.

Once you have added the components, press **ctrl+S** to save the Workshop1A file with the same name.



Components:

Name	Formula	Description
N2	N2	
O2	O2	

Figure 1.17 Adding the defined components to the flowsheet.

1.7.2 Creating a Flowsheet in Aspen Adsorption

Now that we have successfully added several chemical components to Aspen, it is time to begin specifying the layout of our process. Aspen provides a large number of "Models" that are contained in "Model Libraries." These models roughly correspond to common unit operations, but take care not to confuse these models with actual physical process equipment. For example, a physical packed bed might be represented as a combination of three separate "Models" in Aspen. Specifically, two "empty void" models can describe the empty voids at the top and bottom of the packed bed, while the gas-bed model will describe the region of the packed bed, which actually performs separation. In the same way, a single Aspen "Model" might represent several physical pieces of equipment. For example, a single gas_interaction model can be used to represent several identical packed beds.

Step 7: Ensure that the Model Libraries are visible

To begin, ensure that the model libraries are visible by clicking on the "Model Libraries" button in the "View" menu (Figure 1.18).

Once the button has been clicked, the following area shown in Figure 1.19 will be visible on the main window. This area displays all the prebuilt models available in Aspen Adsorption, and are colloquially referred to as "blocks." Each model or block roughly corresponds to a unit operation, such as a packed bed, tank, or valve. However, some models have subtler roles, which we cover as we get to them.

Step 8: Understand an overview of the flowsheet and of implementing the forward-reverse flow reversibility through the pressure setters and flow setters in Aspen Adsorption

Let us first take a look at the final flowsheet of Figure 1.20 that we are to draw and understand the concepts of pressure setters and reversible flow setters within the Aspen Adsorption's dynamic simulation environment.

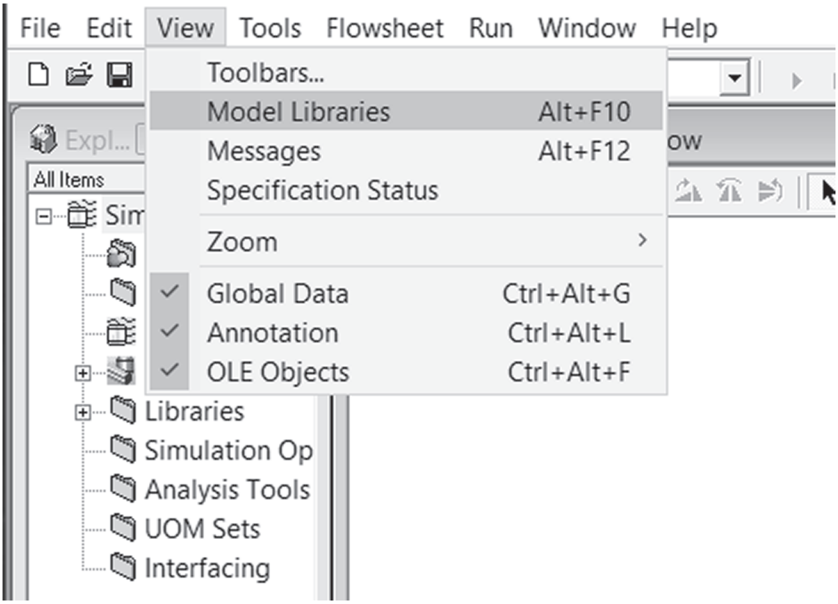


Figure 1.18 Display of the model libraries.

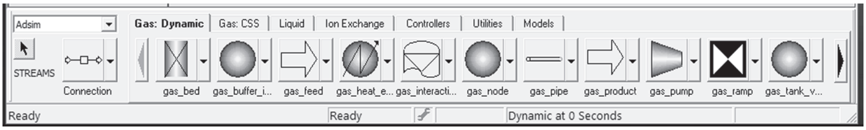


Figure 1.19 The model libraries.

Within the flowsheet, we have the following feed and product "streams":

1) Feed F1 (an air stream; a mixture of N2 and O2)
2) Product P1 (a high-purity O2 product)
3) Waste W1 (a waste mixture of a high-purity N2 and a low-purity O2).

Each stream is defined by $(C + 2)$ specifications, where C is the number of components, and the remaining two specifications are typically temperature and pressure.

The flowsheet also includes the following "blocks," which are models for unit operations, such as mixer, splitter, valve, and adsorption column:

1) Gas_valve model, which serves as a control valve for closing or opening the valve, and as **a "reversible" flow setter** that sets the flow rate and **the forward-reverse direction of flow** through the valve: feed valves VF, VF1, and VF2; waste valves VW1 and VW2; purge valve VPurge; and product valves VP, VP1, and VP2.

   In Aspen Adsorption, valves operate under the assumption that the molar flow rate is linearly related to pressure drop across the valve, as shown in Eq. (1.12):

$$F = \mathrm{Cv}\Delta P \tag{1.12}$$

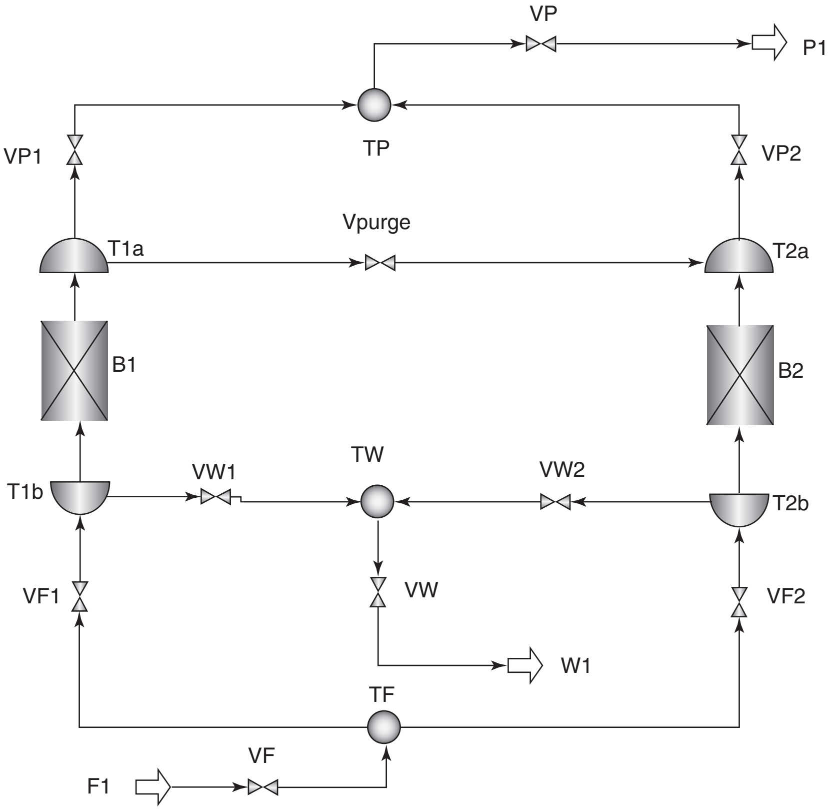


Figure 1.20 An overview of the final flowsheet.

In the equation, F is the molar flow rate in kmol s^{-1} and ΔP is the pressure drop across the valve in bar. This means that the Cv value in Aspen *does not* correspond to the conventional form of the Cv equation shown in Eq. (1.13):

$$\mathrm{Cv} = q\sqrt{\frac{G_\mathrm{f}}{\Delta P}}. \tag{1.13}$$

In the equation, q is the volumetric flow rate in GPM (gallon per minute) and G_f is the specific gravity of the fluid. In Eq. (1.13), ΔP is still the pressure drop across the valve, but it has units of psi.

2) The Gas_tank_void model, serves as a mixer or a splitter, and as **a pressure setter** that sets the pressure to enable the calculation of flow rate through the valve equation based on the pressure drop across the valve, and of the pressure drop across an adsorber bed. We set the initial pressure of each gas_tank_void model through the Presets/Initial form within the block. In the flowsheet, we have the following gas_tank_void blocks: TF, TW, T1a, T1b, T2a, T2b, and TP.
3) Gas_bed model for the absorber, including beds B1 and B2.

The online “Help” section of Aspen Adsorption explains in detail the concept that implements **the forward-reverse flow directions** corresponding to the cyclic adsorption under a dynamic environment. Basically, in the overall flowsheet of Figure 1.20, we do the following:

1) Add a gas_tank_void block TF as a pressure setter to fix the pressure between valves VF and VF1, and between valves VF and VF2. Add a gas_tank_void block TW as a pressure setter to fix the pressure between valves VW1 and VW, and between valves VW2 and VW. Also, add a gas_tank_void block TP as a pressure setter to fix the pressure between valves VP1 and VP, and between valves VP2 and VP.
2) Add gas_tank_void blocks T1a and T1b as pressure setters to fix the pressures at the inlet and outlet of adsorber bed B1. By doing so, we also fix the pressure between valves VF1 and VW1, and between valves VPurge and VP1. Do the same for adsorber bed B2 with gas_tank_void blocks T2a and T2b.

Step 9: Place your first blocks: the adsorber beds

To select the adsorber bed block, click on the first icon in Figure 1.19, labeled gas_bed. To place it in the flowsheet, merely click anywhere in the flowsheet. Click a second time to place a second gas block, then right-click to stop adding repeatedly the same blocks. Once the gas_beds have been placed, an icon will appear that represents a new packed bed. See Figure 1.21.

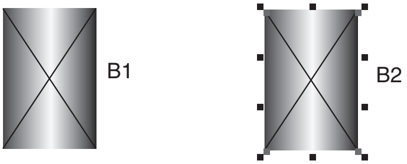


Figure 1.21 Freshly placed gas_beds in the flowsheet.

Step 10: Place the gas_tank blocks

We can repeat this process to add the rest of the blocks to the flowsheet, but there is one additional consideration. Each model has multiple icons that can be used to improve the intelligibility of the flowsheet. To view the extra icons, click on the small arrow beside the button in the model library. Use this arrow to add seven different tanks (gas_tank_void) to the flowsheet, as shown in Figure 1.22. It is important to note that the icons do not change the behavior of the block in any way, and they are purely cosmetic.

Step 11: Place the gas_valves

The gas_valve models are the very last on the list in the Gas: Dynamic tab. Therefore, if you are working on a small screen, you may need to use the arrow on the far right-hand side to scroll the gas_valve button into view. Once you have, place the valves as shown in Figure 1.23.

Step 12: Add the Feed and Product blocks

The final blocks to add to the flowsheet are the "feed" and "product" blocks. These represent points where material may enter or exit the flowsheet. They are not required in all circumstances, but they are needed here. We cover situations where they are not needed in later exercises. Add one feed block (B19) at the lower left of the flowsheet and two product blocks (B20, B21), as shown in Figure 1.24.

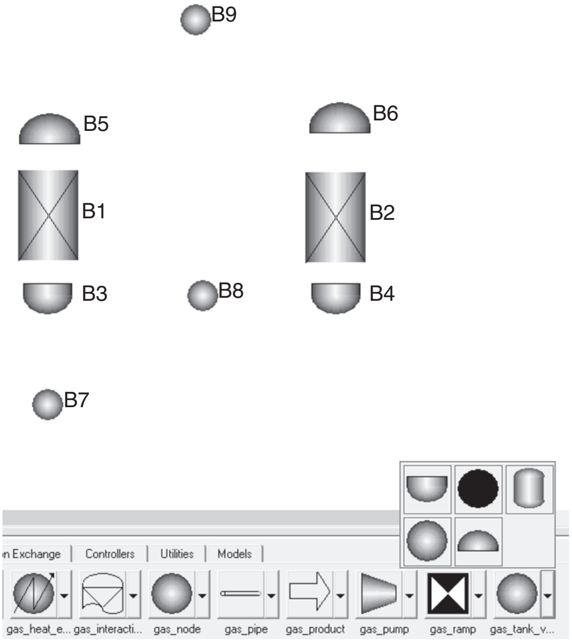


Figure 1.22 Placing gas_tank_voids using the various icon options.

Step 13: Connect the blocks using gas_material_connections

Similarly to the procedure when placing models with different icons, use the small arrow by the "connection" icon to select gas_material_connection. Unlike with the models, the different connection types do have different behaviors, and so it does matter which is selected. After selecting the connection icon, we see that the blocks in the flowsheet show blue and red arrows, indicating points where they can be connected together. You can connect the blocks in any order by clicking on the arrow of one block, and an arrow of a second block. Blocks may accept more than one connection to the same point. For example, a gas_tank_void can accept many inlet and outlet streams simultaneously. If you want to change the location of a connection for esthetics, hold down the mouse button while clicking on the blue or red arrow, and drag it to the desired location before releasing. See Figure 1.25 for the connection options and arrows.

One additional feature that can improve the legibility of flowsheet diagrams is the rotate button at the top of the flowsheet window, which allows blocks (and therefore their connection points) to be rotated (Figure 1.26). Use this feature, along with the gas_material_connection to connect the flowsheet as shown in Figure 1.27. Pay close attention to the direction of the arrows, which indicate the expected direction of fluid flow. These directions are reversible for some, but not all, connection types. While the gas_material_connection is reversible, having the streams in the correct order facilitates initialization.

If the rotation options are not visible, you may enable them by right-clicking on a block in the flowsheet to see "Rotate Icon." Figure 1.26 shows the right-click menu with the option that enables the rotation buttons highlighted.

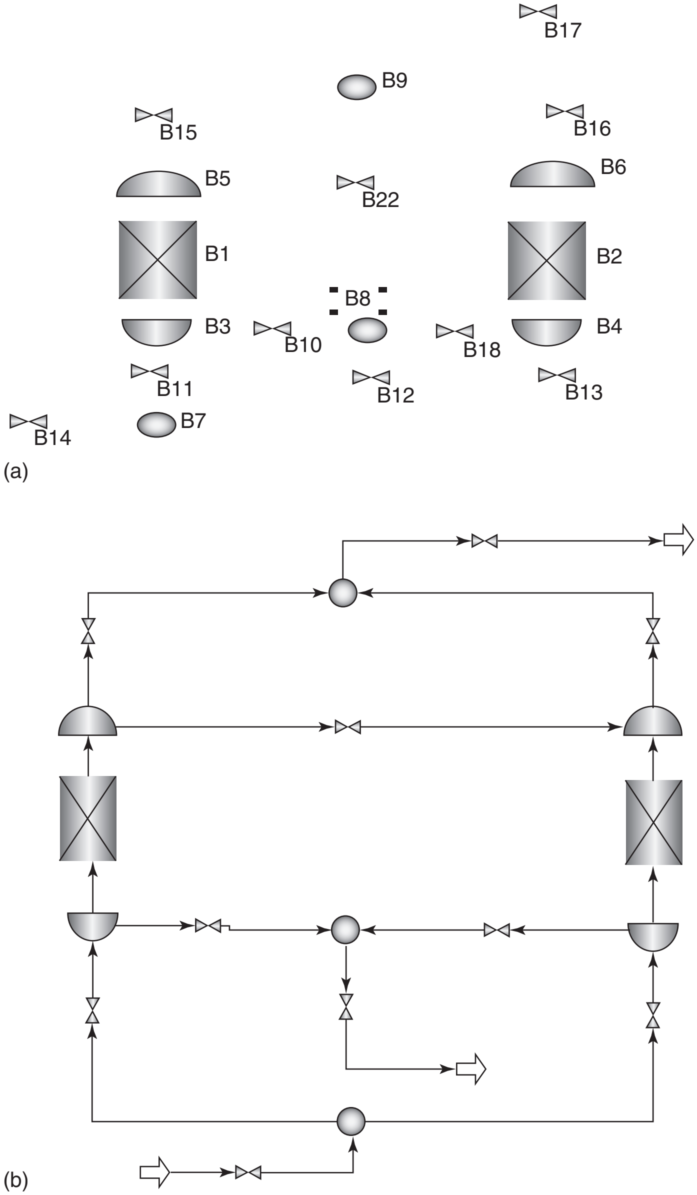


Figure 1.23 The flowsheet with valves added. (a) The valves after initial placement and (b) the valves after "clean up" in step 13.

Step 14: Clean Up

The flowsheet you created may not appear as tidy as that in Figure 1.27. In this step, we cover three tips for cleaning up a new flowsheet, and nearly every model you build will need these.

First: Align blocks and redraw the streams.

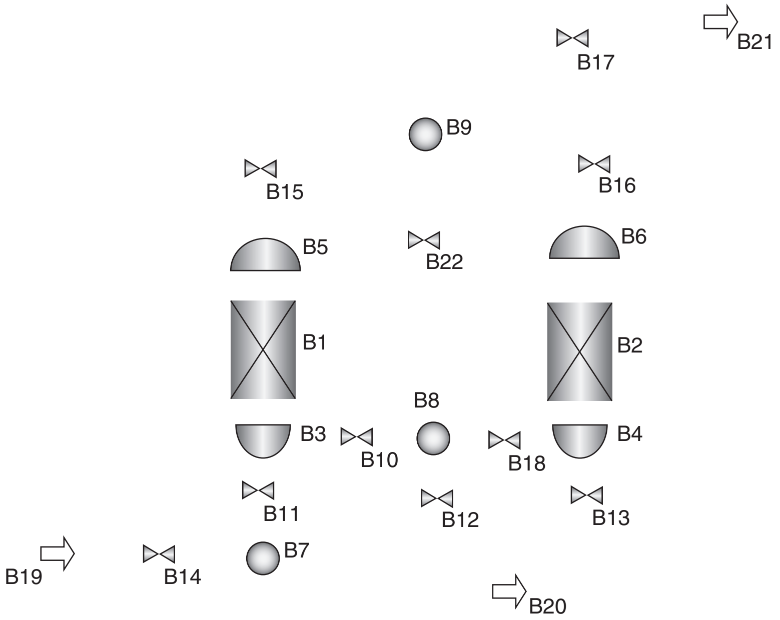


Figure 1.24 The flowsheet with all blocks added.

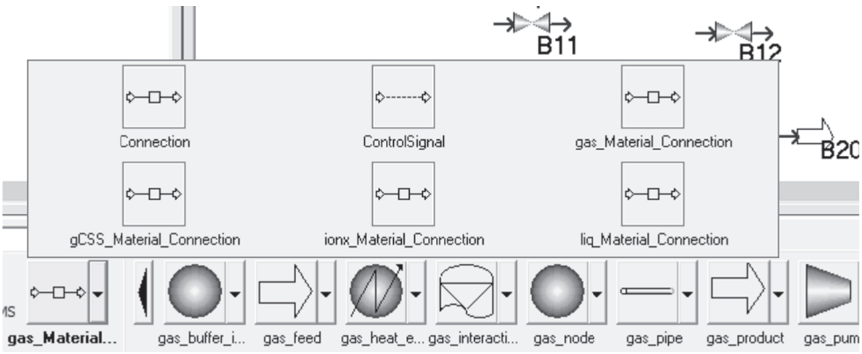


Figure 1.25 Connection options and arrows.

There are two simple ways to align and redraw the blocks in the flowsheet. First, select the stream connecting the two blocks you wish to align, and press **ctrl+B** to align them. Then, press **ctrl+J** to redraw the stream into a more efficient path. You can do this all at once by first using **ctrl+A** to select all the streams, and alternating between **ctrl+B** and **ctrl+J**, although this will not resolve all esthetic issues, and you may need to manually move some blocks and iterate.

Second: Rename the important blocks and streams.

To rename a block or stream, first click on it, then press ctrl+m and enter the new name. Use this process to rename the blocks as shown in Figure 1.28.

Third: Hide the names of unimportant streams or blocks.

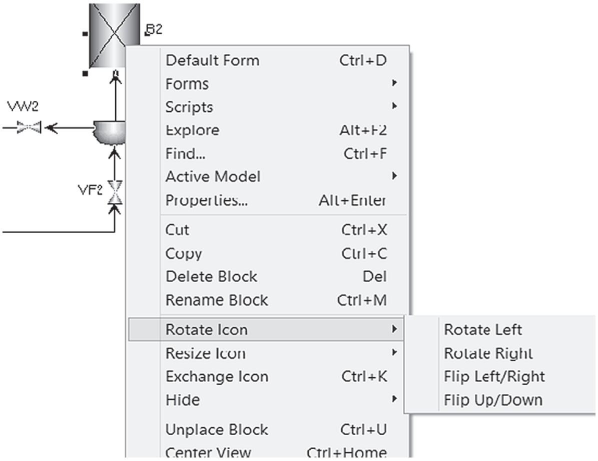


Figure 1.26 The flowsheet right-click menu.

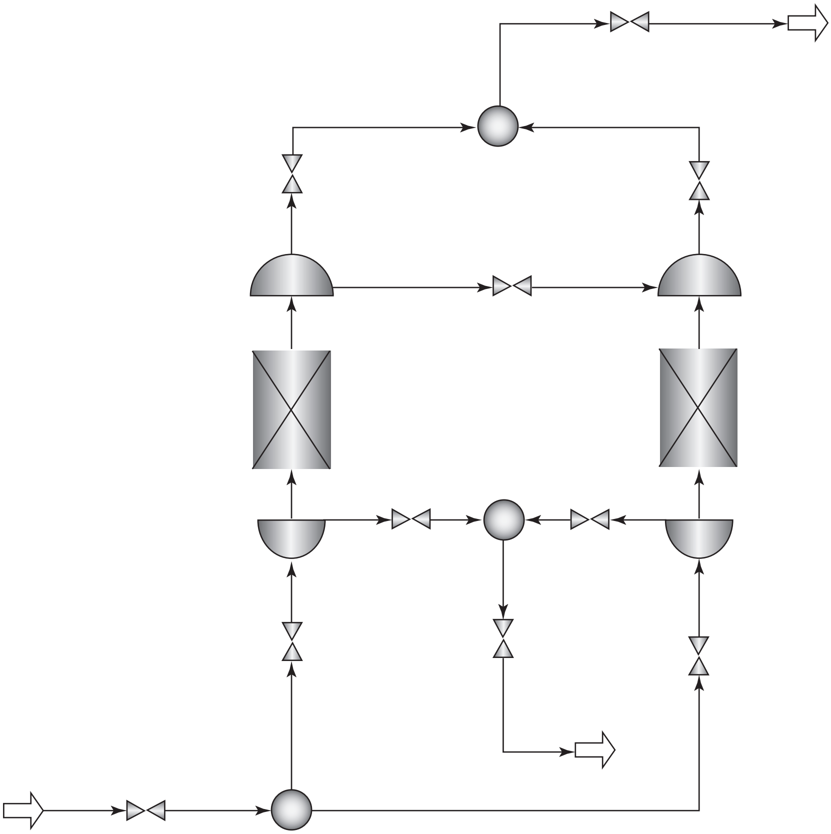


Figure 1.27 The connected flowsheet.

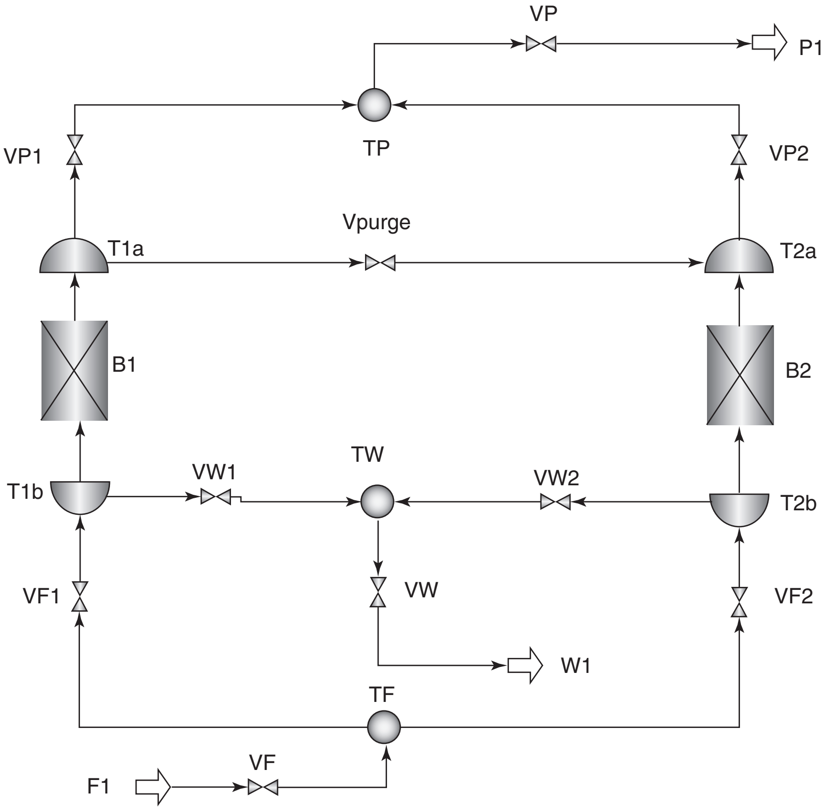


Figure 1.28 The completely labeled and connected flowsheet.

In this flowsheet, the names of the streams will not end up being important. Therefore, we can hide their labels. Do this by selecting the stream, then pressing ctrl+H.

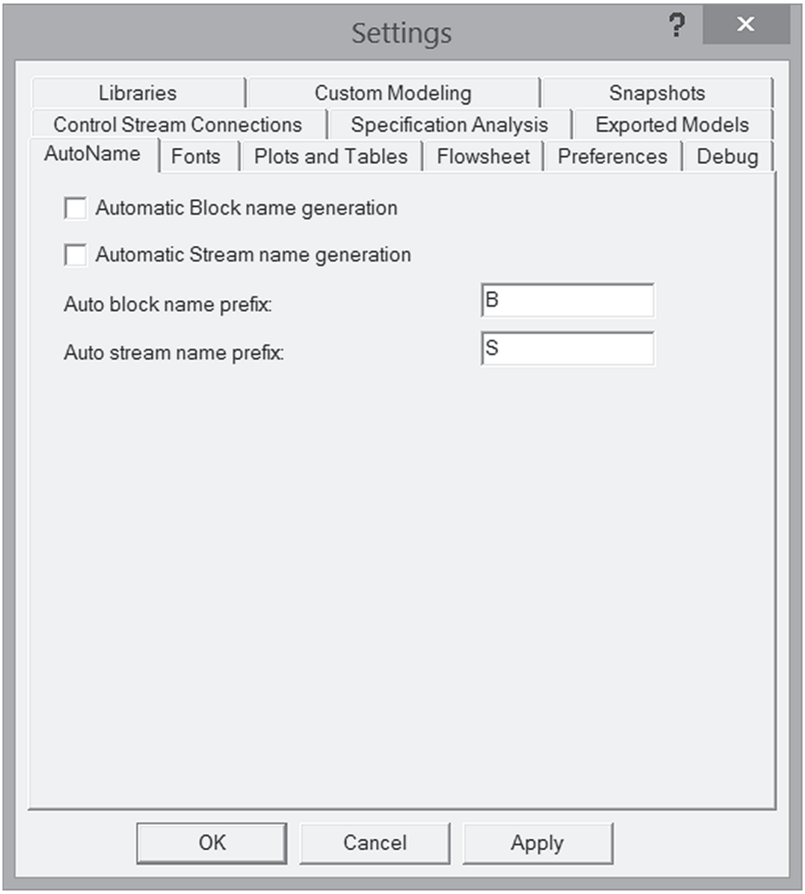
Once you have completed these three "clean up" operations, the flowsheet will look like Figure 1.28.

Once you are satisfied with the layout of the flowsheet, save the file as **Workshop1B.ada**

Step 14a: An alternative approach to drawing the process flowsheet quickly

Now that we have understood how to use the relevant streams and blocks within Aspen Adsorption, and practiced applying various tools in drawing the flowsheet, we can proceed to demonstrate an alternative approach to drawing the flowsheet that is straightforward. We show this in a few steps below.

1) Cancel the automatic name generation for blocks and streams: Tools → Settings → unclick the automatic name generation for blocks and streams → Apply → OK (Figure 1.29).
2) Draw stream F1, valve VF, pressure setter (gas_tank_void) TF, valve VF1, and valve VF2 together with the gas_material_connections S1 to S4. Rotate the blocks appropriately if needed. (Figure 1.30).



☐ Automatic Block name generation

☐ Automatic Stream name generation

Auto block name prefix: B

Auto stream name prefix: S

Figure 1.29 Cancellation of automatic name generation for blocks and streams.

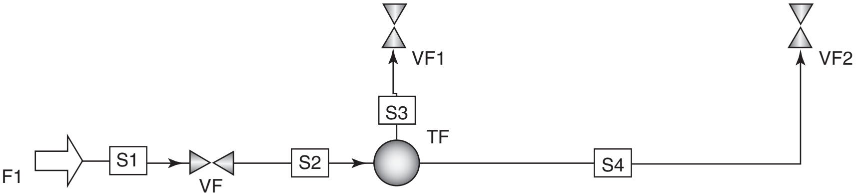


Figure 1.30 An alternative approach to drawing the flowsheet (step 1).

3) Draw the pressure setters (gas_tank_voids) T1b, T2b, and TW, valves VW1, VW2, and VW, and product stream VW, as well as the gas_material_connections S5 to S12. Rotate the blocks appropriately if needed. (Figure 1.31)
4) Draw the adsorber beds B1 and B2, pressure setters (gas_tank_voids) T1a and T1b, and valves VPurge, VP1, and VP2, together with the

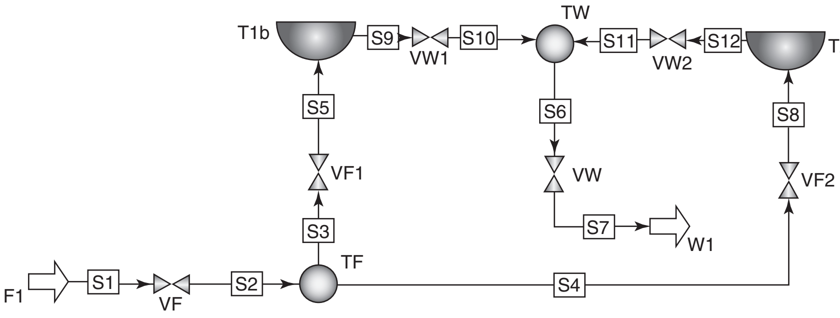


Figure 1.31 An alternative approach to drawing the flowsheet (step 2).

gas_material_connections S13 to S20. Rotate the blocks appropriately if needed. (Figure 1.32)

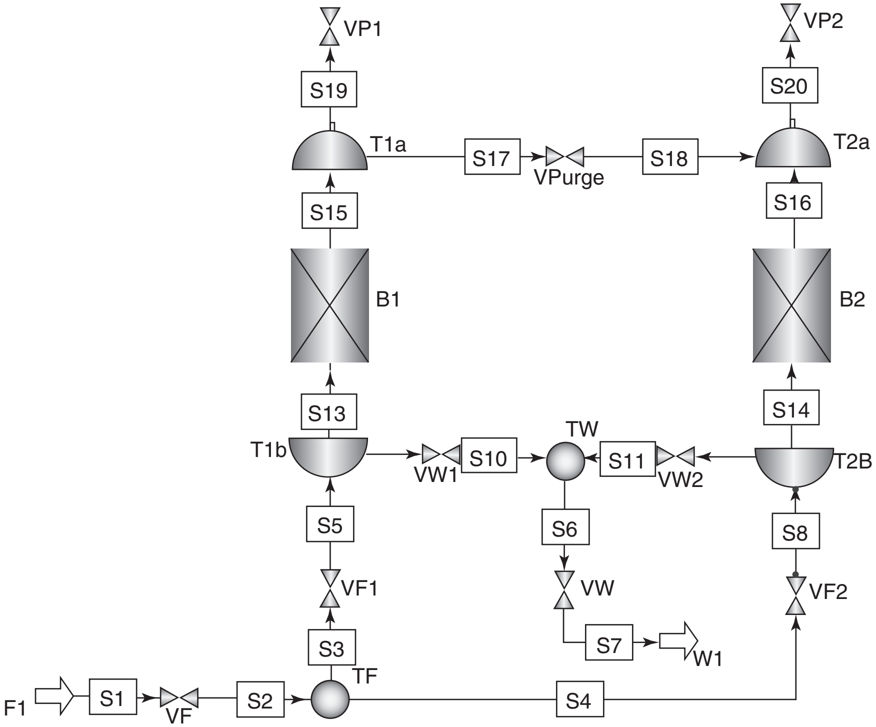


Figure 1.32 An alternative approach to drawing the flowsheet (step 3).

5) Draw the pressure setters (gas_tank_void) TP, and valve VP, product P1, together with the gas_material_connections S21 to S24. Rotate the blocks appropriately if needed. (Figure 1.33)
6) Hide the names of all streams (Figure 1.34). Save the file as **Workshop1B.ada**.

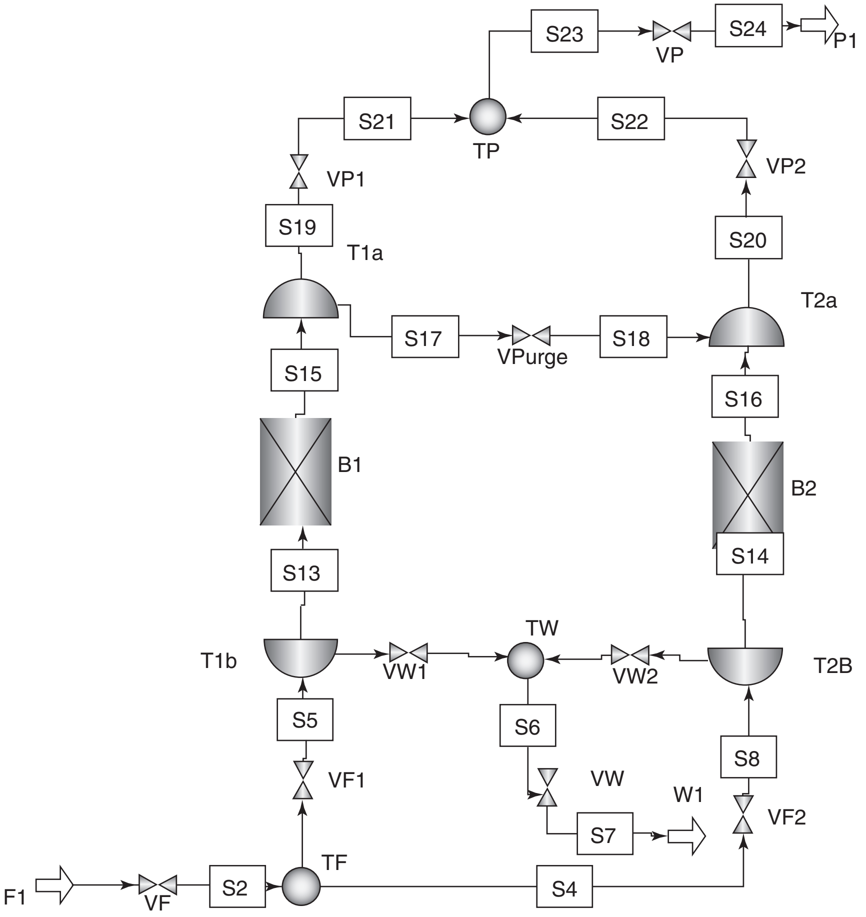


Figure 1.33 An alternative approach to drawing the flowsheet (step 4).

1.7.3 Specifying Operating Conditions: Tables and Forms

There are two main methods for entering values into an Aspen simulation: Tables and Forms, with Tables being the most common. Tables are exactly what you would expect: a window dedicated to tabulating variables and their values. Forms are similar, except Aspen Tech has applied formatting to organize and present the data. To open the default form for a process model, simply double-click on it. It is ***critical*** to be aware that the default form does not always include entries to all the variables you might need to provide data for.

Step 15: Specify the beds B1 and B2

Figure 1.35 shows the specification of the column in the PSA model. It has only one vertical adsorbent layer within the bed with the same packed adsorbent molecular sieve 5A. We choose 1-D (one-dimensional) as the spatial dimensions, since we do not expect there to be any issues with 2-D (two-dimensional)

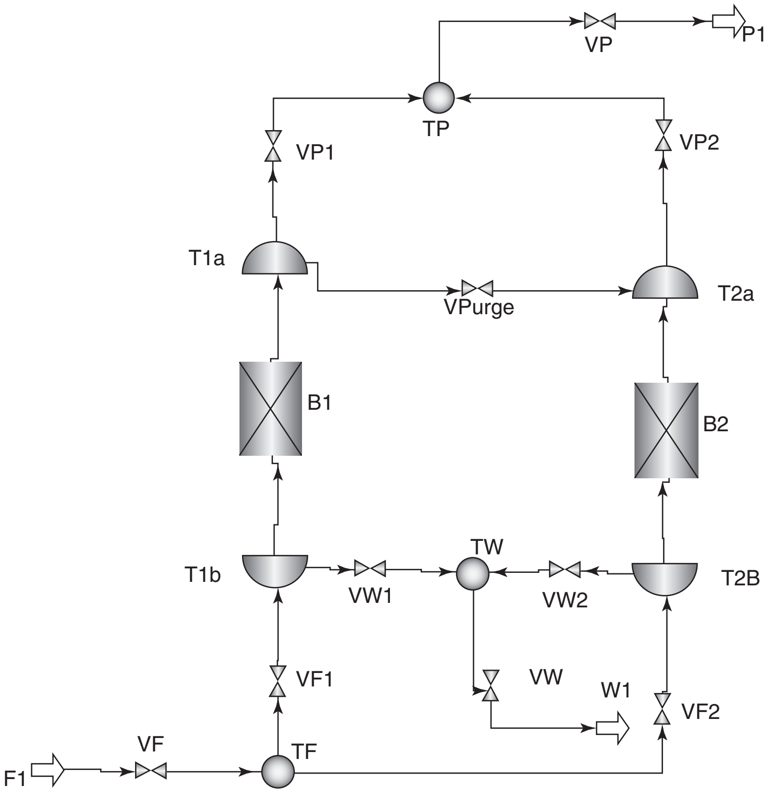


Figure 1.34 An alternative approach to drawing the flowsheet (step 5).

radial mixing. There is no heat exchanger within the adsorbent layer, so we may leave that option alone.

Step 16: Specify the discretization method to be used

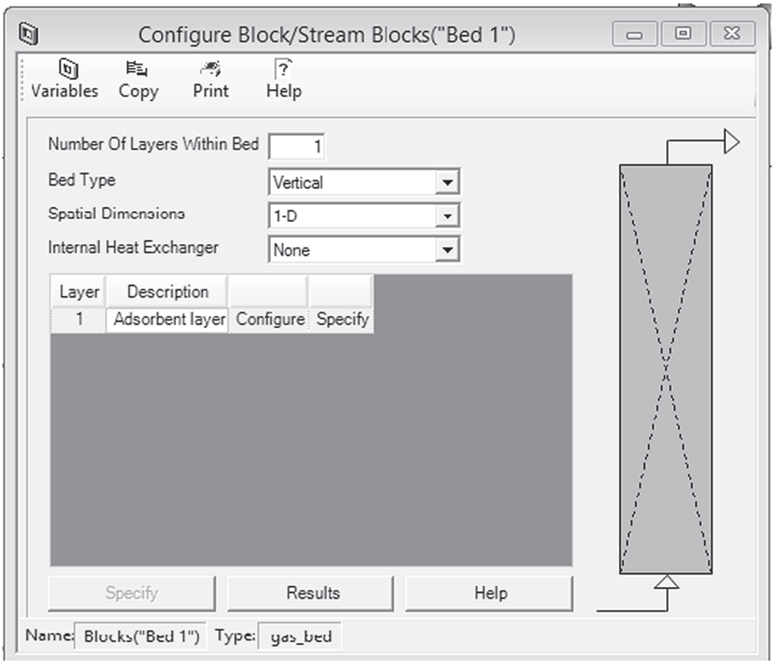
From this point, we want to specify more detailed properties of the adsorption bed. To do this, click on the "Configure" button to the right of "Layer 1." Once this has been clicked, Aspen will show the General tab (Figure 1.36), which allows us to specify the numerical options for solving the partial differential equations (PDEs), and to select the gas model assumption.

Aspen Adsorption uses a set of PDEs, ordinary differential equations (ODEs) and algebraic equations, together with the appropriate initial and boundary conditions, to fully describe the adsorption column.

The *upwind differencing scheme 1* (UDS1) is the preferred option in most cases. We prefer to use UDS1 for this dynamic PSA model because it saves the simulation time and the results are reasonably accurate. Therefore, we use the USD1 with 60 nodes.

Step 17: Provide the Material/Momentum Balance Assumptions

We use the Material/Momentum Balance tab in Figure 1.37 to specify the material and momentum balances, and the dispersive properties. For simplicity, we choose convection only as the mass balance assumption. The

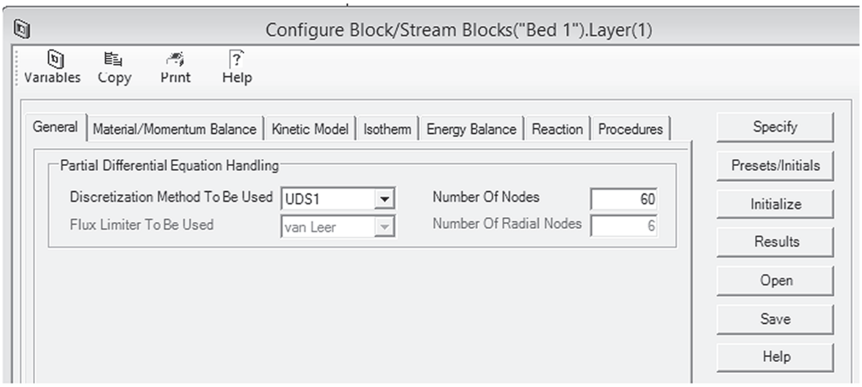


Number Of Layers Within Bed: 1
Bed Type: Vertical
Spatial Dimensions: 1-D
Internal Heat Exchanger: None

Layer	Description		
1	Adsorbent layer	Configure	Specify

Name: Blocks("Bed 1") Type: gas_bed

Figure 1.35 The column configuration specification.

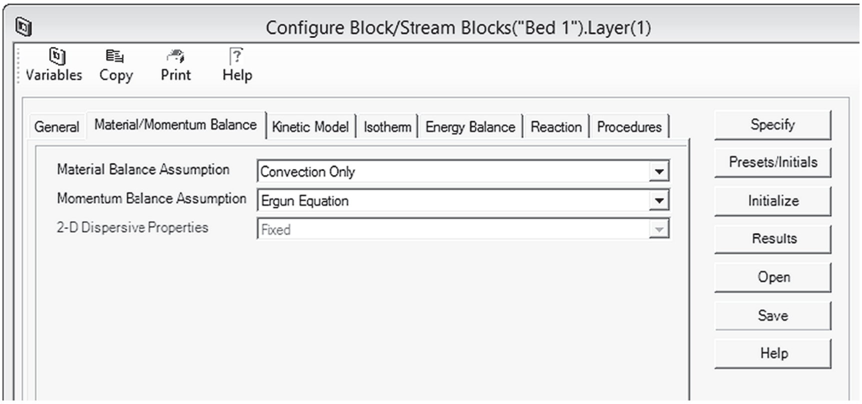


Partial Differential Equation Handling
Discretization Method To Be Used: UDS1
Flux Limiter To Be Used: van Leer
Number Of Nodes: 60
Number Of Radial Nodes: 6

Figure 1.36 The discretization method in the PSA model.

Convection Only option drops the dispersion term from the material balance in Eq. (1.14), so the model represents the plug flow with a zero dispersion coefficient. Local equilibrium is achieved instantaneously between the adsorbent and adsorbates at each axial location.

We use the Momentum Balance Assumption box to specify how the adsorption bed layer model treats gas velocity and pressure. For the calculation of the pressure drops in the PSA system, we use the Ergun equation, Eq. (1.11), which



Material Balance Assumption: Convection Only
Momentum Balance Assumption: Ergun Equation
2-D Dispersive Properties: Fixed

Figure 1.37 The material balance assumption in the PSA model.

is valid for both laminar and turbulent flows and is the most popular option.

$$\frac{\partial C_i}{\partial t} + \frac{(1-\varepsilon)}{\varepsilon}\frac{\partial q_i}{\partial t} + u\frac{\partial C_i}{\partial z} = D_{\mathrm{L}}\frac{\partial^2 C_i}{\partial z^2} = 0. \tag{1.14}$$

In the equation, C_i is the concentration for component i in the gas phase, q_i is the concentration for component i in the solid phase, and ε represents the overall bed voidage, z is the axial distance through the column, and D_{L} is the axial dispersion coefficient. P is the pressure drop within the column, u is the superficial velocity of the gas flow, $\mu =$ fluid viscosity, $r_{\mathrm{p}} =$ particle radius, and $\psi =$ particle shape factor.

Step 18: Specify the Kinetic Model Assumption & Mass-Transfer Coefficients

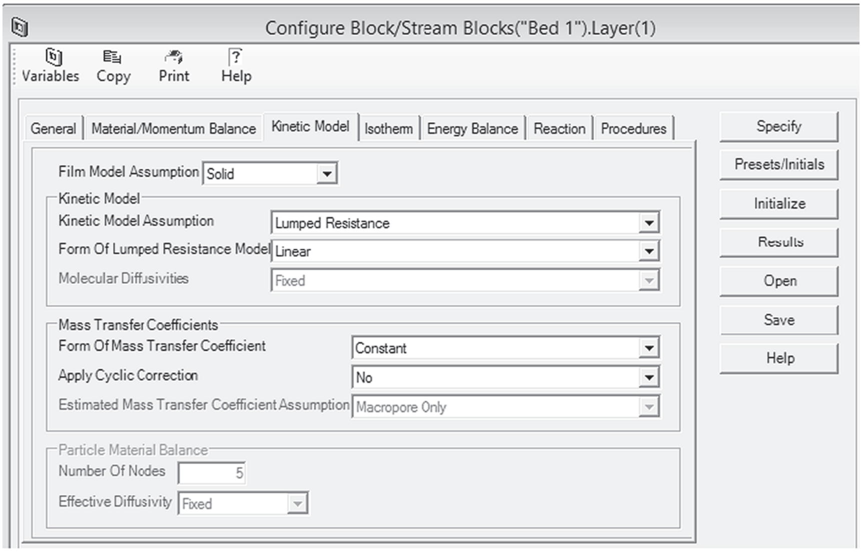
We use the Kinetic Model tab in Figure 1.38 to specify the assumptions made about model kinetics, such as resistances, diffusivities and mass transfer coefficients. In the Film Model Assumption box, we choose the solid form, where the mass transfer driving force is expressed as a function of the solid-phase loading.

Typically, several mass transfer resistances occur in the gas-phase adsorption processes:

- Mass transfer resistance between the bulk gas phase and the gas-solid interface.
- Mass transfer resistance due to the porous structure of the adsorbent.

In our case, we consider the mass transfer resistance as *a lumped and linear resistance* or *a linear driving force (LDF) assumption* in the Kinetic Model Assumption box. It means that we lump these mass transfer resistances as a single overall factor, or one resistance dominates all others. The mass transfer coefficient for each component is constant throughout the bed. The mass transfer driving force for component i is a linear function of the solid-phase loading (solid film) as shown in Eq. (1.15):

$$\frac{\partial q_i}{\partial t} = k_i(q_i^* - q_i), \tag{1.15}$$



Film Model Assumption: Solid

Kinetic Model
Kinetic Model Assumption: Lumped Resistance
Form Of Lumped Resistance Model: Linear
Molecular Diffusivities: Fixed

Mass Transfer Coefficients
Form Of Mass Transfer Coefficient: Constant
Apply Cyclic Correction: No
Estimated Mass Transfer Coefficient Assumption: Macropore Only

Particle Material Balance
Number Of Nodes: 5
Effective Diffusivity: Fixed

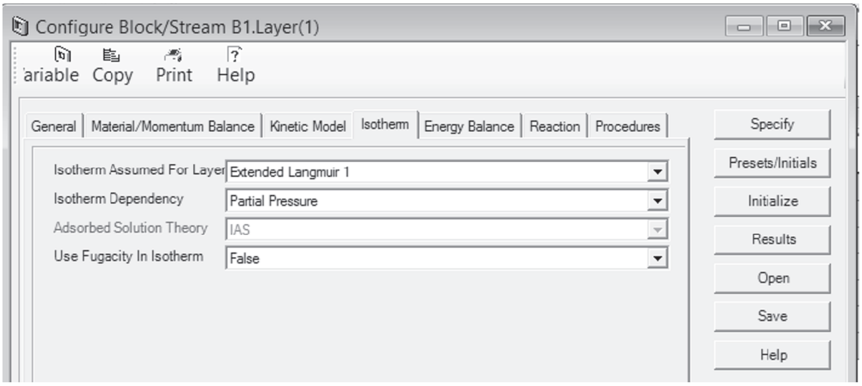
Figure 1.38 The kinetic method in the PSA model.

where k_i is *the linear lumped mass transfer coefficient*, q_i is solute concentrations of the solid phase, and q_i^* represents the adsorbed phase concentration at equilibrium with the gas phase.

Step 19: Specify the isotherm assumptions in the bed

We use the Isotherm tab in Figure 1.39 to choose the assumptions regarding the isotherm of the system.

In an adsorber design, we are usually interested in the adsorption equilibria of mixtures, rather than those of pure components. This is because adsorbed gas components interact on the solid surface, so individual gas components adsorb differently when mixed with other components. Mixture adsorption equilibrium data are not readily available. Although measurements can be made, they are tedious and time consuming to perform, so it is a common



Isotherm Assumed For Layer: Extended Langmuir 1
Isotherm Dependency: Partial Pressure
Adsorbed Solution Theory: IAS
Use Fugacity In Isotherm: False

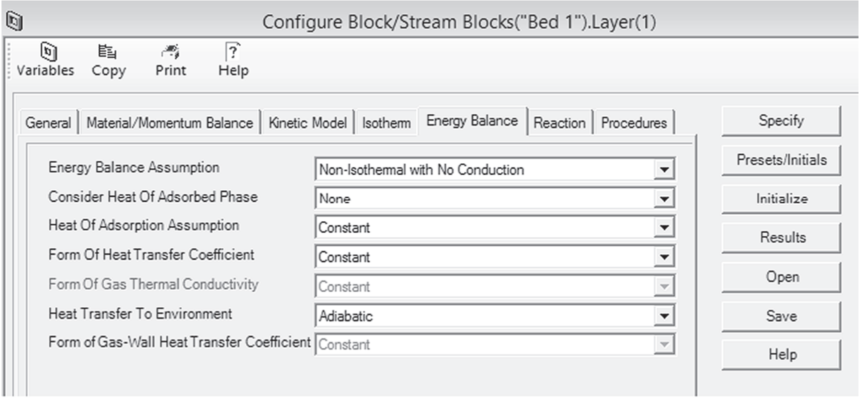
Figure 1.39 The isotherm method in the PSA model.

practice to predict mixture isotherms from pure component isotherms. We use the extended Langmuir isotherm as the isotherm model, which is a function of partial pressure in the system. In this approach, we can predict mixture isotherms from pure component data.

We do not enter the numeric values for the isotherm parameters here, but wait until after all the tabs have been completed

Step 20: Energy Balances

We use the Energy Balance tab in Figure 1.40 to specify how the energy balance is incorporated into the model for this gas adsorption process. We use the nonisothermal with no conduction as the energy assumption. We assume that the beds are adiabatic.

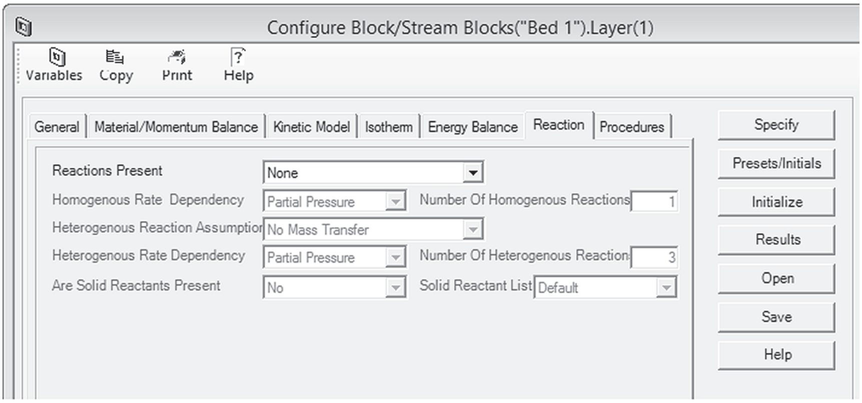


Energy Balance Assumption: Non-Isothermal with No Conduction
Consider Heat Of Adsorbed Phase: None
Heat Of Adsorption Assumption: Constant
Form Of Heat Transfer Coefficient: Constant
Form Of Gas Thermal Conductivity: Constant
Heat Transfer To Environment: Adiabatic
Form of Gas-Wall Heat Transfer Coefficient: Constant

Figure 1.40 The energy balances in the PSA model.

Step 21: Reactions

There are no reactions in this PSA system, and we specify that here (Figure 1.41).

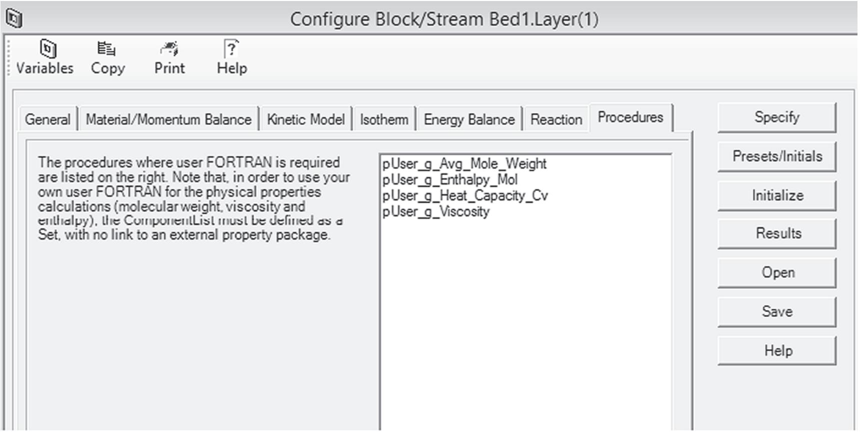


Reactions Present: None
Homogenous Rate Dependency: Partial Pressure
Number Of Homogenous Reactions: 1
Heterogenous Reaction Assumptior: No Mass Transfer
Heterogenous Rate Dependency: Partial Pressure
Number Of Heterogenous Reaction: 3
Are Solid Reactants Present: No
Solid Reactant List: Default

Figure 1.41 The reaction method in the PSA model.

Step 22: User procedures

We can use the Procedures tab in Figure 1.42 to view a list of user procedures within the current adsorption layer model. This is where our choice of Component List pays off. Had we chosen Component Set, we would need to provide our own FORTRAN code to calculate the quantities shown in this list for Aspen to be able to calculate the values and simulate the bed.



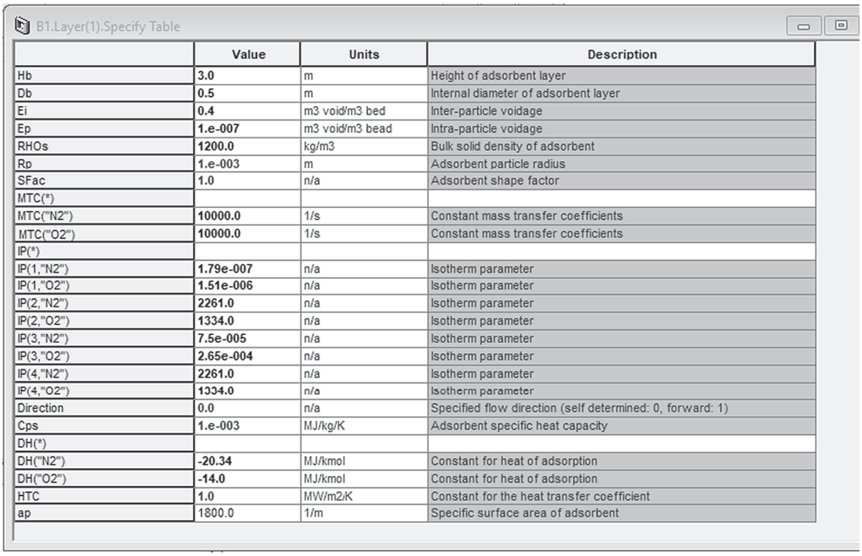
The procedures where user FORTRAN is required are listed on the right. Note that, in order to use your own user FORTRAN for the physical properties calculations (molecular weight, viscosity and enthalpy), the ComponentList must be defined as a Set, with no link to an external property package.

pUser_g_Avg_Mole_Weight
pUser_g_Enthalpy_Mol
pUser_g_Heat_Capacity_Cv
pUser_g_Viscosity

Figure 1.42 The available procedures in the PSA model.

Step 23: The "Specify" button

After defining all assumptions for the layer, we click the "Specify" button in the Configuration form to open the data table containing the required data for the layer. Table 1.6 contains the required data, and Figure 1.43 shows the filled table.



	Value	Units	Description
Hb	3.0	m	Height of adsorbent layer
Db	0.5	m	Internal diameter of adsorbent layer
Ei	0.4	m3 void/m3 bed	Inter-particle voidage
Ep	1.e-007	m3 void/m3 bead	Intra-particle voidage
RHOs	1200.0	kg/m3	Bulk solid density of adsorbent
Rp	1.e-003	m	Adsorbent particle radius
SFac	1.0	n/a	Adsorbent shape factor
MTC(*)			
MTC("N2")	10000.0	1/s	Constant mass transfer coefficients
MTC("O2")	10000.0	1/s	Constant mass transfer coefficients
IP(*)			
IP(1,"N2")	1.79e-007	n/a	Isotherm parameter
IP(1,"O2")	1.51e-006	n/a	Isotherm parameter
IP(2,"N2")	2261.0	n/a	Isotherm parameter
IP(2,"O2")	1334.0	n/a	Isotherm parameter
IP(3,"N2")	7.5e-005	n/a	Isotherm parameter
IP(3,"O2")	2.65e-004	n/a	Isotherm parameter
IP(4,"N2")	2261.0	n/a	Isotherm parameter
IP(4,"O2")	1334.0	n/a	Isotherm parameter
Direction	0.0	n/a	Specified flow direction (self determined: 0, forward: 1)
Cps	1.e-003	MJ/kg/K	Adsorbent specific heat capacity
DH(*)			
DH("N2")	-20.34	MJ/kmol	Constant for heat of adsorption
DH("O2")	-14.0	MJ/kmol	Constant for heat of adsorption
HTC	1.0	MW/m2/K	Constant for the heat transfer coefficient
ap	1800.0	1/m	Specific surface area of adsorbent

Figure 1.43 The specify form of the adsorbent layer in the PSA model.

Table 1.6 The specifications of the adsorbent layer.

Column (adsorbent layer) height (m)		3
Internal diameter of the column (m)		0.5
Interparticle voidage (m^3 void/m^3 bed)		0.4
Intraparticle voidage (m^3 void/m^3 bead)		1.00e−07
Solid density of the adsorbent ($kg\,m^{-3}$)		1200
Adsorbent particle radius (mm)		1.00
Adsorbent shape factor (n/a)		1
Specific surface area ($1\,m^{-1}$)		1800
	Nitrogen (N_2)	Oxygen (O_2)
Mass transfer coefficient ($1\,s^{-1}$)	100 000	100 000
IP1 equilibrium loading	1.79e−07	1.51e−06
IP2 Arrhenius factor	2261	1334
IP3 saturation Factor	7.50e−05	2.65e−04
IP4 Arrhenius factor	2261	1334
Heat of adsorption constant ($kJ\,mol^{-1}$)	−20.34	−14

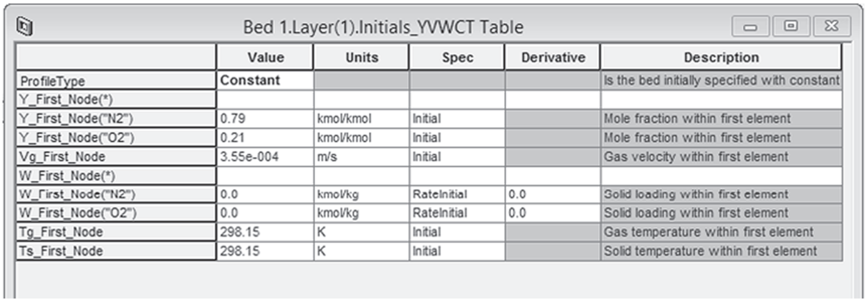
When these numbers are typed into the column, they look like Figure 1.43.

Once the values have all been entered into this table, it may be closed.

Step 24: Set the initial conditions inside the bed

The final step before the bed is completely specified is to press the "Presets/initials" button to set the initial condition of the bed. We want the initial conditions to have the following ratios: nitrogen 0.79, oxygen 0.21. The temperature for both gas and solid phases is 25 °C.

The form shown in Figure 1.44 represents the initial conditions for only one finite-element node in the bed. We will apply this value to all the nodes once we reach the "initialization" step.



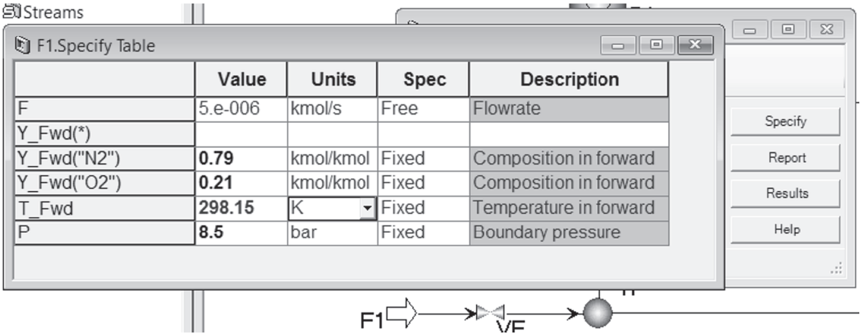
Bed 1.Layer(1).Initials_YVWCT Table

	Value	Units	Spec	Derivative	Description
ProfileType	Constant				Is the bed initially specified with constant
Y_First_Node(*)					
Y_First_Node("N2")	0.79	kmol/kmol	Initial		Mole fraction within first element
Y_First_Node("O2")	0.21	kmol/kmol	Initial		Mole fraction within first element
Vg_First_Node	3.55e-004	m/s	Initial		Gas velocity within first element
W_First_Node(*)					
W_First_Node("N2")	0.0	kmol/kg	RateInitial	0.0	Solid loading within first element
W_First_Node("O2")	0.0	kmol/kg	RateInitial	0.0	Solid loading within first element
Tg_First_Node	298.15	K	Initial		Gas temperature within first element
Ts_First_Node	298.15	K	Initial		Solid temperature within first element

Figure 1.44 The initialization form in the gas_bed.

Step 25: Specify the feed and product blocks

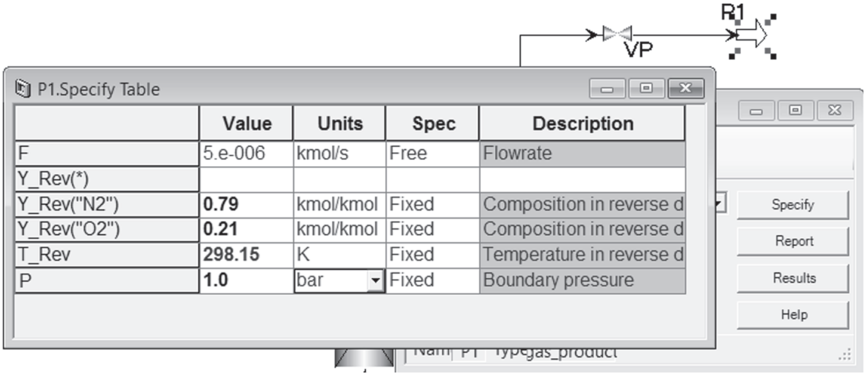
In this PSA model, we set the feed-in flow rate in the "Feed" block as free, because we control the feed flow in the Cycle Organizer through the VF valve. The feed composition is fixed with 0.79 mole fraction nitrogen and 0.21 mole fraction oxygen. The temperature and pressure in the feed are both fixed, with 25 °C and 8.5 bar, respectively (Figure 1.45).



	Value	Units	Spec	Description
F	5.e-006	kmol/s	Free	Flowrate
Y_Fwd(*)				
Y_Fwd("N2")	0.79	kmol/kmol	Fixed	Composition in forward
Y_Fwd("O2")	0.21	kmol/kmol	Fixed	Composition in forward
T_Fwd	298.15	K	Fixed	Temperature in forward
P	8.5	bar	Fixed	Boundary pressure

Figure 1.45 The feed specification in the PSA model.

Just as with the feed block, the valves will decide the product block flow rates. However, we need to specify their pressure, as well as the "reverse" concentrations that get invoked if the flow rate of the product blocks ever becomes negative. Set both product blocks to have a pressure of 1 bar, and reverse concentration that matches the feed block (Figure 1.46).



	Value	Units	Spec	Description
F	5.e-006	kmol/s	Free	Flowrate
Y_Rev(*)				
Y_Rev("N2")	0.79	kmol/kmol	Fixed	Composition in reverse d
Y_Rev("O2")	0.21	kmol/kmol	Fixed	Composition in reverse d
T_Rev	298.15	K	Fixed	Temperature in reverse d
P	1.0	bar	Fixed	Boundary pressure

Figure 1.46 Specifying a product block.

Once you have entered the data, save the flowsheet as **Workshop1C.ada.**

Step 26: Initializing the flowsheet

At this point, we have defined a valid flowsheet. We are not yet done entering information, but Aspen should be able to run what we have so far. Therefore, to check our work, initialize the simulation for a run. The first thing to do is to look at the run controls shown in Figure 1.47. If they are greyed out, Aspen considers our flowsheet to be incomplete (i.e. things are not connected properly) or misconfigured (i.e. we have too many or too few degrees of freedom.) At this stage, the buttons *should* be greyed out.

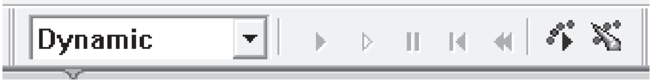
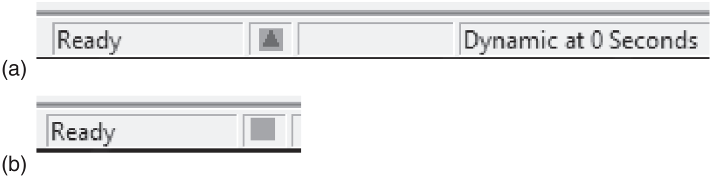


Figure 1.47 The Aspen run controls.

The next step to look at is the "Specification Status," which will tell us why the run controls are unavailable (Figure 1.48).


(a)

Ready | Dynamic at 0 Seconds

(b)

Ready

Figure 1.48 The Specification Status for an overspecified flowsheet (a) and a completely specified flowsheet (b).

If we have failed to connect the blocks correctly, the indicator will show a grey wrench icon. If we have done everything correctly, we should see an upward pointing triangle that indicates that we have an over-specified simulation. Why is our simulation overspecified? Because we have not yet *initialized* the gas beds and tanks. Initialization changes various internal variables according to how the flowsheet is connected and configured (dynamic/steady state). To perform the initialization, use the Flowsheet menu to pick "Check & Initial" (Figure 1.49). This initialization will, among other things, set the gas beds to have a uniform composition, precisely the composition we chose in Step 24:

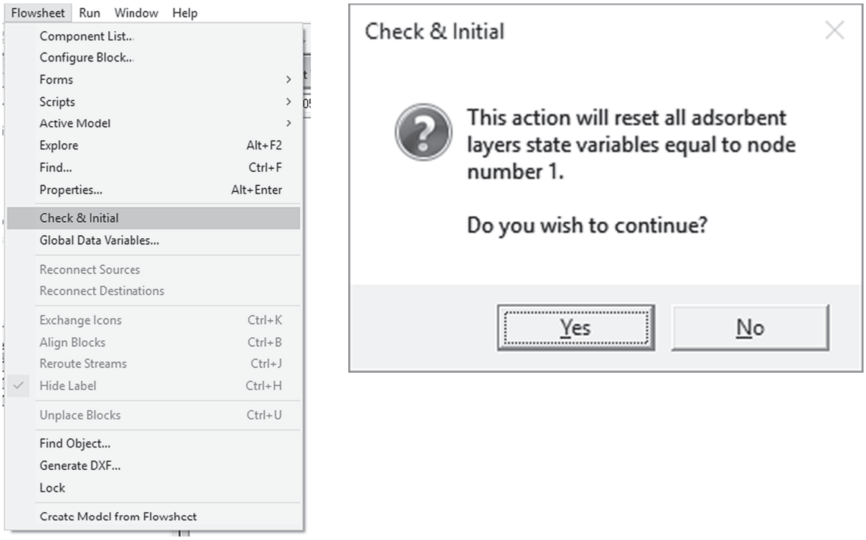
Once the flowsheet has been successfully initialized, save the file as **Workshop1D.ada.**

1.7.4 Scheduling Events with the Cycle Organizer

We have not yet provided any information about the valves, and that is because they will be controlled through the "Cycle Organizer." This block makes it easy to program schedules into our simulation, so that we can achieve the dynamic valve opening and closing required to simulate our PSA process.

The way we have placed the valves in our flowsheet, Figure 1.28, will allow us to employ the following strategies:

- Flow rates are set by the VF, VP, and VW valves, and they will not close during any step. That is to say, they will behave as valves with constant flow coefficient, so that the flow rate through them is a function of the pressure drop across them.



This action will reset all adsorbent layers state variables equal to node number 1.

Do you wish to continue?

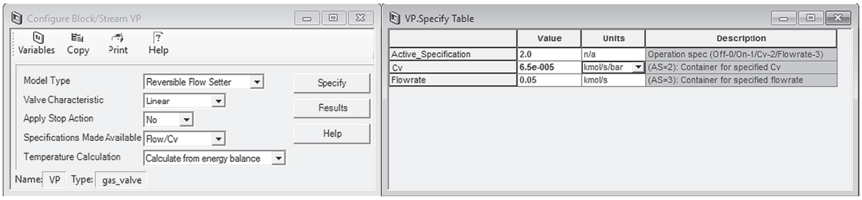
Figure 1.49 The Check and Initial function.

- The VPurge valve will also function as a Cv valve, but will only be open during purge steps.
- All other valves (VF1, VF2, VW1, VW2, VP1, and VP2) are either completely open or completely closed, and simply select which bed the gas will flow through.

Step 27: Specify the VF, VW, VPurge, and VP valves

We have previously explained, in Tables 1.4 and 1.5, the four active specifications (ASs) for valves within Aspen Adsorption: (1) AS = 0, valve is fully closed; (2) AS = 1, valve is fully open; (3) AS = 3, the gas flow rate through the valve is linearly dependent on the pressure drop across the valve according to Eq (1.12); and (4) AS = 3, the valve has a fixed flow rate.

Since the Cv values of these valves do not change over time, we can specify them before working with the Cycle Organizer. To change the Cv value of a valve, double-click on it, then press the "Specify" button (Figure 1.50).



Model Type: Reversible Flow Setter
Valve Characteristic: Linear
Apply Stop Action: No
Specifications Made Available: Flow/Cv
Temperature Calculation: Calculate from energy balance
Name: VP Type: gas_valve

	Value	Units	Description
Active_Specification	2.0	n/a	Operation spec (Off-0/On-1/Cv-2/Flowrate-3)
Cv	6.5e-005	kmol/s/bar	(AS=2): Container for specified Cv
Flowrate	0.05	kmol/s	(AS=3): Container for specified flowrate

Figure 1.50 Specifying the VP valve.

Set the valve Cv values according to Table 1.7. Note that the valve acts as **a flow setter** according to Eqs. (1.12) and (1.13) presented previously in Step 8.

Table 1.7 Cv valve settings.

Valve	Cv setting (kmol/(s bar^{-1}))
VF	0.0095
VP	6.5e−6
Vpurge	4.5e−5
VW	0.065

The VP and Vpurge valve Cv values are significantly lower than the feed and waste valves. This is because we are always collecting the product and purge from the high-pressure tank. Having a more restricted flow rate prevents the bed from depressurizing too quickly and contaminating the product.

Step 28: Add the Cycle Organizer

It is now time to think about the valve scheduling. To add a Cycle Organizer to the flowsheet, press the "tools" button, then click on "Cycle Organizer" (Figure 1.51).

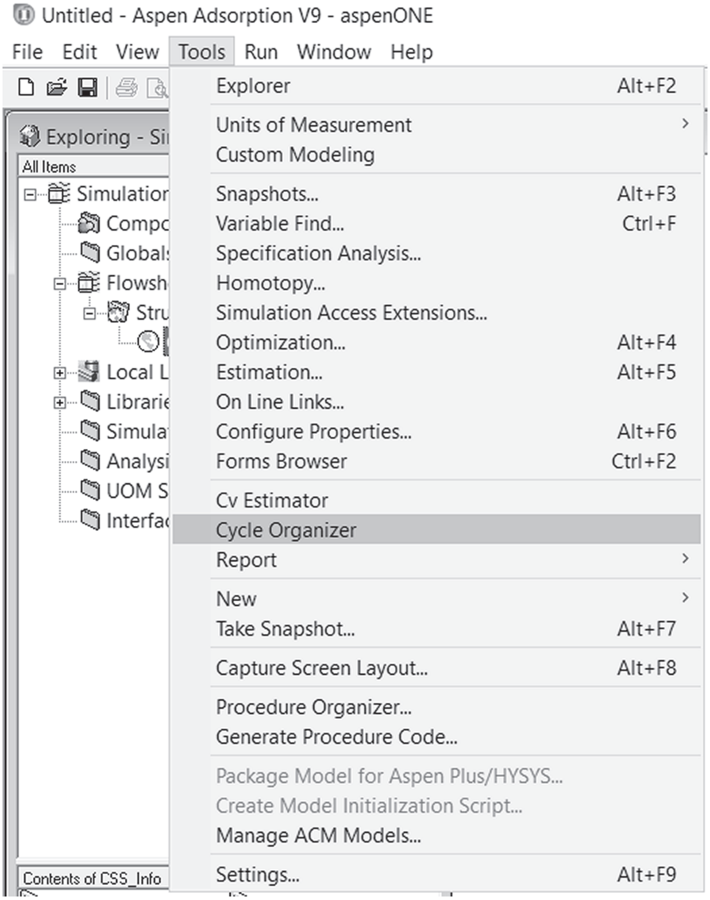
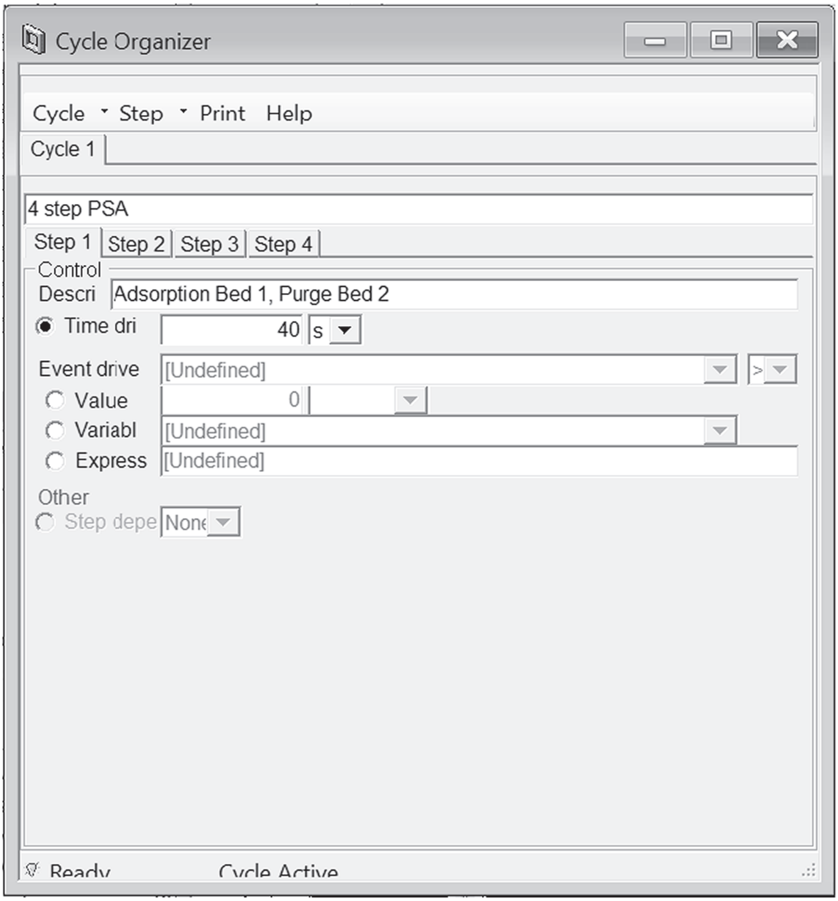


Figure 1.51 Adding the Cycle Organizer.

Step 29: Specifying a step in the Cycle Organizer

After adding a Cycle Organizer, we need to specify the various steps that the Cycle Organizer will go through. The input form for the Cycle Organizer presents one undefined step. There are many options to control these steps. They can be triggered by events that occur in the flowsheet, time, or even other cycles. To specify the first step, we put in a description and indicate that the step will simply run for 40 s, as shown in Figure 1.52.



4 step PSA

Descri: Adsorption Bed 1, Purge Bed 2

● Time dri: 40 s

Event drive: [Undefined] >

○ Value: 0

○ Variabl: [Undefined]

○ Express: [Undefined]

○ Step depe: None

Figure 1.52 Specifying the first step (adsorption bed 1, purge bed 2).

Of course, we also need to specify which valves will be open and closed during this step. To do this, click on the “step” button and select “Manipulated” (Figure 1.53).

Now we need to know what variables to manipulate. Double-click on any valve icon to see what settings are available. Figure 1.54 shows the high-level options, and common numerical variables that define the valve. For the Cycle Organizer, we will try to configure the flowsheet so that we only need to modify the Active_Specification for simplicity’s sake.

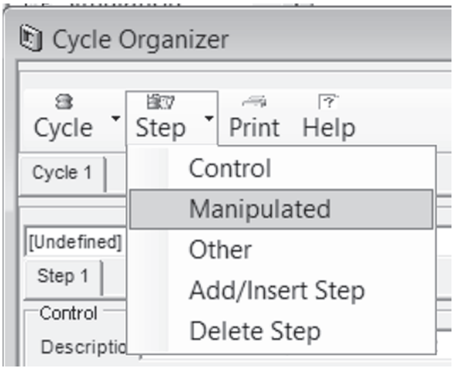
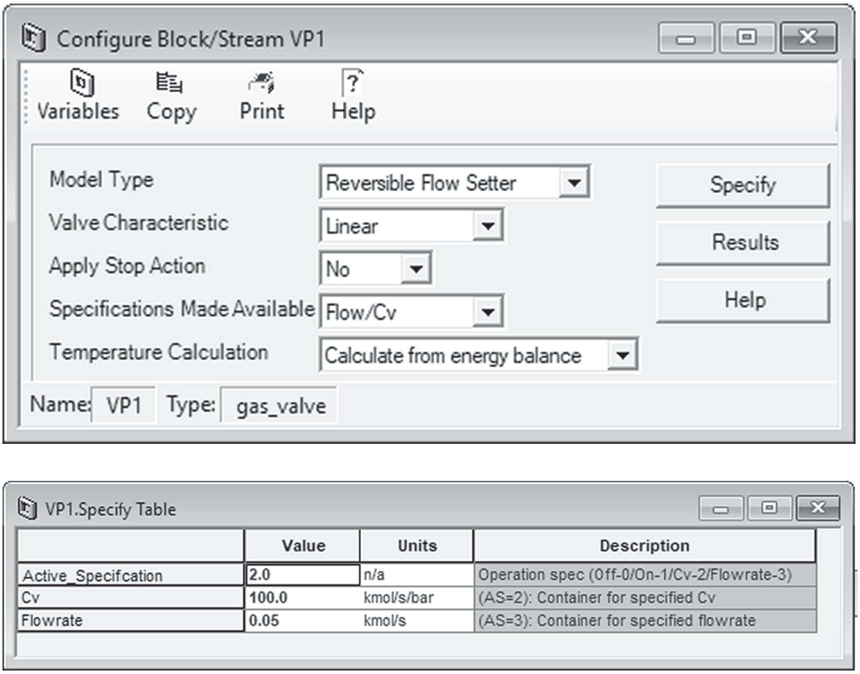


Figure 1.53 Viewing manipulated variables in the cycle organizes.



Model Type: Reversible Flow Setter
Valve Characteristic: Linear
Apply Stop Action: No
Specifications Made Available: Flow/Cv
Temperature Calculation: Calculate from energy balance
Name: VP1 Type: gas_valve

	Value	Units	Description
Active_Specifcation	2.0	n/a	Operation spec (Off-0/On-1/Cv-2/Flowrate-3)
Cv	100.0	kmol/s/bar	(AS=2): Container for specified Cv
Flowrate	0.05	kmol/s	(AS=3): Container for specified flowrate

Figure 1.54 The valve settings for VP1.

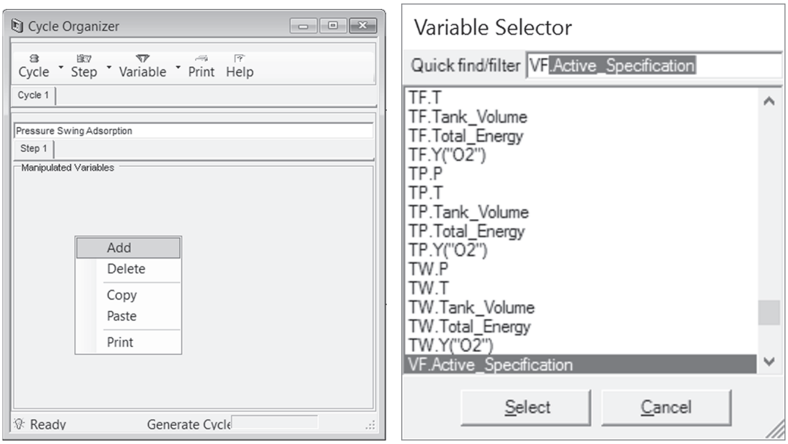
To add variables, right-click and choose “Add” (Figure 1.55).

Following Figure 1.7 and Table 1.4 in Section 1.7, we specify the variables and values for Step 1 (adsorption bed 1, purge bed 2) of the PSA cycle (Figure 1.56).

What do these “Active_Specification” variables mean? We have defined these previously in Table 1.4. They tell Aspen that the valves will behave according to Table 1.4.

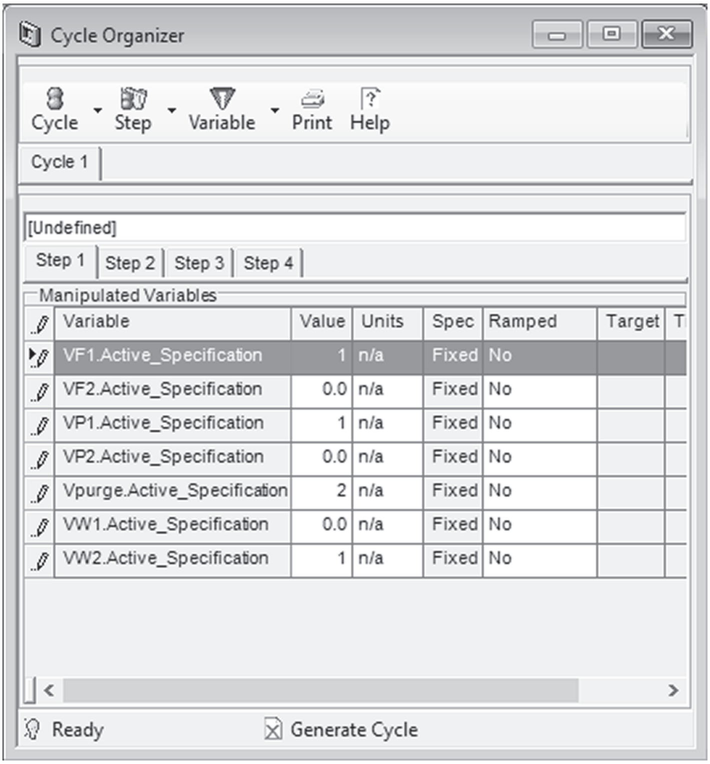
Step 30: Adding steps to the Cycle Organizer

To add more steps, use the step button and select “Add/Insert Step” (Figure 1.57).



Quick find/filter: VF.Active_Specification

Figure 1.55 Adding manipulated variables.



[Undefined]

Manipulated Variables

Variable	Value	Units	Spec	Ramped	Target	T
VF1.Active_Specification	1	n/a	Fixed	No		
VF2.Active_Specification	0.0	n/a	Fixed	No		
VP1.Active_Specification	1	n/a	Fixed	No		
VP2.Active_Specification	0.0	n/a	Fixed	No		
Vpurge.Active_Specification	2	n/a	Fixed	No		
VW1.Active_Specification	0.0	n/a	Fixed	No		
VW2.Active_Specification	1	n/a	Fixed	No		

Figure 1.56 Variables manipulated during step 1(adsorption bed 1, purge bed 2).

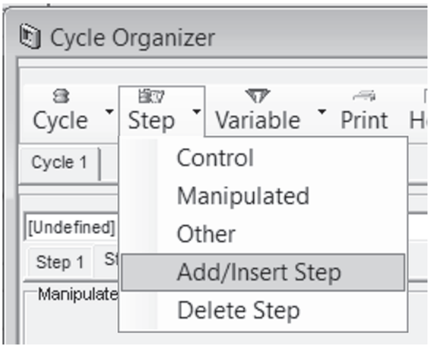


Figure 1.57 Adding steps to the cycle.

Add three additional steps for the total of four steps. Make sure to copy the manipulated variables to save yourself some work.

In this pressurization step, we would like to end the step as soon as the bed pressure reaches some fraction of the maximum pressure (8.5 bar). To do this, we can create an event that will trigger the step change once the void pressure at the top of the bed reaches 8.4 bar. To find the Aspen variable that represents tank pressure, we will use the variable finder. To open the variable finder, press ctrl+f while on the flowsheet, or use the tools menu and select "Variable Find…" as shown in Figure 1.58.

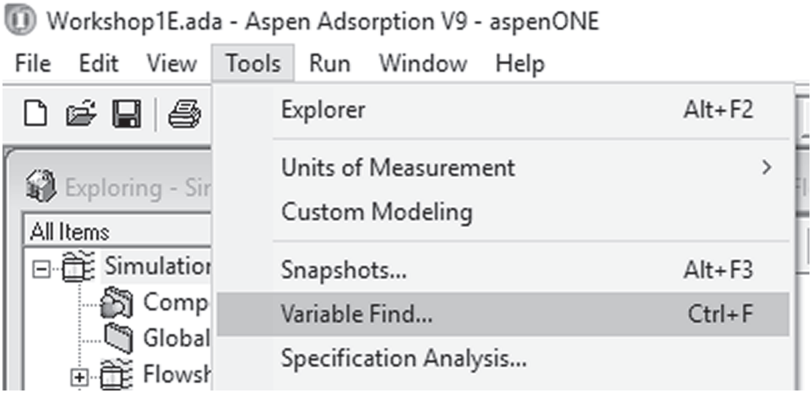


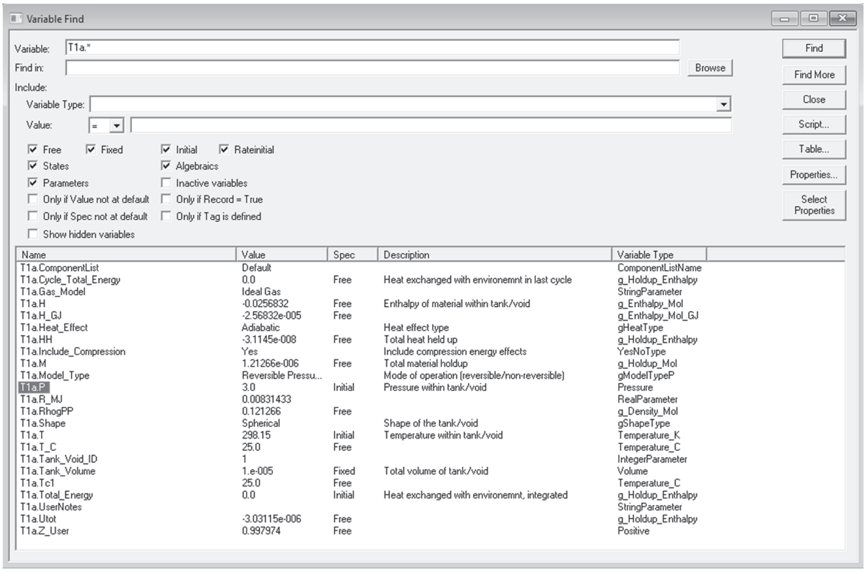
Figure 1.58 Opening the variable finder.

Once the finder is open, search for variable T1a.* as shown in Figure 1.59.

As you can see, the variable representing the tank pressure is called T1a.P, so we can now create an event to control the step time.

We make the second step to be controlled by an event, as shown in Figure 1.60. Aspen will warn you that the expression you enter will not be checked for correctness, so be very careful to enter the equations correctly. This expression indicates that step 2 will run until bed 2 has been pressurized to a pressure greater than 8.4 bar, and bed 1 has been depressurized to less than 1.1 bar.

For step 2, we choose the manipulated variables listed in Figure 1.61.



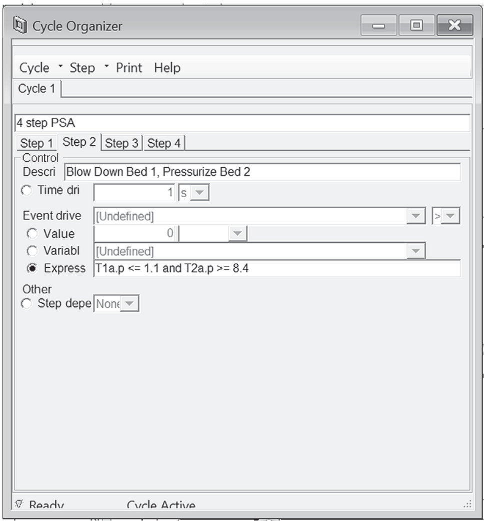
Variable: T1a.*
Find in:
Include:
Variable Type:
Value: =

☑ Free ☑ Fixed ☑ Initial ☑ Rateinitial
☑ States ☑ Algebraics
☑ Parameters ☐ Inactive variables
☐ Only if Value not at default ☐ Only if Record = True
☐ Only if Spec not at default ☐ Only if Tag is defined
☐ Show hidden variables

Name	Value	Spec	Description	Variable Type
T1a.ComponentList	Default			ComponentListName
T1a.Cycle_Total_Energy	0.0	Free	Heat exchanged with environemnt in last cycle	g_Holdup_Enthalpy
T1a.Gas_Model	Ideal Gas			StringParameter
T1a.H	-0.0256832	Free	Enthalpy of material within tank/void	g_Enthalpy_Mol
T1a.H_GJ	-2.56832e-005	Free		g_Enthalpy_Mol_GJ
T1a.Heat_Effect	Adiabatic		Heat effect type	gHeatType
T1a.HH	-3.1145e-008	Free	Total heat held up	g_Holdup_Enthalpy
T1a.Include_Compression	Yes		Include compression energy effects	YesNoType
T1a.M	1.21266e-006	Free	Total material holdup	g_Holdup_Mol
T1a.Model_Type	Reversible Pressu...		Mode of operation (reversible/non-reversible)	gModelTypeP
T1a.P	3.0	Initial	Pressure within tank/void	Pressure
T1a.R_MJ	0.00831433			RealParameter
T1a.RhogPP	0.121266	Free		g_Density_Mol
T1a.Shape	Spherical		Shape of the tank/void	gShapeType
T1a.T	298.15	Initial	Temperature within tank/void	Temperature_K
T1a.T_C	25.0	Free		Temperature_C
T1a.Tank_Void_ID	1			IntegerParameter
T1a.Tank_Volume	1.e-005	Fixed	Total volume of tank/void	Volume
T1a.Tc1	25.0	Free		Temperature_C
T1a.Total_Energy	0.0	Initial	Heat exchanged with environemnt, integrated	g_Holdup_Enthalpy
T1a.UserNotes				StringParameter
T1a.Utot	-3.03115e-006	Free		g_Holdup_Enthalpy
T1a.Z_User	0.997974	Free		Positive

Figure 1.59 The variable finder.

Figure 1.60 The event-controlled step 2 (blowdown bed 1, pressurize bed 2).



4 step PSA

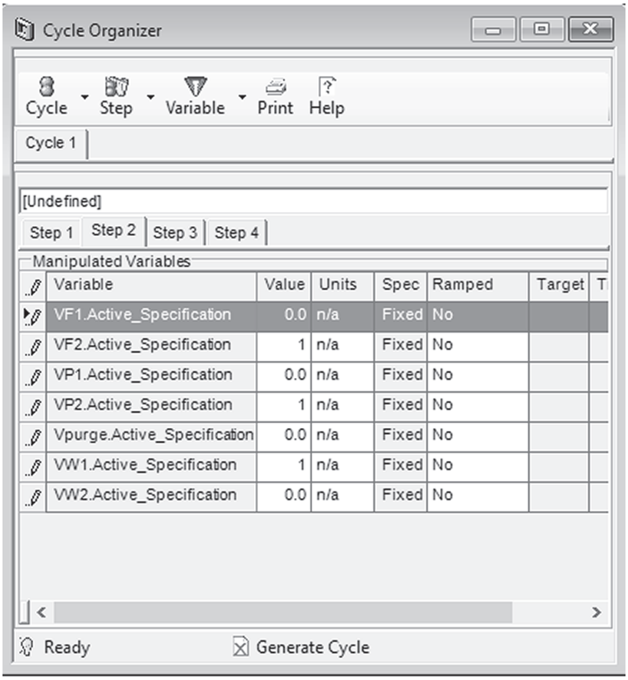
Descri: Blow Down Bed 1, Pressurize Bed 2
○ Time dri: 1 s
Event drive: [Undefined] >
○ Value: 0
○ Variabl: [Undefined]
● Express: T1a.p <= 1.1 and T2a.p >= 8.4
○ Step depe: None

Step 3 is a mirror of step 1, which runs for 40 s (Figure 1.62).

Since we only need to change two valves, we can remove all the other variables, if we wish (Figure 1.63).

And step 4 is a mirror of step 2 (Figure 1.64).

The manipulated variables are also reversed (Figure 1.65).



[Undefined]

Variable	Value	Units	Spec	Ramped	Target	T
VF1.Active_Specification	0.0	n/a	Fixed	No		
VF2.Active_Specification	1	n/a	Fixed	No		
VP1.Active_Specification	0.0	n/a	Fixed	No		
VP2.Active_Specification	1	n/a	Fixed	No		
Vpurge.Active_Specification	0.0	n/a	Fixed	No		
VW1.Active_Specification	1	n/a	Fixed	No		
VW2.Active_Specification	0.0	n/a	Fixed	No		

Figure 1.61 Manipulated variables in step 2 (blowdown bed 1, pressurize bed 2).

Step 31: Setting the Cycle Options

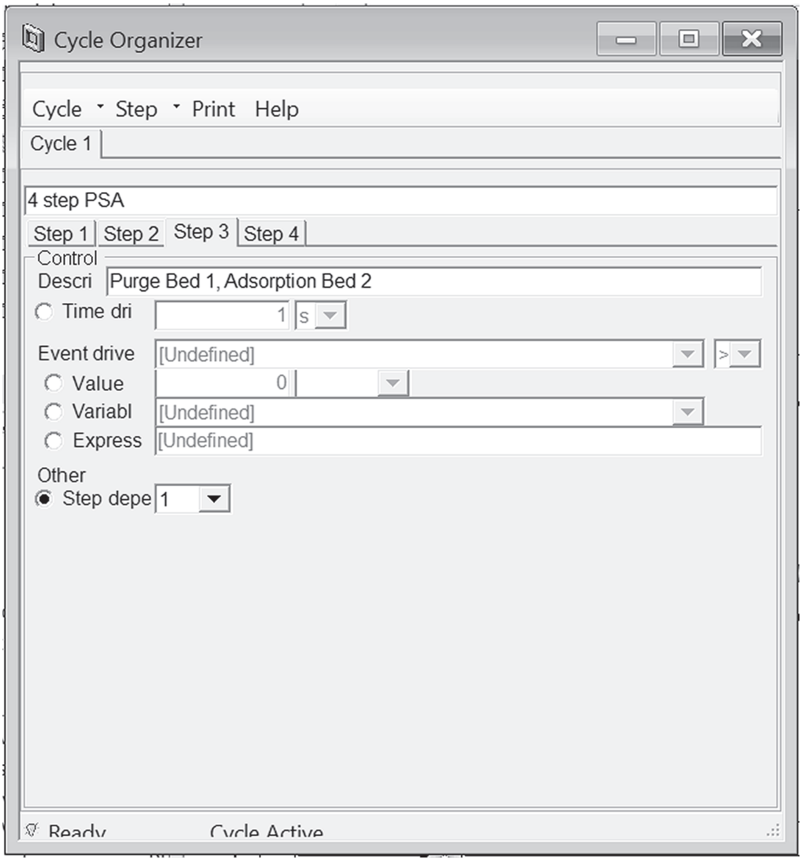
Now that we have defined all our steps, we will look at the overall cycle options. The only one we are really interested in is the maximum number of steps. This will impose an endpoint on our simulation. To set this value, click on the "Cycle" button and enter 10 in the Maximum cycles box (Figure 1.66)

Step 32: Finalizing the Cycle Organizer

After entering the cycle data, it is important to "generate" and "activate" the Cycle Organizer. To do this, use the "Cycle" button and press the "Generate Task" menu item (Figure 1.67).

This step reveals what the Cycle Organizer really is: a code generator. The Cycle Organizer is simply a user interface to make it easier to write tasks that will periodically make changes to the flowsheet. It is possible to skip the Cycle Organizer altogether and create your own task, which will perform the exact functions as the task generated by the Cycle Organizer.

After generating this task, navigate to the Flowsheet and look for the "Cycle1" task (Figure 1.68).



4 step PSA

Descri: Purge Bed 1, Adsorption Bed 2

○ Time dri: 1 s

Event drive: [Undefined] >

○ Value: 0

○ Variabl: [Undefined]

○ Express: [Undefined]

● Step depe: 1

Ready   Cycle Active

Figure 1.62 Step 3 (purge bed 1, adsorption bed 2).

1.7.5 Running an Aspen Simulation

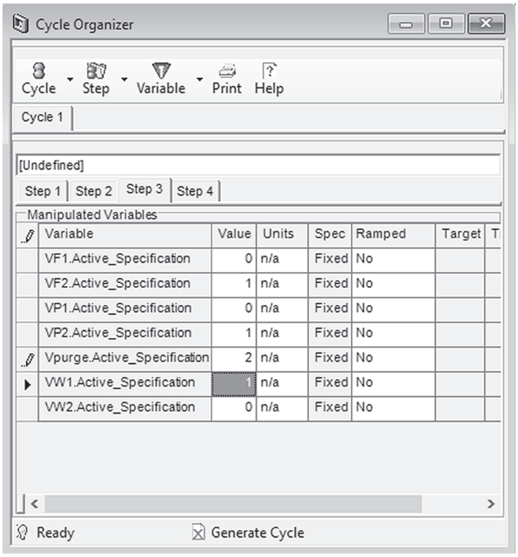
Before you run the simulation, save the simulation as **Workshop1E.ada**.

Step 33: Run the simulation in Dynamic mode using the "play" button

To begin the simulation, ensure that the dropdown menu says "Dynamic," then press the solid blue "play" button (Figure 1.69). This will perform an initialization run followed by a dynamic simulation.

1.7.6 Viewing and Exporting Simulation Results

Once the simulation has completed, we want to view some results.

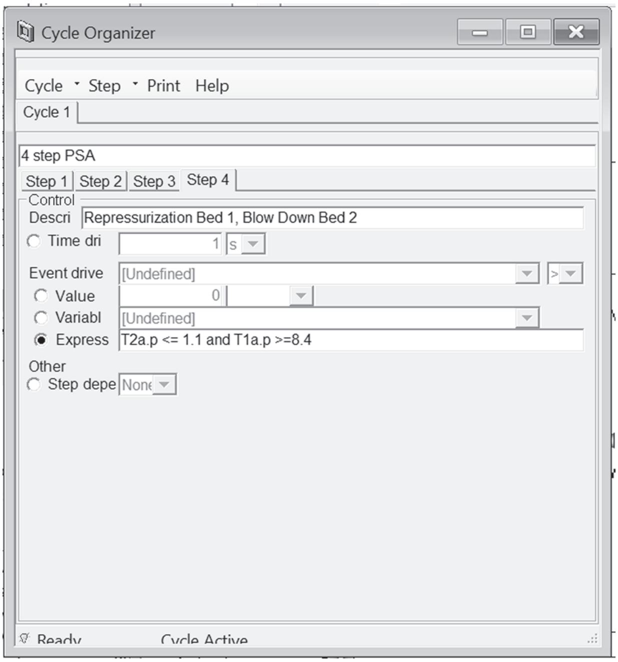


[Undefined]

Manipulated Variables

Variable	Value	Units	Spec	Ramped	Target	T
VF1.Active_Specification	0	n/a	Fixed	No		
VF2.Active_Specification	1	n/a	Fixed	No		
VP1.Active_Specification	0	n/a	Fixed	No		
VP2.Active_Specification	1	n/a	Fixed	No		
Vpurge.Active_Specification	2	n/a	Fixed	No		
VW1.Active_Specification	1	n/a	Fixed	No		
VW2.Active_Specification	0	n/a	Fixed	No		

Figure 1.63 Manipulated variables in step 3 (purge bed 1, adsorption bed 2).



4 step PSA

Descri: Repressurization Bed 1, Blow Down Bed 2

○ Time dri: 1 s

Event drive: [Undefined] >

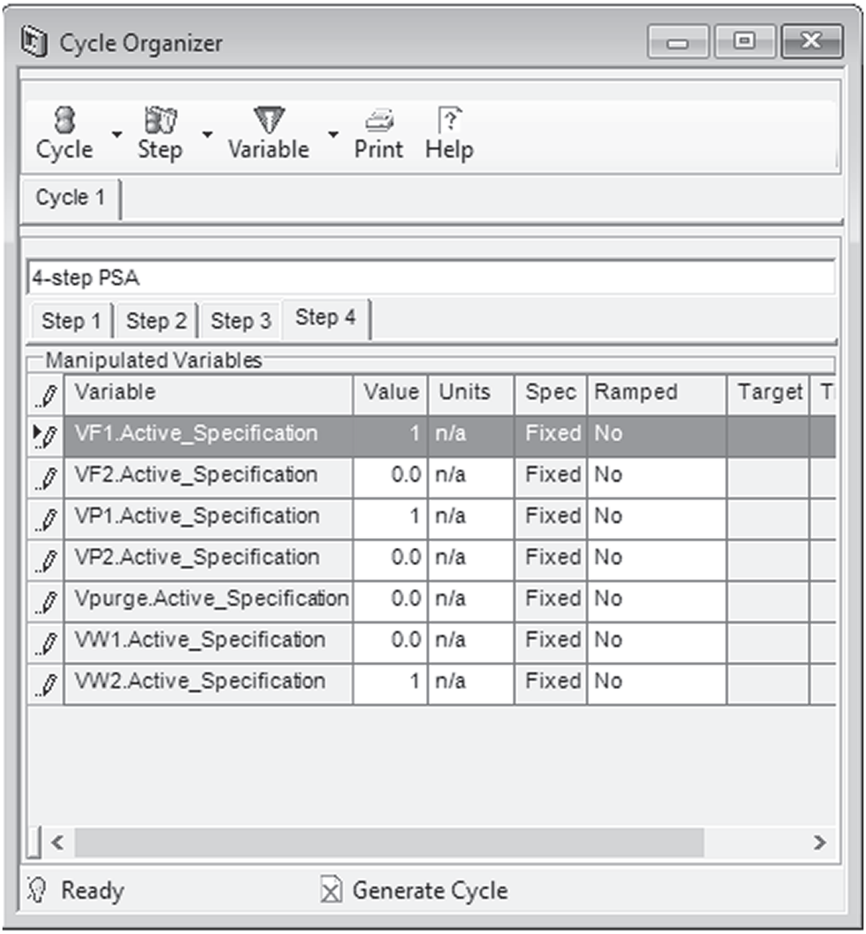
○ Value: 0

○ Variabl: [Undefined]

● Express: T2a.p <= 1.1 and T1a.p >=8.4

○ Step depe: None

Figure 1.64 The event driving step 4 (pressurize bed 1, blowdown bed 2).



4-step PSA

Variable	Value	Units	Spec	Ramped	Target	T
VF1.Active_Specification	1	n/a	Fixed	No		
VF2.Active_Specification	0.0	n/a	Fixed	No		
VP1.Active_Specification	1	n/a	Fixed	No		
VP2.Active_Specification	0.0	n/a	Fixed	No		
Vpurge.Active_Specification	0.0	n/a	Fixed	No		
VW1.Active_Specification	0.0	n/a	Fixed	No		
VW2.Active_Specification	1	n/a	Fixed	No		

Figure 1.65 Step 4 manipulated variables (pressurize bed 1, blowdown bed 2).

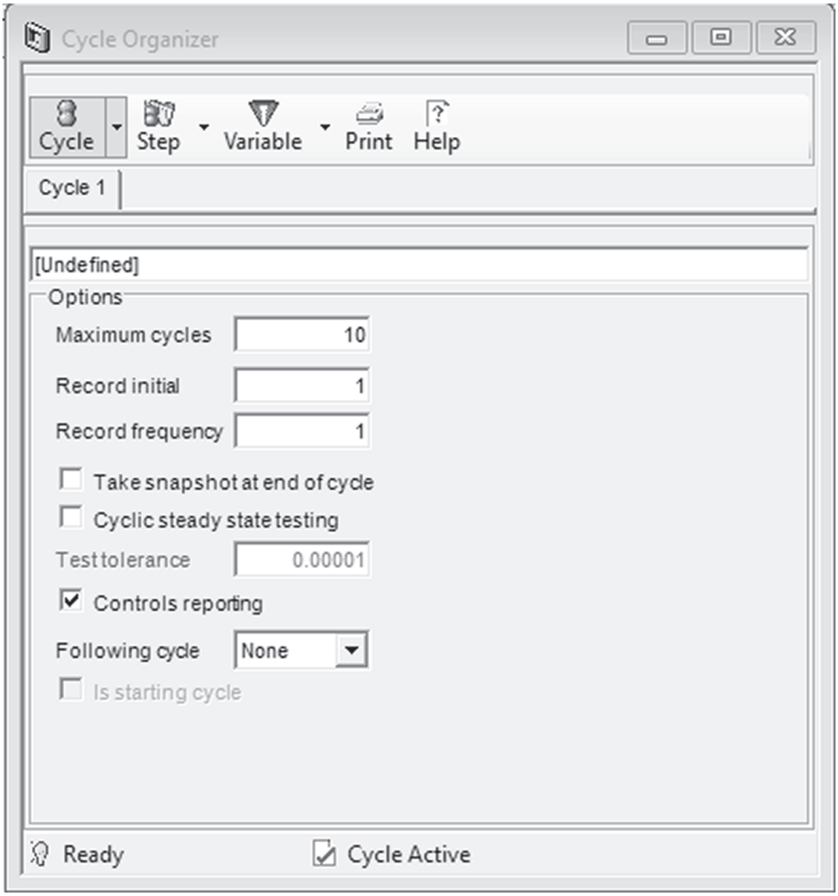
Step 34: Add a plot of the oxygen product composition

To add a plot of the oxygen composition over time, open the flowsheet in the Explorer and click on the "Add Form" (Figure 1.70).

Once the form is created, drag the variables from the P1 block's "Results" table into the plot (Figure 1.71).

Right-click on the plot and "Zoom Full" in order to see the full time history of the oxygen product composition (Figure 1.72).

Step 35: Create an axial composition plot (Figure 1.73)



[Undefined]

Options

Maximum cycles: 10

Record initial: 1

Record frequency: 1

☐ Take snapshot at end of cycle

☐ Cyclic steady state testing

Test tolerance: 0.00001

☑ Controls reporting

Following cycle: None

☐ Is starting cycle

Figure 1.66 The Cycle Options.

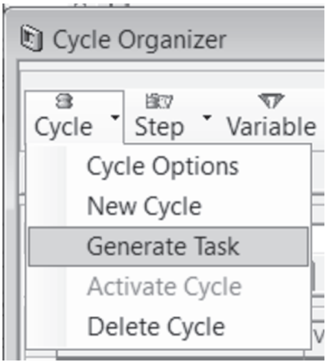


Figure 1.67 Generating the Cycle Organizer task.

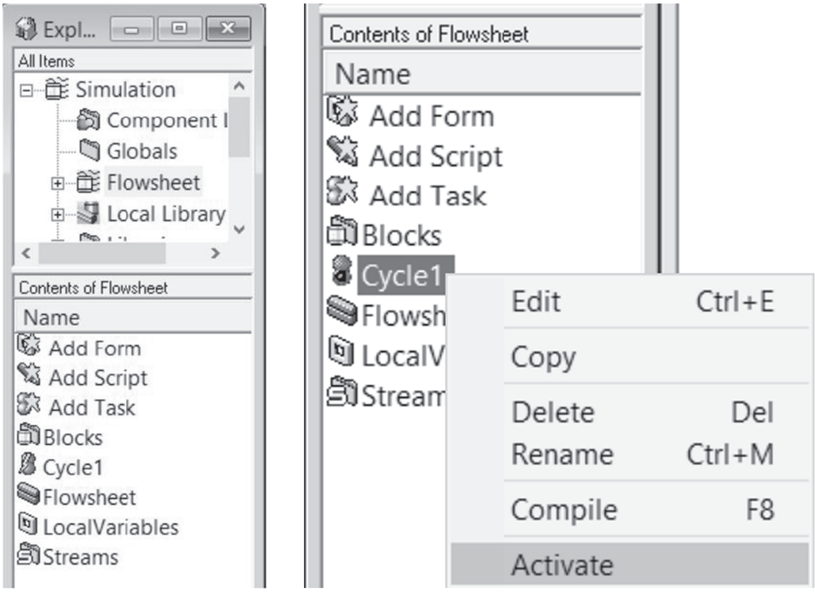
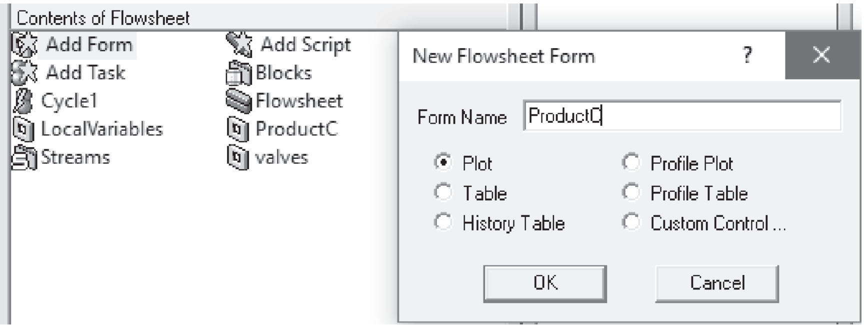


Figure 1.68 If the cycle task does not have a lightning bolt icon, use the right mouse button to activate it.

Figure 1.69 The run control buttons.


Dynamic



Form Name: ProductC

● Plot ○ Profile Plot
○ Table ○ Profile Table
○ History Table ○ Custom Control ...

Figure 1.70 Adding a product composition plot.

Step 36: Profile Editor for the Axial_Composition profile plot

Position: B1. Layer(*).Axial_Distance(*)

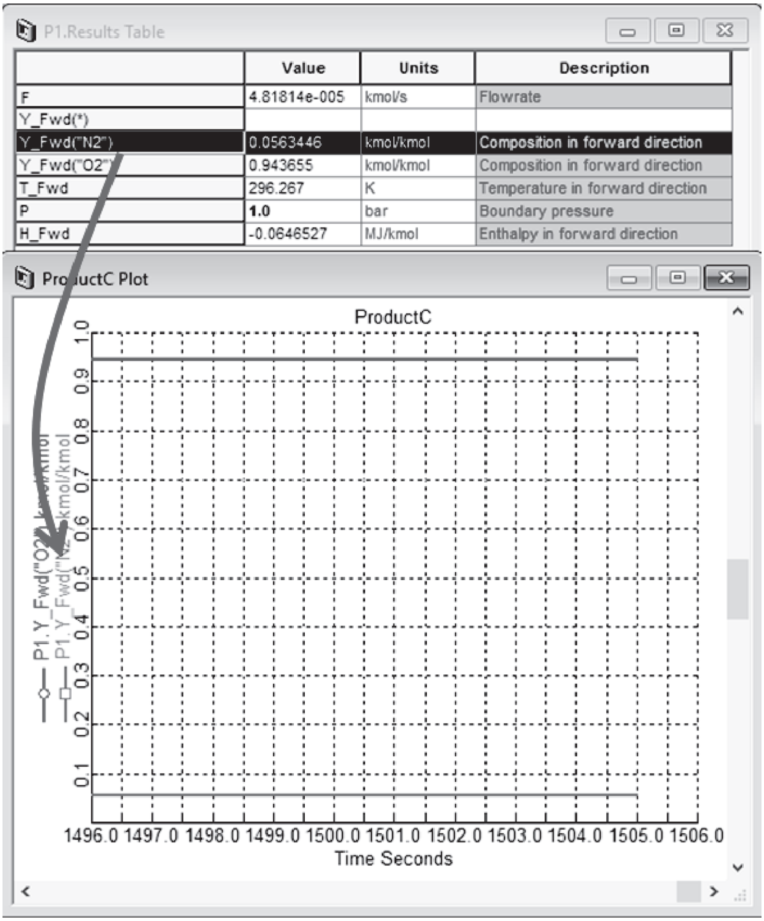
N2 Partial Pressure: B1. Layer(*).Y (*,“N2”)

O2 Partial Pressure: B1. Layer(*).Y (*,“O2”)

Since our column has one layer, you could use Layer(1), instead of Layer(*); however, it is good practice to always use Layer(*) so that you always view the full column profile (Figure 1.74).

Step 37: Conclusion

Save the file as **Workshop1F.ada.**



P1.Results Table

	Value	Units	Description
F	4.81814e-005	kmol/s	Flowrate
Y_Fwd(*)			
Y_Fwd("N2")	0.0563446	kmol/kmol	Composition in forward direction
Y_Fwd("O2")	0.943655	kmol/kmol	Composition in forward direction
T_Fwd	296.267	K	Temperature in forward direction
P	**1.0**	bar	Boundary pressure
H_Fwd	-0.0646527	MJ/kmol	Enthalpy in forward direction

Figure 1.71 Dragging variables into the plot.

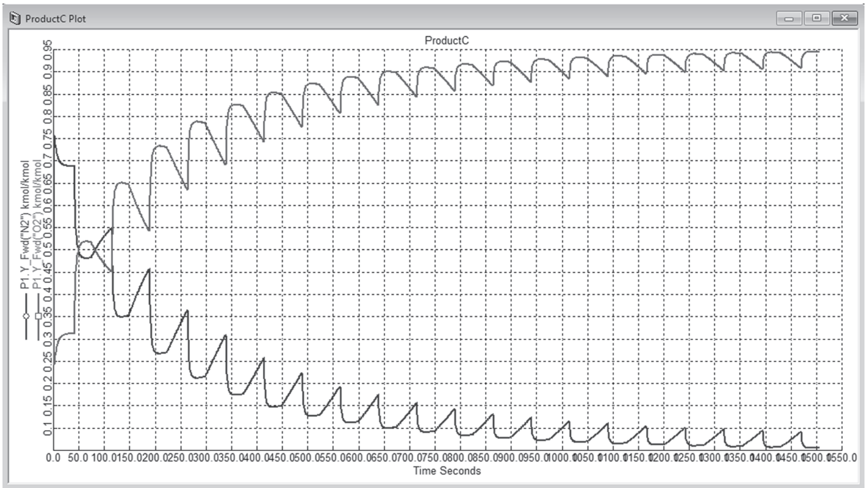
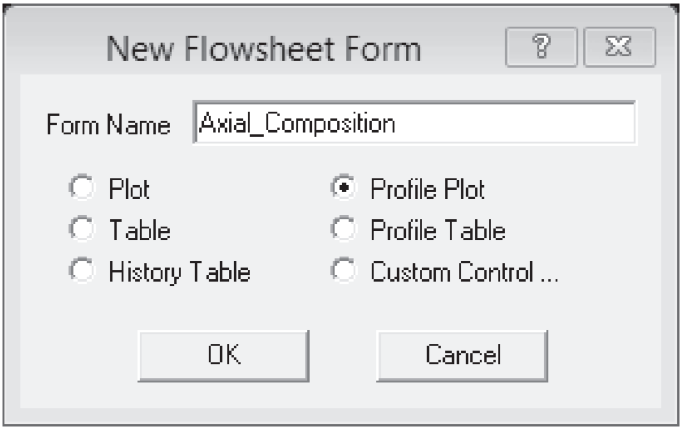


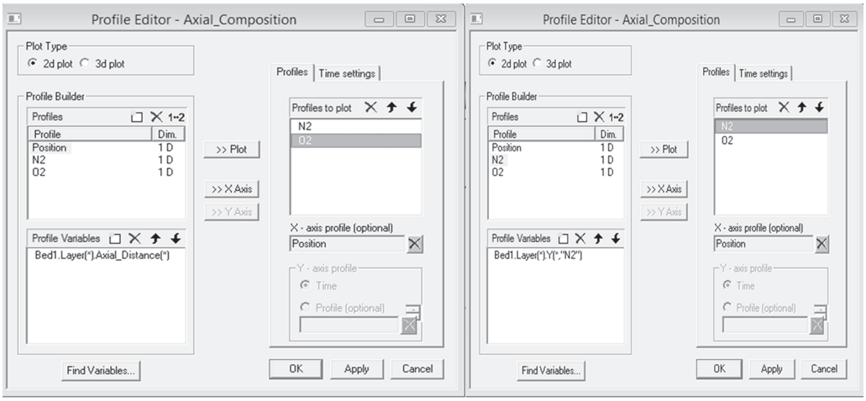
Figure 1.72 The composition plot in the light product stream (raffinate or "waste"stream or nitrogen-rich stream) over time in the PSA model.



Form Name: Axial_Composition

○ Plot
○ Table
○ History Table
● Profile Plot
○ Profile Table
○ Custom Control ...

Figure 1.73 The generation of a concentration profile within the column.



Plot Type: ● 2d plot ○ 3d plot

Profile	Dim.
Position	1 D
N2	1 D
02	1 D

Profile Variables: Bed1.Layer(*).Axial_Distance(*)

Profiles to plot: N2, 02

X - axis profile (optional): Position

Y - axis profile: ● Time ○ Profile (optional)

Plot Type: ● 2d plot ○ 3d plot

Profile	Dim.
Position	1 D
N2	1 D
02	1 D

Profile Variables: Bed1.Layer(*).Y(*,"N2")

Profiles to plot: N2, 02

X - axis profile (optional): Position

Y - axis profile: ● Time ○ Profile (optional)

Figure 1.74 The axial composition profile plot in the PSA model.

In this workshop, we developed a two-bed PSA model for a binary separation of an O2/N2 mixture. Figure 1.75 shows how the composition of the gas phase changes during adsorption. In practice, you may consider also creating graphs of the axial pressure, or tank pressures over time.

1.8 PSA Workshop: Hydrogen Separation in Aspen Adsorption

Hydrogen isolation is an important component of several refinery processes, such as cleaning coke oven gas. In most cases, hydrogen is present alongside combustion products (CO/CO_2) and/or light hydrocarbons like methane. In this workshop, we will simulate a variety of hydrogen separation processes, and learn about Aspen Adsorption as we proceed.

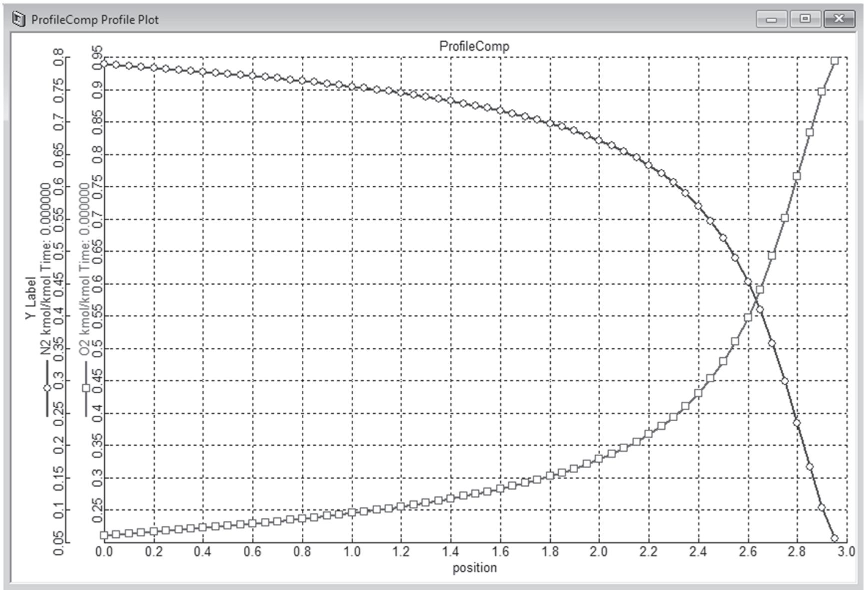


Figure 1.75 The resulting bed concentration plot in the PSA model.

1.8.1 Define the Components and Property Model

Step 1: Open and Configure Aspen

Using the file menu shown in Figure 1.76 create a new, blank flowsheet.

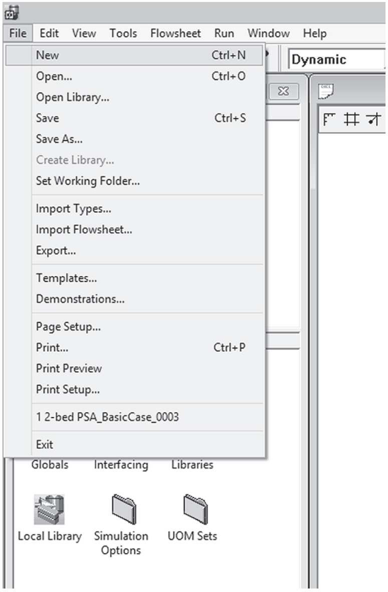
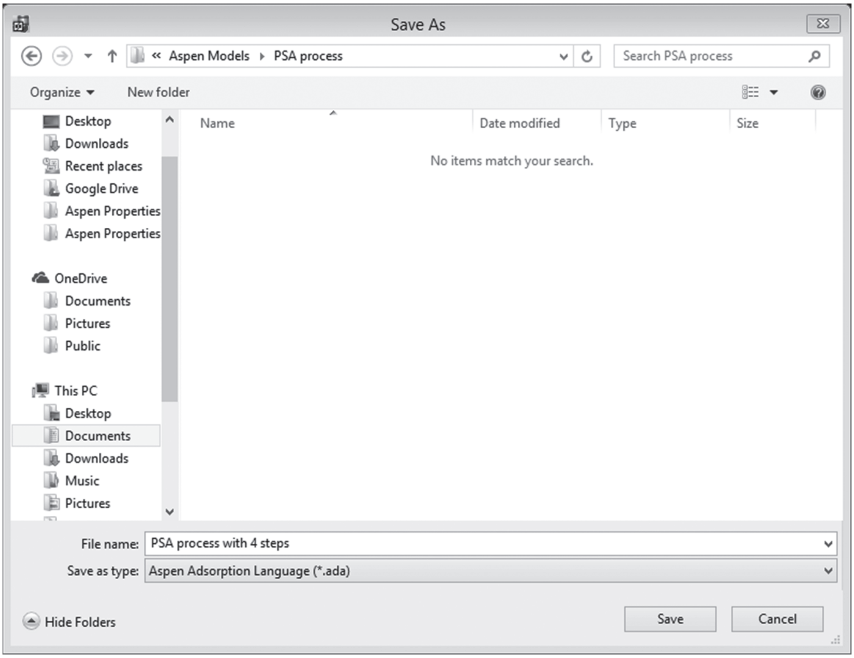


Figure 1.76 A new file in Aspen Adsorption.

Step 2: It is important to save Aspen simulations frequently

Save the file as `H2Workshop1.ada`. We will be saving the file after each major change; it is good practice to remember to save the file under a new name each time. That way, if a change you have made results in incorrect flowsheet behavior at a later time, you will not have to completely start over (Figure 1.77).



No items match your search.

File name: PSA process with 4 steps

Save as type: Aspen Adsorption Language (*.ada)

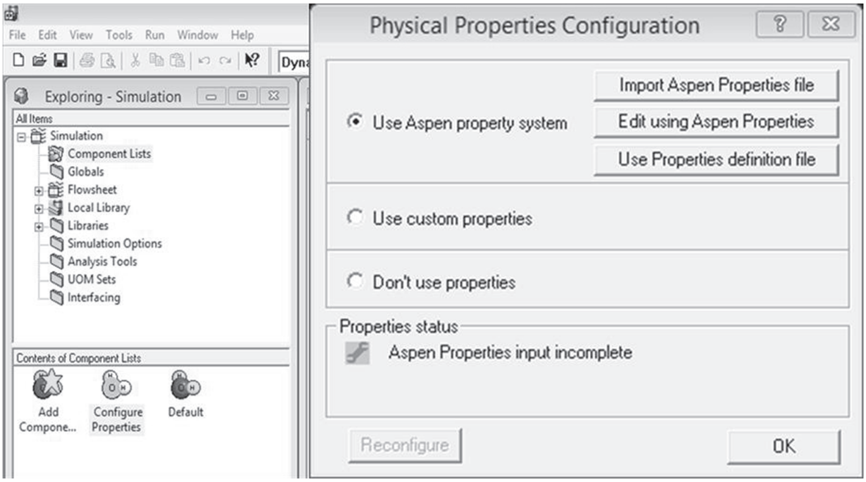
Figure 1.77 The PSA process with four steps for air separation.

Step 3: Add chemical components to Aspen's component list

The first thing to do in a simulation is to tell Aspen which chemicals will be present in our simulation. As we have seen in the previous workshop, Aspen Adsorption will automatically prompt the user to supply components as soon as a new flowsheet has been created. There are two methods for adding chemical components into the model: component list and component set, as discussed in Section 1.7.1.

When we use Aspen Properties for physical properties, we can invoke the Aspen Properties user interface directly if we have it installed. In order to edit physical property options, we need to follow the steps in Figure 1.78:

1) In the Simulation Explorer, click "**Component Lists"**.
2) In the **Explorer of the Component Lists folder**, double-click the "**Configure Properties" node**.
3) In the **Physical Properties Configuration** dialog box, choose "Use Aspen property system" option, and then click "**Edit using Aspen Properties" button to launch the user interface**.
4) **Step 4: Add component names in Aspen Properties**



● Use Aspen property system

○ Use custom properties

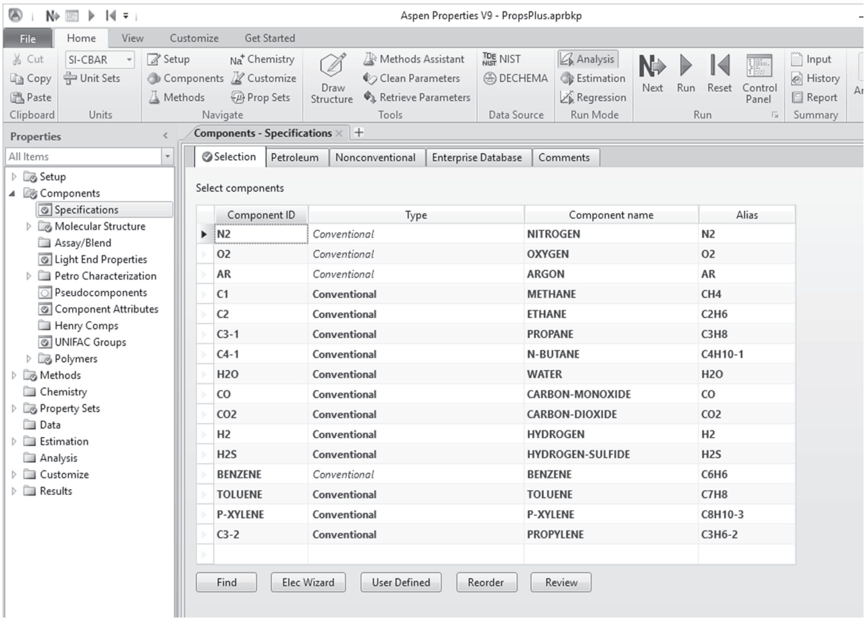
○ Don't use properties

Properties status

Aspen Properties input incomplete

Figure 1.78 The physical properties configuration pane.

After we click "**Edit using Aspen Properties**" in the **Physical Properties Configuration** pane, it automatically opens the Aspen Properties for us to add component names and edit their physical and chemical properties. Figure 1.79 shows all the compounds that might be relevant for our hydrogen separation. To enter these yourself, you can type the names into the Component ID column. For most common chemicals, Aspen will know right away what chemical you have entered. For less common components, you'll need to use the "Find"

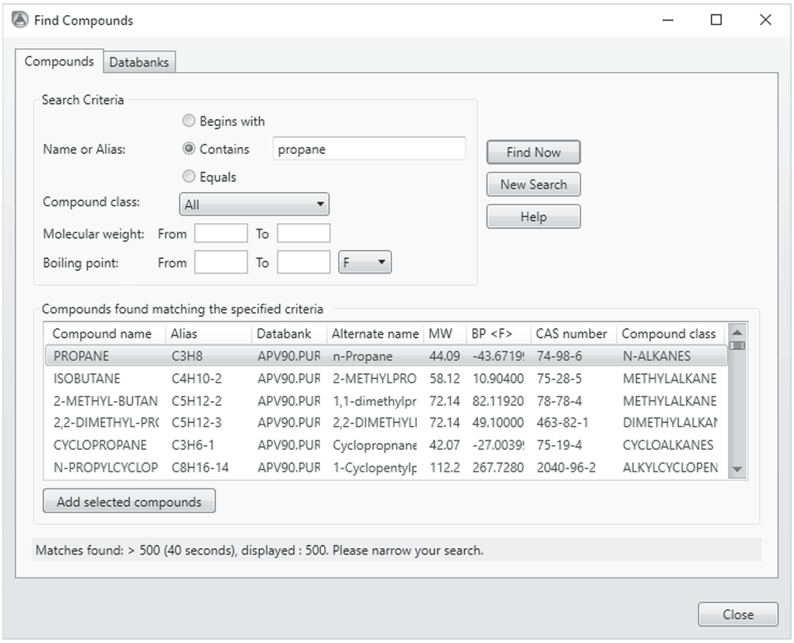


Select components

Component ID	Type	Component name	Alias
N2	Conventional	NITROGEN	N2
O2	Conventional	OXYGEN	O2
AR	Conventional	ARGON	AR
C1	Conventional	METHANE	CH4
C2	Conventional	ETHANE	C2H6
C3-1	Conventional	PROPANE	C3H8
C4-1	Conventional	N-BUTANE	C4H10-1
H2O	Conventional	WATER	H2O
CO	Conventional	CARBON-MONOXIDE	CO
CO2	Conventional	CARBON-DIOXIDE	CO2
H2	Conventional	HYDROGEN	H2
H2S	Conventional	HYDROGEN-SULFIDE	H2S
BENZENE	Conventional	BENZENE	C6H6
TOLUENE	Conventional	TOLUENE	C7H8
P-XYLENE	Conventional	P-XYLENE	C8H10-3
C3-2	Conventional	PROPYLENE	C3H6-2

Figure 1.79 The Aspen Properties interface.

button to search. Figure 1.80 shows how to use the “Find” tool to get components from Aspen’s databanks. Once you select propane in the list of matches, click on the “Add selected compounds” button to add it to the list. You may then search for more compounds if you wish. Use the “Find” tool to add all the components in Figure 1.79.



Name or Alias: ● Contains propane

Compound class: All

Boiling point: F

Compounds found matching the specified criteria

Compound name	Alias	Databank	Alternate name	MW	BP <F>	CAS number	Compound class
PROPANE	C3H8	APV90.PUR	n-Propane	44.09	-43.6719	74-98-6	N-ALKANES
ISOBUTANE	C4H10-2	APV90.PUR	2-METHYLPRO	58.12	10.90400	75-28-5	METHYLALKANE
2-METHYL-BUTAN	C5H12-2	APV90.PUR	1,1-dimethylpr	72.14	82.11920	78-78-4	METHYLALKANE
2,2-DIMETHYL-PR	C5H12-3	APV90.PUR	2,2-DIMETHYLI	72.14	49.10000	463-82-1	DIMETHYLALKA
CYCLOPROPANE	C3H6-1	APV90.PUR	Cyclopropnane	42.07	-27.0039	75-19-4	CYCLOALKANES
N-PROPYLCYCLOP	C8H16-14	APV90.PUR	1-Cyclopentylp	112.2	267.7280	2040-96-2	ALKYLCYCLOPEN

Matches found: > 500 (40 seconds), displayed : 500. Please narrow your search.

Figure 1.80 Searching the Aspen Property Databanks for Propane.

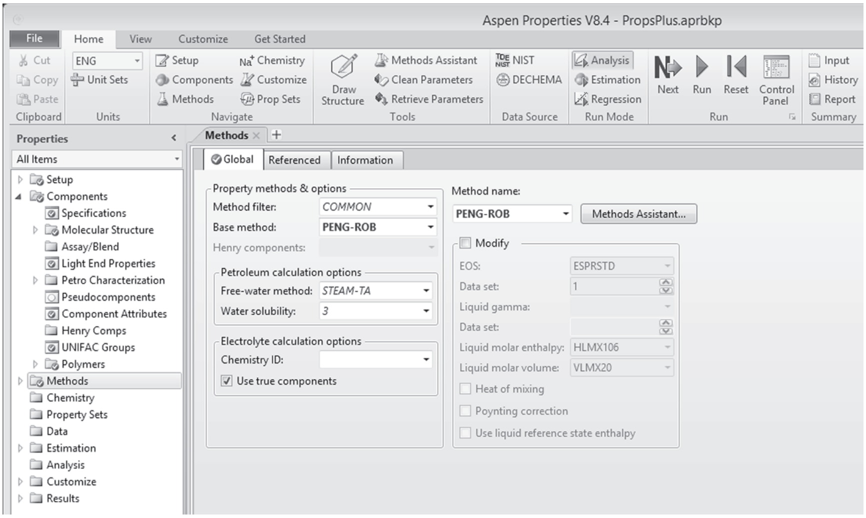
Step 5: Select the appropriate property method

In this step, we specify the methods that calculate the thermodynamic properties for our simulation. The “Base method” and “Method name” drop-down menus are essentially redundant, although the “Base method” option allows you to filter the long list of methods by application. For example, PENG-ROB shows up when the method-filter is set to COMMON; however, specialized variants of the Peng–Robinson method (such as PR-BM) do not show up unless the filter is set to “GasProc.”

To edit components’ physical properties in Aspen Properties, we follow the steps in Figure 1.81:

1) In the “All Items” pane of the “Properties”, click “Specification” in the “Methods” folder.
2) Select “PENG-ROB” as the base method.
3) In the pane of “Home”, click “Run” button.
4) Save the file until the run is completed in the Control Panel, as shown in Figure 1.82.

Once you have completed these steps, close the Aspen properties window and choose “yes” when asked to save the properties file.



Property methods & options

Method filter: COMMON

Base method: PENG-ROB

Henry components:

Petroleum calculation options

Free-water method: STEAM-TA

Water solubility: 3

Electrolyte calculation options

Chemistry ID:

☑ Use true components

Method name: PENG-ROB

☐ Modify

EOS: ESPRSTD

Data set: 1

Liquid gamma:

Data set:

Liquid molar enthalpy: HLMX106

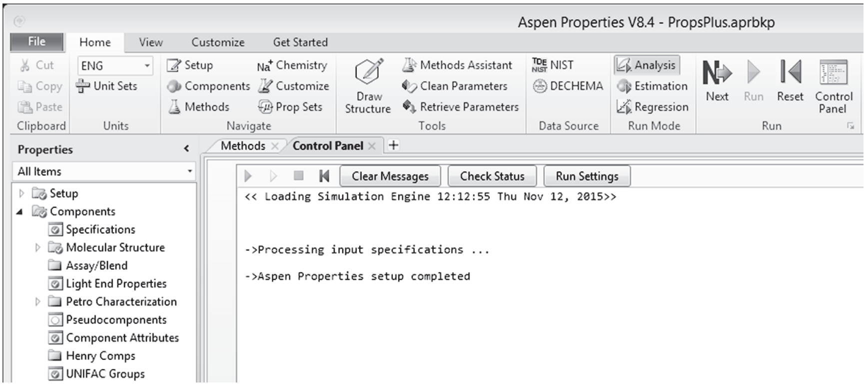
Liquid molar volume: VLMX20

☐ Heat of mixing

☐ Poynting correction

☐ Use liquid reference state enthalpy

Figure 1.81 The specification of the components in Aspen Properties.



```
<< Loading Simulation Engine 12:12:55 Thu Nov 12, 2015>>


->Processing input specifications ...

->Aspen Properties setup completed
```

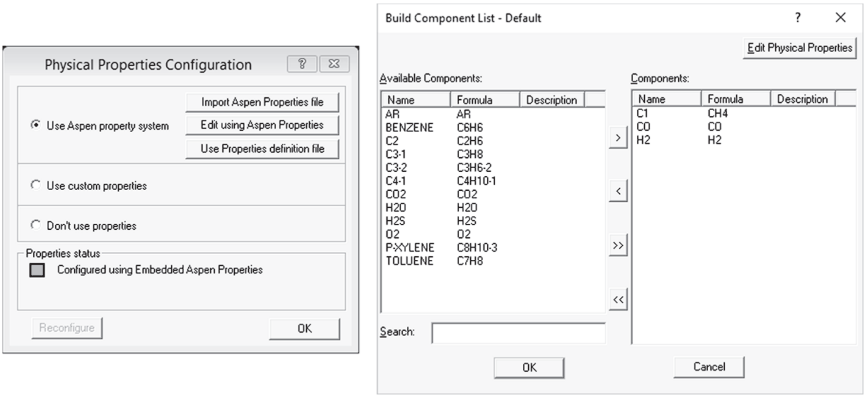
Figure 1.82 The completion in control panel in Aspen Properties.

Step 6: Tell Aspen Adsorption to use the Aspen Properties file we created

Once we have done the import in Aspen Properties, the Aspen Properties input file, **PropsPlus.aprbkp**, will be included in the file when we save the simulation file. Then go back to the Physical Properties Configuration panel, and the Properties status should show a green square next to "Configured using Embedded Aspen Properties" (Figure 1.83).

Click ok on the properties configuration window to be presented with the resulting component list. In order to make the components actually available in the flowsheet, they need to be moved into the right-hand column. To do this, click on the component you want, then press the right arrow, >. Add H2, CO and methane to the right-hand column, then click "ok".

Once you have completed this step, save the file as `H2Workshop2.ada`.



Physical Properties Configuration

● Use Aspen property system

○ Use custom properties

○ Don't use properties

Properties status

☐ Configured using Embedded Aspen Properties

Build Component List - Default

Available Components:

Name	Formula	Description
AR	AR	
BENZENE	C6H6	
C2	C2H6	
C3-1	C3H8	
C3-2	C3H6-2	
C4-1	C4H10-1	
CO2	CO2	
H2O	H2O	
H2S	H2S	
O2	O2	
P-XYLENE	C8H10-3	
TOLUENE	C7H8	

Components:

Name	Formula	Description
C1	CH4	
CO	CO	
H2	H2	

Figure 1.83 The completion of the physical properties configuration.

1.8.2 Creating a Flowsheet in Aspen Adsorption

Now that we have successfully added several chemical components to Aspen, it is time to begin specifying the layout of our process. Aspen provides a large number of "Models" that are contained in "Model Libraries." These models roughly correspond to common unit operations, but take care not to confuse these models with actual physical process equipment. For example, a physical packed bed might be represented as a combination of three separate "Models" in Aspen. Specifically, two gas_tank_void models can describe the empty voids at the top and bottom of the packed bed, and also serve as **pressure setters** to fix the pressure drop across the adsorption bed; while the gas-bed model will describe the region of the packed bed that actually performs the separation. In the same way, a single Aspen "Model" might represent several physical pieces of equipment. For example, a single gas_interaction model can be used to represent several identical packed beds.

Step 7: Ensure that the model libraries are visible

To begin, ensure that the model libraries are visible by clicking on the "Model Libraries" button in the "View" menu (Figure 1.84).

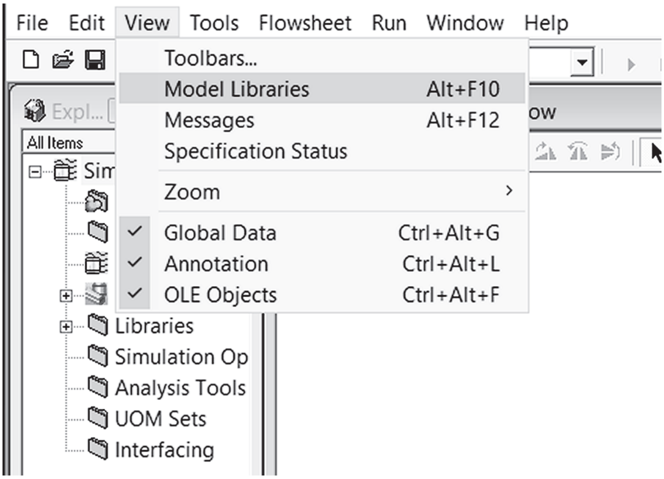


Figure 1.84 Display of the model libraries.

Once the button has been clicked, the area shown in Figure 1.85 will be visible on the main window. This area displays all the prebuilt models available in Aspen Adsorption, and are colloquially referred to as “blocks.” Each model or block roughly corresponds to a unit operation, such as a packed bed, tank or valve. However, some models have subtler roles, which we will cover as we get to them.

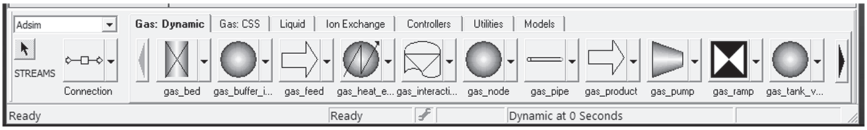


Figure 1.85 The model libraries.

Step 8: Place the first blocks on the flowsheet

To place these blocks on the flowsheet, first click on the block in the model library, then click on the flowsheet. You can add as many blocks of that type as you want by clicking multiple times. Click with the right mouse button to stop adding blocks. For our first step, we will add three blocks to the flowsheet, a gas_bed, a gas_feed, and a gas_product. Add them as shown in Figure 1.86. Note that you may want to rename the blocks; you can do this by clicking on a block, then pressing ctrl+m. This is especially useful here since there is no visual way to differentiate between the feed and product blocks.

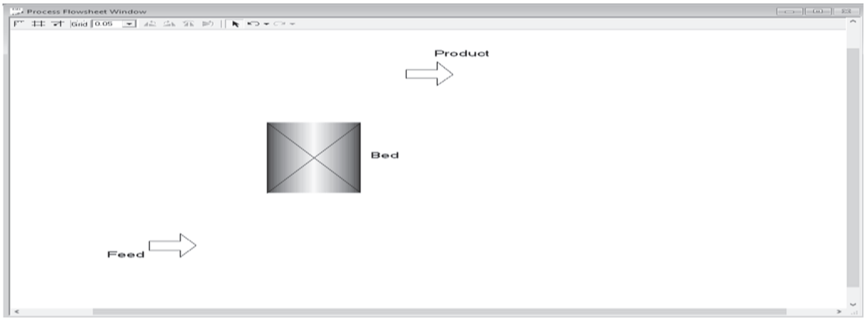


Figure 1.86 Placing the first blocks on the flowsheet.

Step 9: Connect the blocks using gas_material_connections

Similarly to placing models with different icons, use the small arrow by the “connection” icon to select gas_material_connection. Unlike with the models, the different connection types DO have different behaviors, and so it does matter which is selected. Once the connection icon has been selected, the blocks in the flowsheet will expose blue and red arrows, indicating points where they can be connected together. You can connect the blocks in any order by clicking on the arrow of one block, and an arrow of a second block. Blocks may accept more than one connection to the same point (for example, a gas_tank_void can accept many inlet and outlet streams simultaneously.) If you want to change the location of a connection for aesthetics, hold down the mouse button while clicking on the blue or red arrow, and drag it to the desired location before releasing. The connection options and arrows, are shown in Figure 1.87.

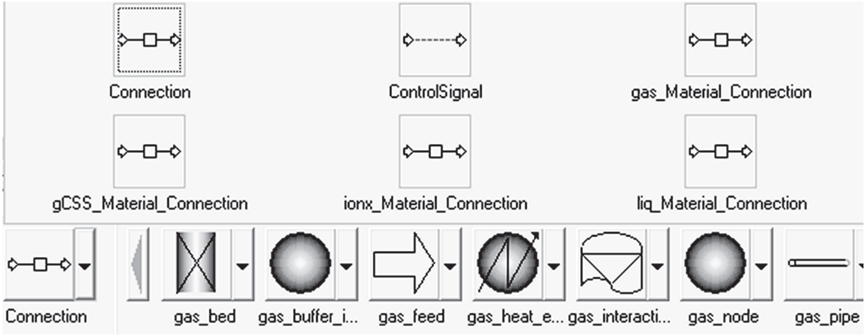
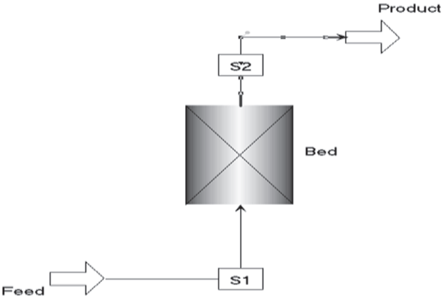


Figure 1.87 The methods for connecting blocks.

Connect the blocks as shown in Figure 1.88.

Figure 1.88 The connected blocks.



Save the resulting simulation as `H2Workshop3.ada`.

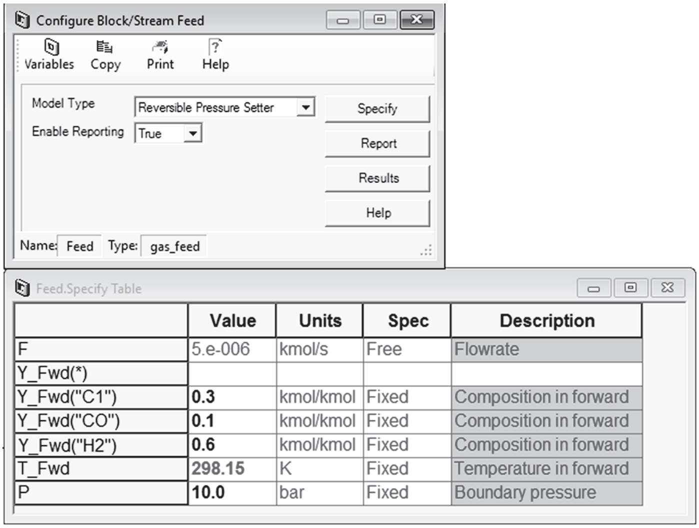
1.8.3 Run a Breakthrough Simulation

Step 10: Specify the feed block and the product block

What we have specified so far is clearly not a PSA process. All we have done is to create a model of a gas stream flowing through an adsorber bed. However, this is still a useful model. We can use this model to predict breakthrough curves. In order to do this, we need to first tell Aspen about the gas stream that will be flowing through the bed. Double-click on the “Feed” block to open the default form. This shows us some options for the feed block. For right now, all we want is to “Specify” the values using the “Specify” button (Figure 1.89). Note that the feed block also serves as a pressure setter to fix the inlet pressure of the adsorber bed.

Enter the values shown in Figure 1.89, then close the windows.

Specify the “Product” block in the same way. The Product block also sets the outlet pressure for the adsorber bed (Figure 1.90).



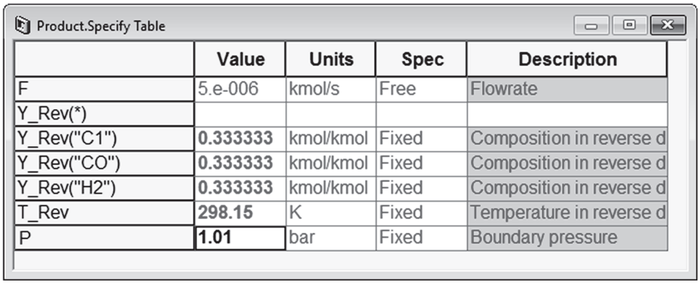
Model Type: Reversible Pressure Setter

Enable Reporting: True

Name: Feed Type: gas_feed

	Value	Units	Spec	Description
F	5.e-006	kmol/s	Free	Flowrate
Y_Fwd(*)				
Y_Fwd("C1")	0.3	kmol/kmol	Fixed	Composition in forward
Y_Fwd("CO")	0.1	kmol/kmol	Fixed	Composition in forward
Y_Fwd("H2")	0.6	kmol/kmol	Fixed	Composition in forward
T_Fwd	298.15	K	Fixed	Temperature in forward
P	10.0	bar	Fixed	Boundary pressure

Figure 1.89 Specifying the feed block.



	Value	Units	Spec	Description
F	5.e-006	kmol/s	Free	Flowrate
Y_Rev(*)				
Y_Rev("C1")	0.333333	kmol/kmol	Fixed	Composition in reverse d
Y_Rev("CO")	0.333333	kmol/kmol	Fixed	Composition in reverse d
Y_Rev("H2")	0.333333	kmol/kmol	Fixed	Composition in reverse d
T_Rev	298.15	K	Fixed	Temperature in reverse d
P	1.01	bar	Fixed	Boundary pressure

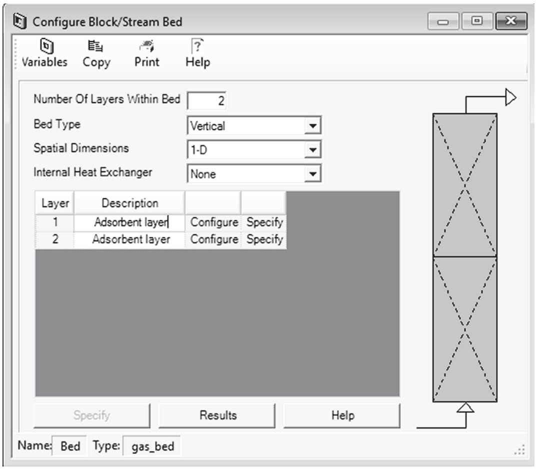
Figure 1.90 Set the product pressure to 1.01 bar.

Step 11: Specify the Adsorber bed

Double-click on the gas_bed to open its default form. This form is different from the feed block, since the gas_bed model is more complex. The gas_bed form allows you to create packed beds consisting of any number of adsorbent layers. For this separation, we will use two layers, to represent the layered bed from Jee et al. [24], which used zeolite 5A and activated carbon. To create a two-layer bed, simply enter 2 in the Number of Layers box, as shown in Figure 1.91.

Now, each layer has its own "configure" and "specify" buttons. Generally speaking, the Configure tab is where you choose the assumptions you make about the physical behavior of the layer. The Specify tab is where you provide the numeric values for the layer's physical properties. Changing the assumptions in the configure tab can change what variables are present in the specify tab.

Step 12: Specify the first layer



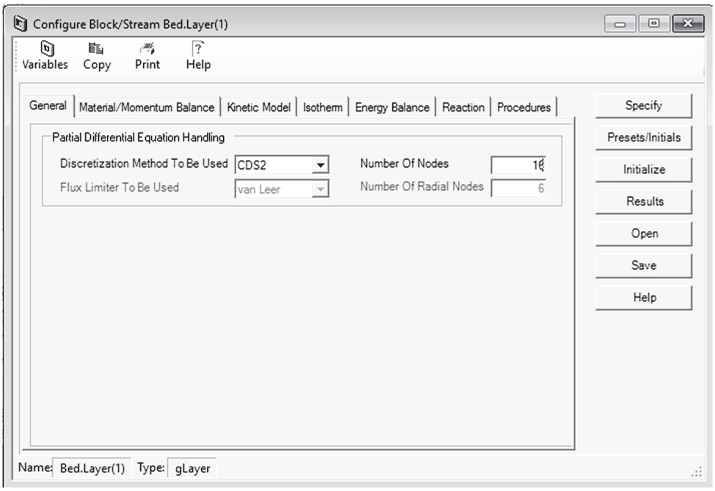
Number Of Layers Within Bed: 2
Bed Type: Vertical
Spatial Dimensions: 1-D
Internal Heat Exchanger: None

Layer	Description		
1	Adsorbent layer	Configure	Specify
2	Adsorbent layer	Configure	Specify

Name: Bed Type: gas_bed

Figure 1.91 Configuring the gas_bed block.

Click on the "configure" button for Layer 1. The first tab that appears is the Finite Element discretization method options. In this tab, you can specify exactly how the PDE defined by the gas_bed will be solved. For this example, we will use *a Central Differencing Scheme, CDS2* with 16 nodes. This will allow for very fast simulation times when we include axial dispersion term in our momentum balance according to the online help file in Aspen Adsorption. Figure 1.92 shows this selection.

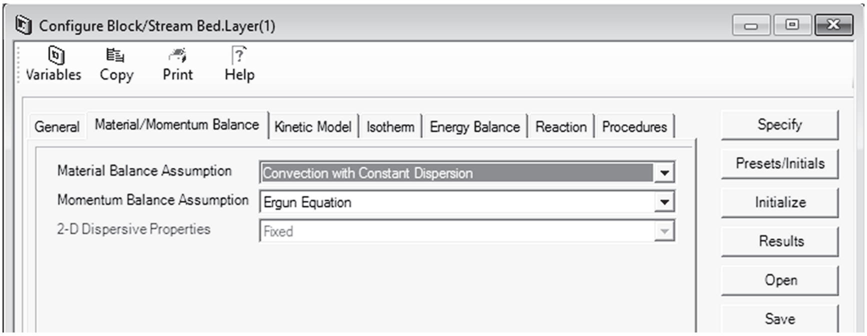


Partial Differential Equation Handling
Discretization Method To Be Used: CDS2
Number Of Nodes: 16
Flux Limiter To Be Used: van Leer
Number Of Radial Nodes: 6

Name: Bed.Layer(1) Type: gLayer

Figure 1.92 Choose the second-order central difference scheme (CDS2) to improve the simulation efficiency with axial dispersion effect.

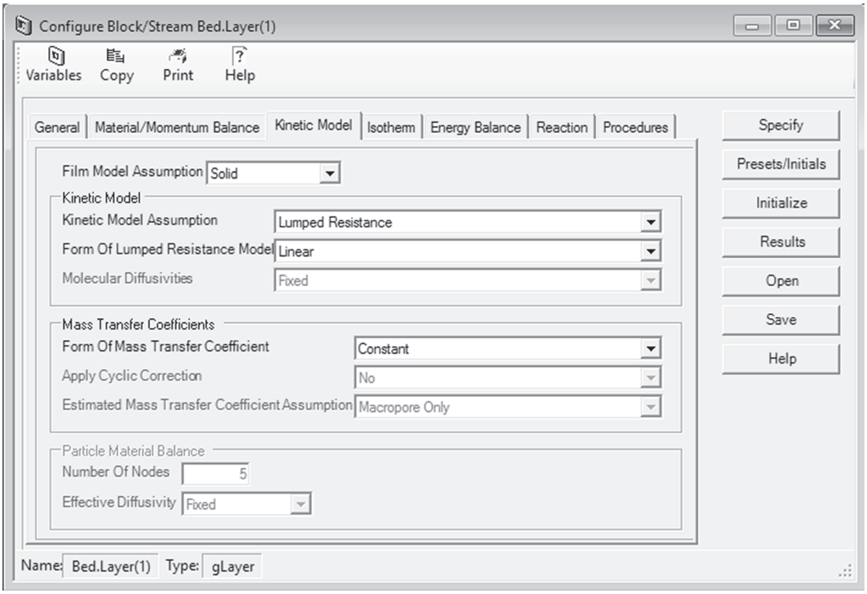
The next tab allows us to choose the momentum and material balances we wish to calculate for the system. Both of our layers will use "convection with constant dispersion" and the Ergun Equation, Eq. (1.11), for pressure drop (Figure 1.93).



Material Balance Assumption: Convection with Constant Dispersion
Momentum Balance Assumption: Ergun Equation
2-D Dispersive Properties: Fixed

Figure 1.93 Specifying the material balances within the bed.

The next tab allows us to choose the assumptions regarding the kinetics of the system. For our case, the default linear-lumped resistance or LDF assumption is acceptable, and the resistance should be based on the solid-phase concentrations. Refer to Eq. (1.14) in Section 1.7.3 about the LDF assumption (Figure 1.94).



Film Model Assumption: Solid

Kinetic Model
Kinetic Model Assumption: Lumped Resistance
Form Of Lumped Resistance Model: Linear
Molecular Diffusivities: Fixed

Mass Transfer Coefficients
Form Of Mass Transfer Coefficient: Constant
Apply Cyclic Correction: No
Estimated Mass Transfer Coefficient Assumption: Macropore Only

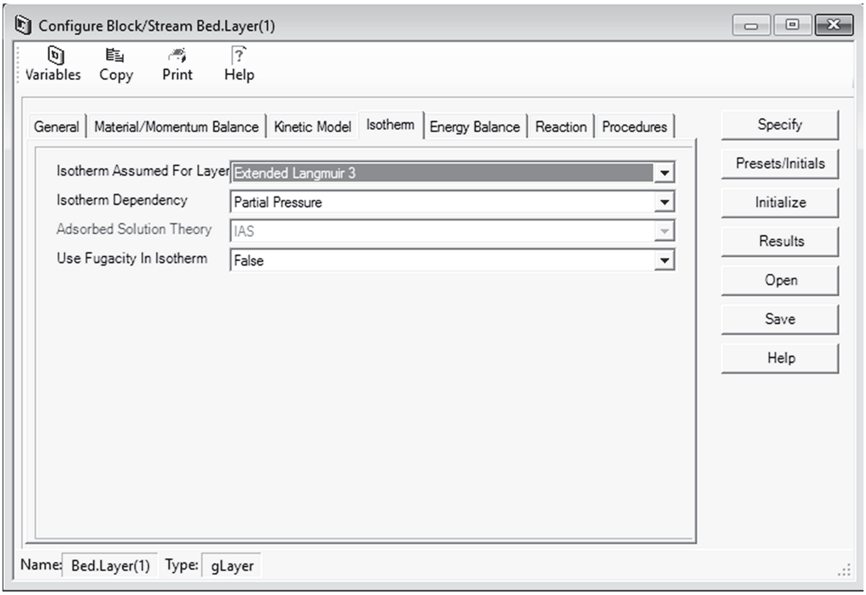
Particle Material Balance
Number Of Nodes: 5
Effective Diffusivity: Fixed

Name: Bed.Layer(1) Type: gLayer

Figure 1.94 The kinetic assumptions.

Next, we choose the equilibrium behavior, the isotherm assumptions. For both layers, an Extended Langmuir 3 model based on partial pressure is appropriate. Note that this isotherm does not perfectly match that reported in Jee et al. [24], and we will revisit this discrepancy later. After choosing the isotherm, you should see Figure 1.95.

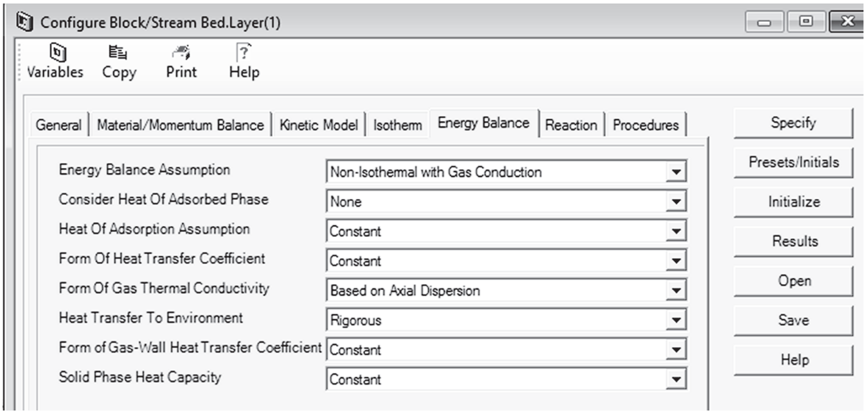
The final tab we will make changes to is the energy balance tab. This tab allows a wide range of assumptions about the heat transfer in the system. For



Isotherm Assumed For Layer: Extended Langmuir 3
Isotherm Dependency: Partial Pressure
Adsorbed Solution Theory: IAS
Use Fugacity In Isotherm: False
Name: Bed.Layer(1) Type: gLayer

Figure 1.95 Isotherm selection.

this bed, the only heat transfer occurs by conduction in the gas phase. We will be performing a rigorous energy balance with the wall, but all heat capacities and heats of adsorption are constant. The thermal conductivity of the gas is a function of the axial dispersion. To make these assumptions, choose the options shown in Figure 1.96.



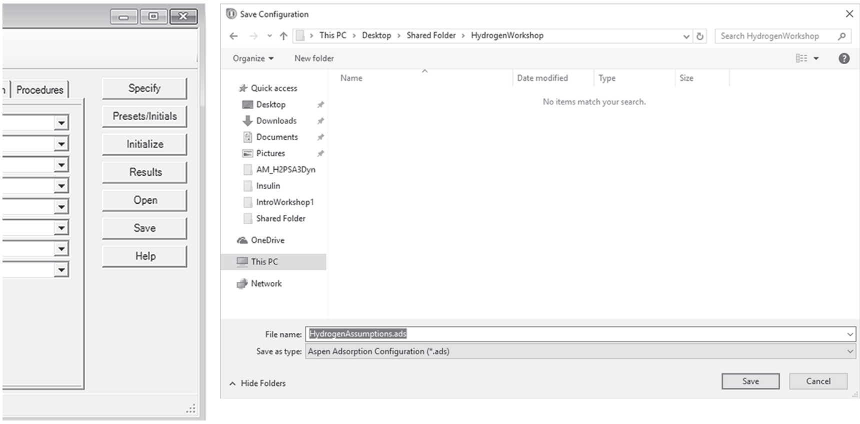
Energy Balance Assumption: Non-Isothermal with Gas Conduction
Consider Heat Of Adsorbed Phase: None
Heat Of Adsorption Assumption: Constant
Form Of Heat Transfer Coefficient: Constant
Form Of Gas Thermal Conductivity: Based on Axial Dispersion
Heat Transfer To Environment: Rigorous
Form of Gas-Wall Heat Transfer Coefficient: Constant
Solid Phase Heat Capacity: Constant

Figure 1.96 The energy balance and heat transfer assumptions.

With this, we have completed the assumption configuration for the first layer. Do not close the configure window yet though!

Step 13: Specify the assumptions for the second layer

The assumptions for this layer are identical to the first. To quickly copy the settings from one layer to the next, we will use the "Save" button in the right-hand panel to create a file that contains all the assumptions (Figure 1.97). Save the file as **HydrogenAssumptions.ada**.



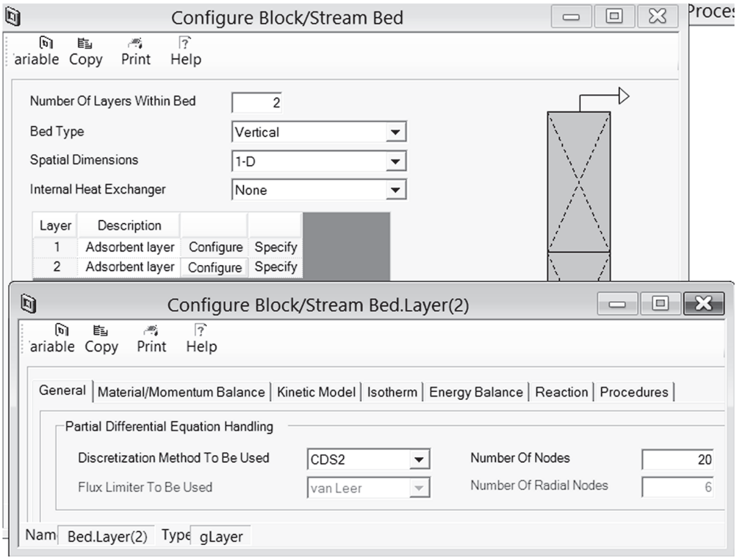
No items match your search.

File name: HydrogenAssumptions.ads

Save as type: Aspen Adsorption Configuration (*.ads)

Figure 1.97 Saving the assumptions for the layer.

Once we have created the assumption file, we can open it in the second layer (Figures 1.98 and 1.99).



Number Of Layers Within Bed: 2

Bed Type: Vertical

Spatial Dimensions: 1-D

Internal Heat Exchanger: None

Layer	Description		
1	Adsorbent layer	Configure	Specify
2	Adsorbent layer	Configure	Specify

Discretization Method To Be Used: CDS2

Flux Limiter To Be Used: van Leer

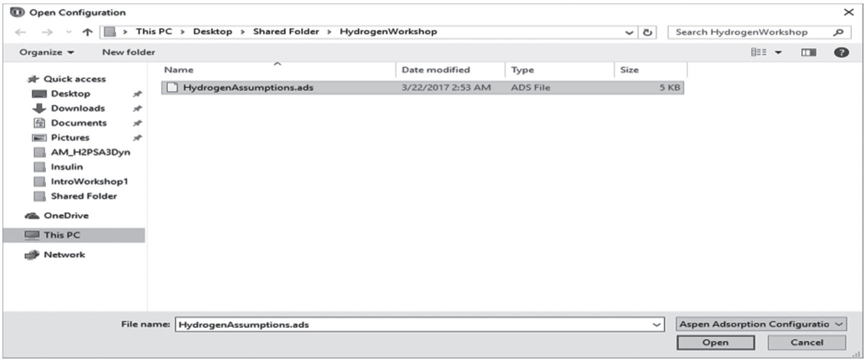
Number Of Nodes: 20

Number Of Radial Nodes: 6

Nam: Bed.Layer(2) Type: gLayer

Figure 1.98 Opening the configure form for layer 2.

Once we have opened the file, confirm that all the parameters match what were specified in step 13. Pay attention to the number of nodes in the PDE discretization method.



Name	Date modified	Type	Size
HydrogenAssumptions.ads	3/22/2017 2:53 AM	ADS File	5 KB

File name: HydrogenAssumptions.ads

Aspen Adsorption Configuratio

Figure 1.99 Selecting the configuration file from the first layer.

Step 14: Specify the numeric values

So far we have only specified assumptions about the layers, but it is now time to provide the numbers required for the various models we chose. To do this, click on the "specify" button for both layers. Enter the information in Tables 1.8 and 1.9 into the layer specification forms.

Table 1.8 Data shared between layers 1 and 2.

Bed height	0.5 m
Bed diameter	0.1855 m
Bed wall thickness	0.00134 m
Dispersion coefficient (all components)	1.5e−005
Heat of adsorption (CO)	−22.175 MJ kmol^{-1}
Heat of adsorption (C1)	−20.92 MJ kmol^{-1}
Heat of adsorption (H2)	−11.715 MJ kmol^{-1}
Fluid/solid heat transfer coefficient	1 MW/(m^2 K^{-1})
Fluid/wall heat transfer coefficient	3.851e−005 MW/(m^2 K^{-1})
Wall/Env heat transfer coefficient	1.423e−005 MW/(m^2 K^{-1})
Wall thermal conductivity	1e−20 MW/(m K^{-1})
Wall material heat capacity	5.0232e−4 MJ/(kg K^{-1})
Wall material density	7830 kg m^{-3}

Once these values have been entered, save the simulation as `H2Workshop4.ada` (Figure 1.100).

Double-click on the green–red–triangle button. We see the specification status indicating that the current simulation is underspecified by 12 initial variables. See Figure 1.101.

Step 15: Initialize the simulation

Now that the values have all been entered, the simulation should be ready to run. Unfortunately, there is one final impediment. Double-click on the green–red–triangle button. We see the specification status indicating that the

Table 1.9 Data that are distinct for each layer.

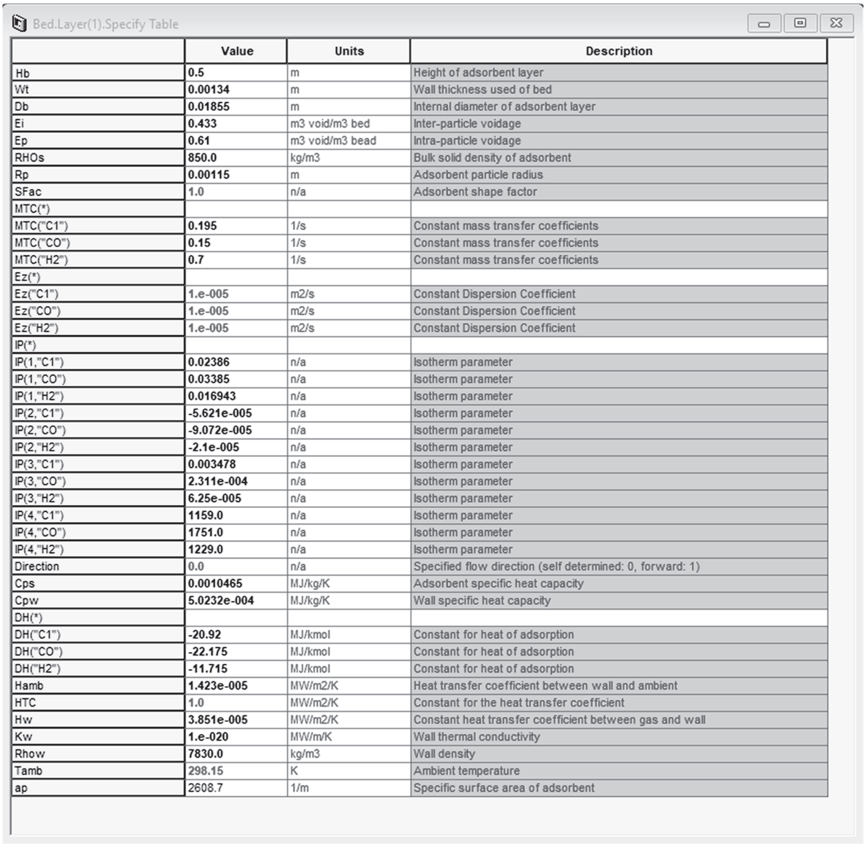
Variable	Layer 1	Layer 2	Units
Particle radius	0.001 15	0.001 57	m
Bed voidage	0.433	0.357	—
Intraparticle voidage	0.61	0.65	—
Surface area/volume ratio	2608.7	1910.83	$1\,m^{-1}$
Particle density	850	1160	$kg\,m^{-3}$
Mass transfer coefficient (CO)	0.15	0.063	$1\,s^{-1}$
Mass transfer coefficient (C1)	0.195	0.147	$1\,s^{-1}$
Mass transfer coefficient (H2)	0.7	0.7	$1\,s^{-1}$
Solid phase heat capacity	0.001 046 5	9.209e−004	$MJ/(kg\,K^{-1})^{-1}$
IP(1,"C1")	0.023 86	0.005 833	Isotherm parameter
IP(1,"CO")	0.033 85	0.011 845	Isotherm parameter
IP(1,"H2")	0.016 943	0.004 314	Isotherm parameter
IP(2,"C1")	−5.62e−05	−1.19e−05	Isotherm parameter
IP(2,"CO")	−9.07e−05	−3.13e−05	Isotherm parameter
IP(2,"H2")	−2.10e−05	−1.06e−05	Isotherm parameter
IP(3,"C1")	0.003 478	6.51e−04	Isotherm parameter
IP(3,"CO")	2.31e−04	0.020 2	Isotherm parameter
IP(3,"H2")	6.25e−05	0.002 515	Isotherm parameter
IP(4,"C1")	1159	1731	Isotherm parameter
IP(4,"CO")	1751	763	Isotherm parameter
IP(4,"H2")	1229	458	Isotherm parameter

current simulation is underspecified by 12 initial variables. See Figure 1.101. This message means that the degrees-of-freedom analysis has found that the model we have built needs additional information before Aspen can solve it.

Now that it certainly looks like we have provided all the required information, we need to see what is missing. The answer is that the gas_bed block needs to be "initialized" so that a few additional internal variables will automatically be set. To do this, use the "flowsheet" menu to click on "Check and Initial" Following this, the simulation should be ready to run, because the initialization logic will have fixed the underspecification problem (Figure 1.102).

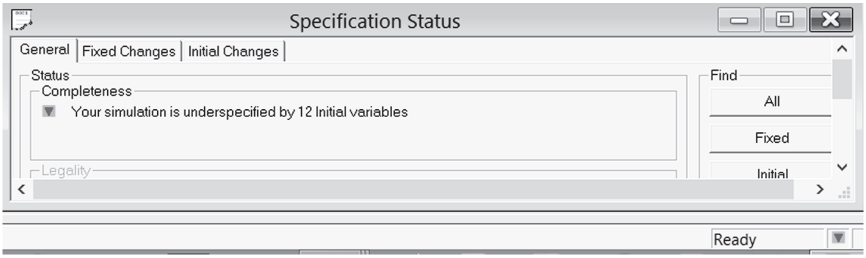
Step 16: Run the simulation

Figure 1.103 shows the controls for running simulations. As it stands, our simulation has no defined "end" criteria. If we run the simulation using the solid blue "play" icon, it would run until we manually stop it with the "pause" button. So first, click on the "run options" button represented by the play button with red circles. Here, we tell the simulation to pause after 100 s.



	Value	Units	Description
Hb	0.5	m	Height of adsorbent layer
Wt	0.00134	m	Wall thickness used of bed
Db	0.01855	m	Internal diameter of adsorbent layer
Ei	0.433	m3 void/m3 bed	Inter-particle voidage
Ep	0.61	m3 void/m3 bead	Intra-particle voidage
RHOs	850.0	kg/m3	Bulk solid density of adsorbent
Rp	0.00115	m	Adsorbent particle radius
SFac	1.0	n/a	Adsorbent shape factor
MTC(*)			
MTC("C1")	0.195	1/s	Constant mass transfer coefficients
MTC("CO")	0.15	1/s	Constant mass transfer coefficients
MTC("H2")	0.7	1/s	Constant mass transfer coefficients
Ez(*)			
Ez("C1")	1.e-005	m2/s	Constant Dispersion Coefficient
Ez("CO")	1.e-005	m2/s	Constant Dispersion Coefficient
Ez("H2")	1.e-005	m2/s	Constant Dispersion Coefficient
IP(*)			
IP(1,"C1")	0.02386	n/a	Isotherm parameter
IP(1,"CO")	0.03385	n/a	Isotherm parameter
IP(1,"H2")	0.016943	n/a	Isotherm parameter
IP(2,"C1")	-5.621e-005	n/a	Isotherm parameter
IP(2,"CO")	-9.072e-005	n/a	Isotherm parameter
IP(2,"H2")	-2.1e-005	n/a	Isotherm parameter
IP(3,"C1")	0.003478	n/a	Isotherm parameter
IP(3,"CO")	2.311e-004	n/a	Isotherm parameter
IP(3,"H2")	6.25e-005	n/a	Isotherm parameter
IP(4,"C1")	1159.0	n/a	Isotherm parameter
IP(4,"CO")	1751.0	n/a	Isotherm parameter
IP(4,"H2")	1229.0	n/a	Isotherm parameter
Direction	0.0	n/a	Specified flow direction (self determined: 0, forward: 1)
Cps	0.0010465	MJ/kg/K	Adsorbent specific heat capacity
Cpw	5.0232e-004	MJ/kg/K	Wall specific heat capacity
DH(*)			
DH("C1")	-20.92	MJ/kmol	Constant for heat of adsorption
DH("CO")	-22.175	MJ/kmol	Constant for heat of adsorption
DH("H2")	-11.715	MJ/kmol	Constant for heat of adsorption
Hamb	1.423e-005	MW/m2/K	Heat transfer coefficient between wall and ambient
HTC	1.0	MW/m2/K	Constant for the heat transfer coefficient
Hw	3.851e-005	MW/m2/K	Constant heat transfer coefficient between gas and wall
Kw	1.e-020	MW/m/K	Wall thermal conductivity
Rhow	7830.0	kg/m3	Wall density
Tamb	298.15	K	Ambient temperature
ap	2608.7	1/m	Specific surface area of adsorbent

Figure 1.100 The Layer(1) specify table.



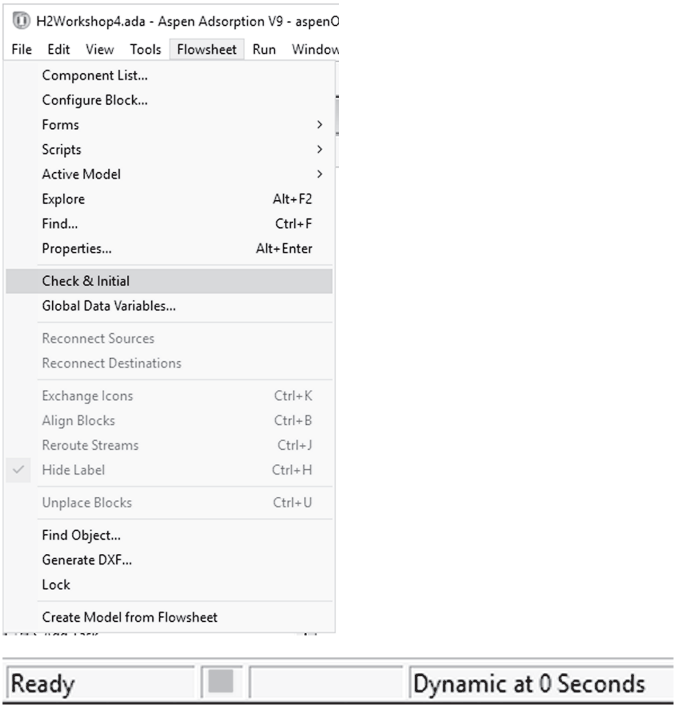
Your simulation is underspecified by 12 Initial variables

Figure 1.101 An underspecified simulation.

Before running the simulation, save the file as `H2Workshop5.ada`. Once you run the simulation, you should see messages like those shown in Figure 1.104.

Step 17: View breakthrough results

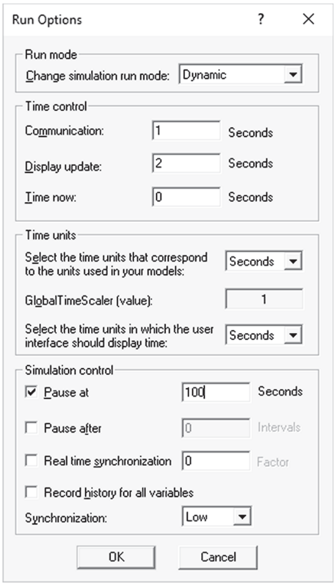
To view a plot of the concentration profile, we need to create a plot in the Flowsheet section of the Explorer window. Double-click on the "Add Form" tool



Ready

Dynamic at 0 Seconds

Figure 1.102 Initializing the flowsheet.



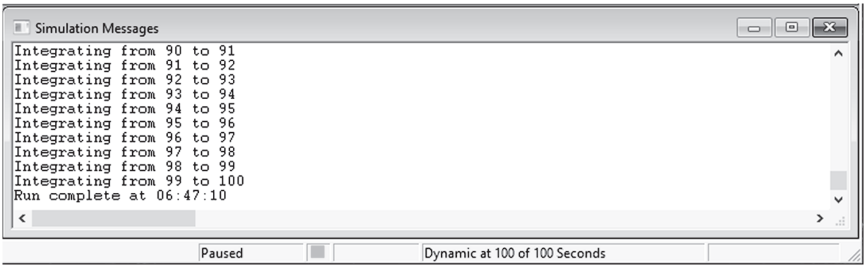
Run mode
Change simulation run mode: Dynamic

Time control
Communication: 1 Seconds
Display update: 2 Seconds
Time now: 0 Seconds

Time units
Select the time units that correspond to the units used in your models: Seconds
GlobalTimeScaler (value): 1
Select the time units in which the user interface should display time: Seconds

Simulation control
☑ Pause at 100 Seconds
☐ Pause after 0 Intervals
☐ Real time synchronization 0 Factor
☐ Record history for all variables
Synchronization: Low

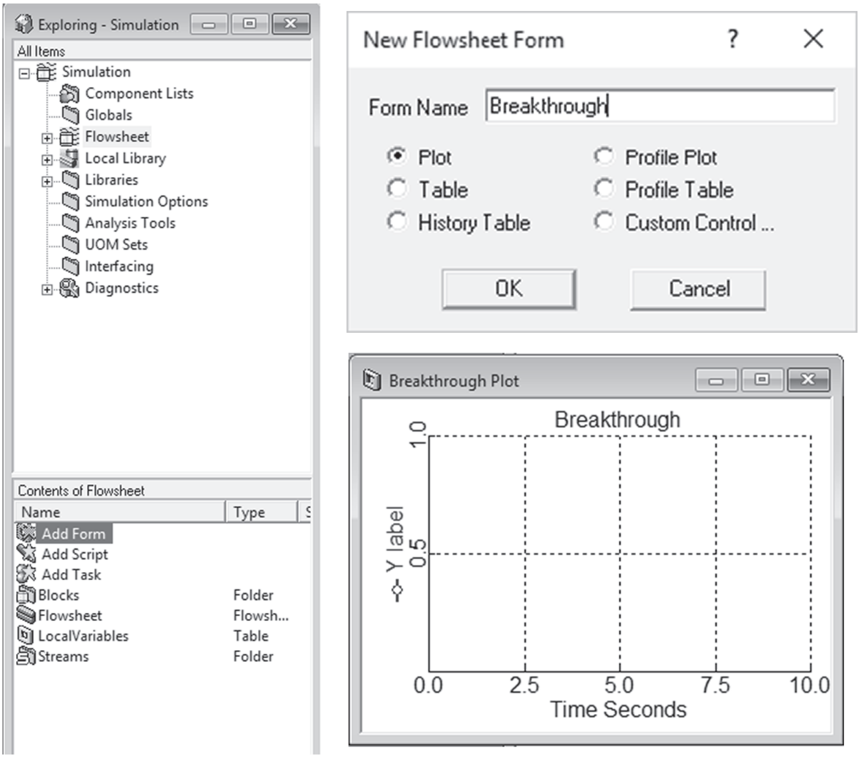
Figure 1.103 Run controls and options.



```
Integrating from 90 to 91
Integrating from 91 to 92
Integrating from 92 to 93
Integrating from 93 to 94
Integrating from 94 to 95
Integrating from 95 to 96
Integrating from 96 to 97
Integrating from 97 to 98
Integrating from 98 to 99
Integrating from 99 to 100
Run complete at 06:47:10
```

Figure 1.104 Messages from a successful simulation.

shown within Contents of Flowsheet in Figure 1.105 to begin the process of adding a plot.



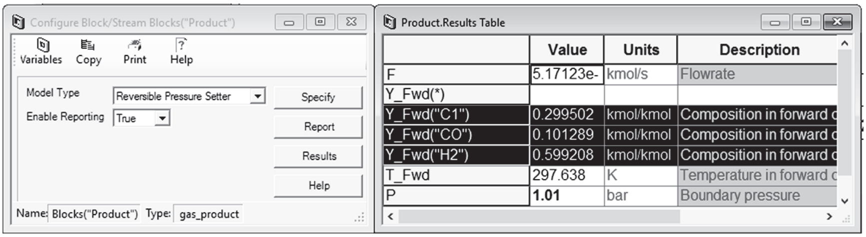
Form Name Breakthrough

● Plot

Name	Type
Add Form	
Add Script	
Add Task	
Blocks	Folder
Flowsheet	Flowsh...
LocalVariables	Table
Streams	Folder

Figure 1.105 The “Add form” tool.

Name the new form “Breakthrough” and ensure that the “Plot” radio button is selected. The result will be a blank plot. In order to add data to this plot, we can click and drag variables from any other form. In this case, we want to see the “Results” from the product block. Double-click on the “Product” block, then click on “Results” to view the results table. Select the three variables shown in Figure 1.106 and drag them onto the y-axis of the plot that is created.



Model Type: Reversible Pressure Setter
Enable Reporting: True
Name: Blocks("Product") Type: gas_product

	Value	Units	Description
F	5.17123e-	kmol/s	Flowrate
Y_Fwd(*)			
Y_Fwd("C1")	0.299502	kmol/kmol	Composition in forward c
Y_Fwd("CO")	0.101289	kmol/kmol	Composition in forward c
Y_Fwd("H2")	0.599208	kmol/kmol	Composition in forward c
T_Fwd	297.638	K	Temperature in forward c
P	**1.01**	bar	Boundary pressure

Figure 1.106 The product results.

Once the variables have been added, we need to show the full simulation history. To do this, right-click on the graph and choose "Zoom Full" as shown in Figure 1.107.

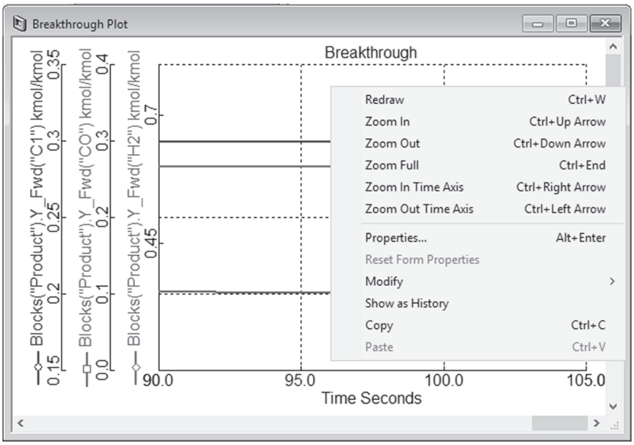


Figure 1.107 View the full history.

Now we see the full results, but they are not quite what we might have expected (Figure 1.108). Why does the result not look like a traditional breakthrough curve, with those sudden jumps in the first few seconds? The answer is that *we initialized the simulation "blindly"* without checking what the simulation would be initialized to. The gas_bed was initialized to have an equimolar mixture of all the components, instead of the composition we might have expected (i.e. equal to the feed)

Step 18: Rewind the simulation

There are two ways of resetting a simulation to its initial conditions. The first is the use of "Rewind using snapshots" and the second is the use of the "Restart" button. Snapshots are useful if you have several initial conditions, and want to switch between them. The restart button, on the other hand, simply resets the values to those used to initialize the simulation. Note that these buttons become inactive if you make *structural* changes to the simulation after a run. That is, if you run a simulation for 100 s and then add a new valve, you will

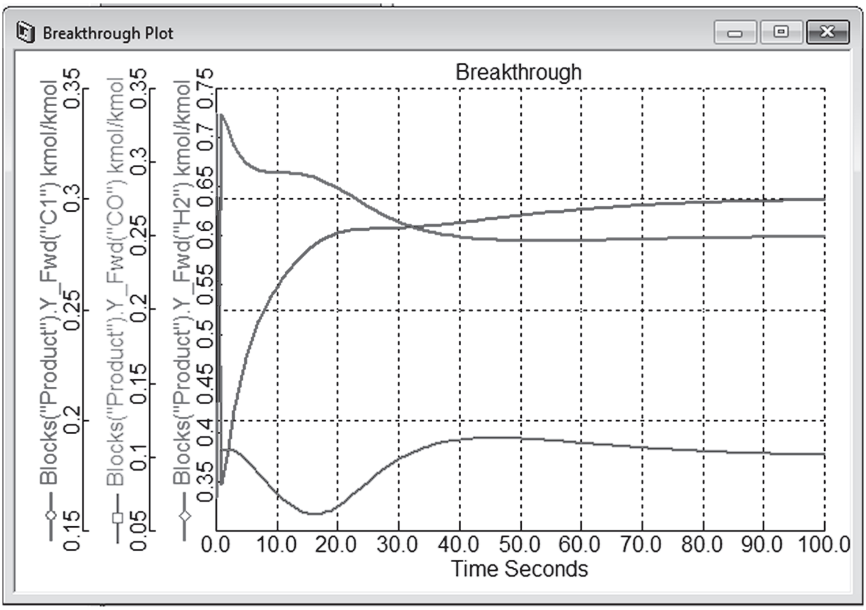


Figure 1.108 The simulation results plotted.

not be able to rewind to t = 0 s anymore. **Always remember to rewind before making changes after a run** (Figure 1.109).

Restart

Rewind using snapshots

Figure 1.109 The rewinding options in Aspen Adsorption.

Using the "restart" button, rewind the simulation.

Step 19: Set the initial conditions correctly

Open the configuration forms for both bed layers. Click on the "presets/initials" button and set the Y_First_Node(*) values to match the feed (Figure 1.110). Do this for both layers.

Once you have entered the values, repeat the "Check and Initial" process we used in Step 15.

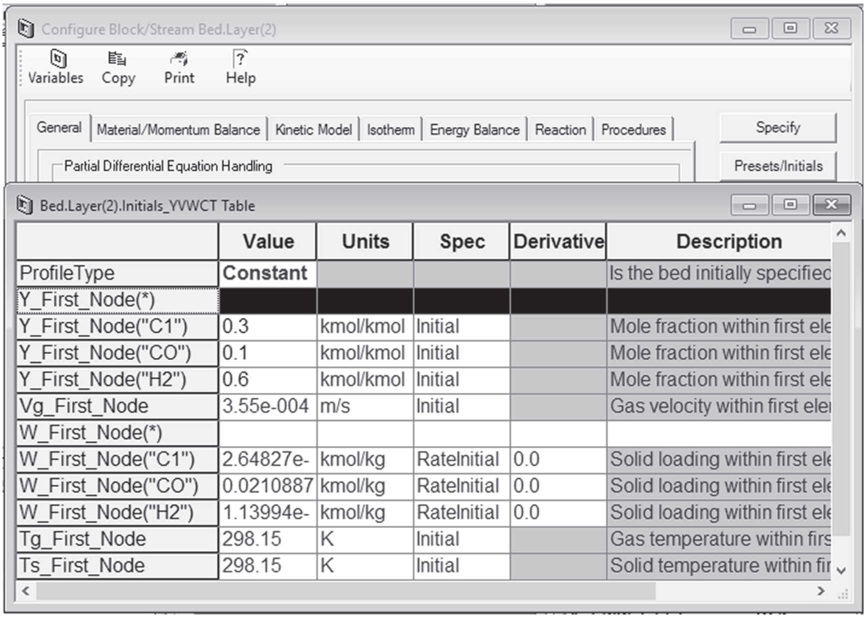
Step 20: Rerun the simulation

This time, the breakthrough curve looks normal. CO and C1 get adsorbed initially, resulting in a higher fraction of H2 in the product stream. However, the bed eventually becomes saturated, and the yield matches the feed.

Rewind the simulation, then save it as `H2Workshop6.ada`.

1.8.4 Create the PSA Flowsheet

Now that we understand the key aspects of building an Aspen Adsorption simulation, let us move on to building the complete PSA process. Starting with `H2Workshop6.ada`, we will add additional blocks to the flowsheet.



	Value	Units	Spec	Derivative	Description
ProfileType	Constant				Is the bed initially specifiec
Y_First_Node(*)					
Y_First_Node("C1")	0.3	kmol/kmol	Initial		Mole fraction within first ele
Y_First_Node("CO")	0.1	kmol/kmol	Initial		Mole fraction within first ele
Y_First_Node("H2")	0.6	kmol/kmol	Initial		Mole fraction within first ele
Vg_First_Node	3.55e-004	m/s	Initial		Gas velocity within first ele
W_First_Node(*)					
W_First_Node("C1")	2.64827e-	kmol/kg	RateInitial	0.0	Solid loading within first ele
W_First_Node("CO")	0.0210887	kmol/kg	RateInitial	0.0	Solid loading within first ele
W_First_Node("H2")	1.13994e-	kmol/kg	RateInitial	0.0	Solid loading within first ele
Tg_First_Node	298.15	K	Initial		Gas temperature within firs
Ts_First_Node	298.15	K	Initial		Solid temperature within fir

Figure 1.110 Specifying the initial bed composition.

Before we begin to describe the PSA process in Aspen, we should make a plan for what we want to do. In this workshop, we will be using a "single bed" approach for simulating a pressure swing adsorber. Specifically, we want to simulate the process shown in Figure 1.111. We will introduce the use of a gas_interaction block in this model.

Step 21: Add the blocks required for PSA

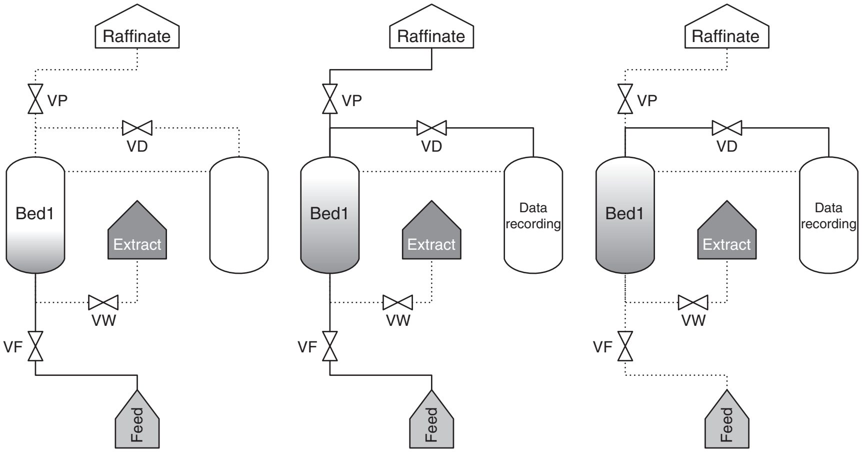
Following Step 8, Section 1.7.2, we add two gas_tank_void blocks as our pressure setters, and add four valves as our reversible flow setters. We also add an extra product block, and a gas_interaction block; we connect them as shown in Figure 1.112. We explain the gas_interaction block in the next step.

If we review Figure 1.111, we can now plan out how to schedule the valves in order to achieve the scheme we described. See Table 1.10.

Previously in Figure 1.7 and Table 1.5, we have explained the four ASs for valves within Aspen Adsorption: (1) AS = 0, valve is fully closed; (2) AS = 1, valve is fully open; (3) AS = 2 the gas flow rate through the valve is linearly dependent on the pressure drop across the valve according to Eq. (1.12); and (4) AS = 3, the valve has a fixed flow rate.

Step 22: Specify the gas_interaction block (D1)

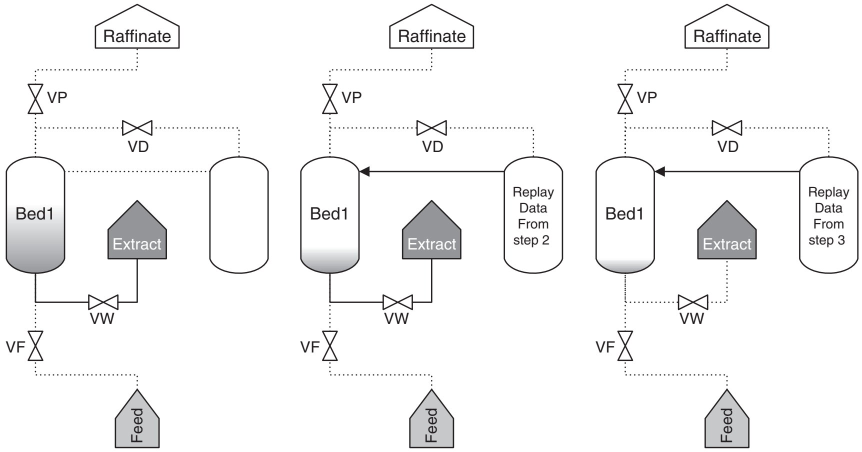
We use the gas_interaction model as a part of the single-bed modeling approach, to record the profile of the material received, and later replay this profile to simulate the returned material. The model records: (1) molar flow rate, (2) mole fraction composition, (3) temperature, (4) upstream bed



1. Bed 1 pressurization

2. Bed 1 adsorption (purge data are recorded)

3. Pressure equalization (data are recorded)



4. Bed 1 blowdown

5. Bed 1 purge (purge data played back)

6. Pressure equalization (equilibration data played back)

Figure 1.111 The steps of this H2 separation process (identical to PSA steps in Figure 1.7, except that the gas_intercation block replaces bed 2).

pressure, and (5) specific enthalpy. The gas_interaction block will automatically "replay" input from the "Bed" block based on our Cycle Organizer settings. Before we configure what data get recorded, however, we should specify a few properties of the block. Specifically, we should set the values that are used for initial guesses on the first iteration, before data have been recorded.

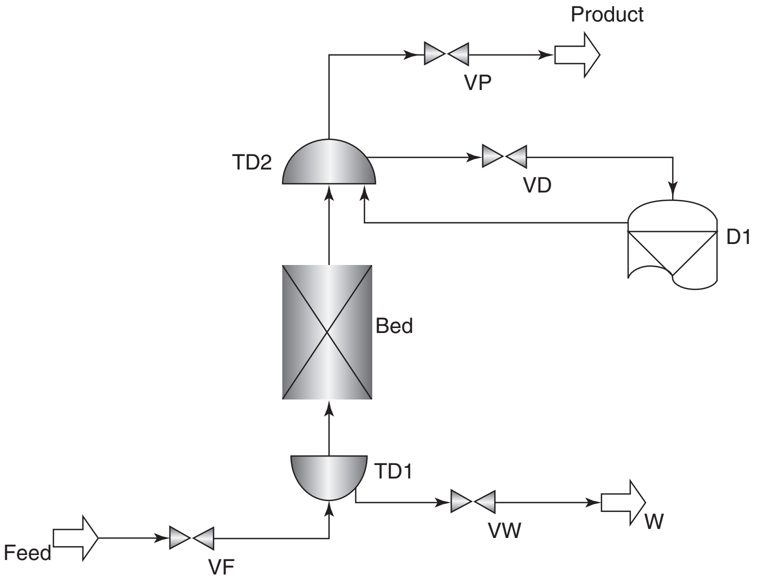
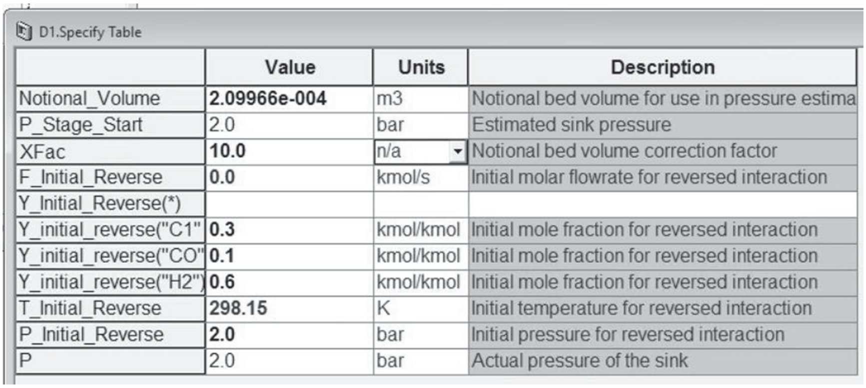


Figure 1.112 The additional blocks required for a PSA separation.

Table 1.10 Valve scheduling and active specifications (ASs) for the hydrogen PSA process.

Step	Function	VF	VD	VP	VW
Step 1	Pressurize the bed	2	0	0	0
Step 2	Adsorb bed 1 – fully load the bed	2	2	2	0
Step 3	Equalize the pressure of bed 1 and "data recorder" (gas_interaction_block)	0	2	0	0
Step 4	Depressurize (blowdown) bed 1	0	0	0	2
Step 5	Purge bed 1 to remove the strongly adsorbed component	0	0	0	2
Step 6	Repressurize bed 1 using pressure from the "data recorder" (gas_interaction_block)	0	0	0	0

Specifically, we should set the XFac number to adjust the effective volume of the interaction block. In our case, a XFac of 10 works well, since it makes the effective volume approximately equal to that of our bed. The pressure values are also important to set; in this case, we set them to 2 bar (Figure 1.113).


D1.Specify Table

	Value	Units	Description
Notional_Volume	2.09966e-004	m3	Notional bed volume for use in pressure estima
P_Stage_Start	2.0	bar	Estimated sink pressure
XFac	10.0	n/a	Notional bed volume correction factor
F_Initial_Reverse	0.0	kmol/s	Initial molar flowrate for reversed interaction
Y_Initial_Reverse(*)			
Y_initial_reverse("C1"	0.3	kmol/kmol	Initial mole fraction for reversed interaction
Y_initial_reverse("CO"	0.1	kmol/kmol	Initial mole fraction for reversed interaction
Y_initial_reverse("H2")	0.6	kmol/kmol	Initial mole fraction for reversed interaction
T_Initial_Reverse	298.15	K	Initial temperature for reversed interaction
P_Initial_Reverse	2.0	bar	Initial pressure for reversed interaction
P	2.0	bar	Actual pressure of the sink

Figure 1.113 Configuring the Gas_interaction block.

Step 23: Add a Cycle Organizer

Use the tools menu to add a Cycle Organizer (Figure 1.114).

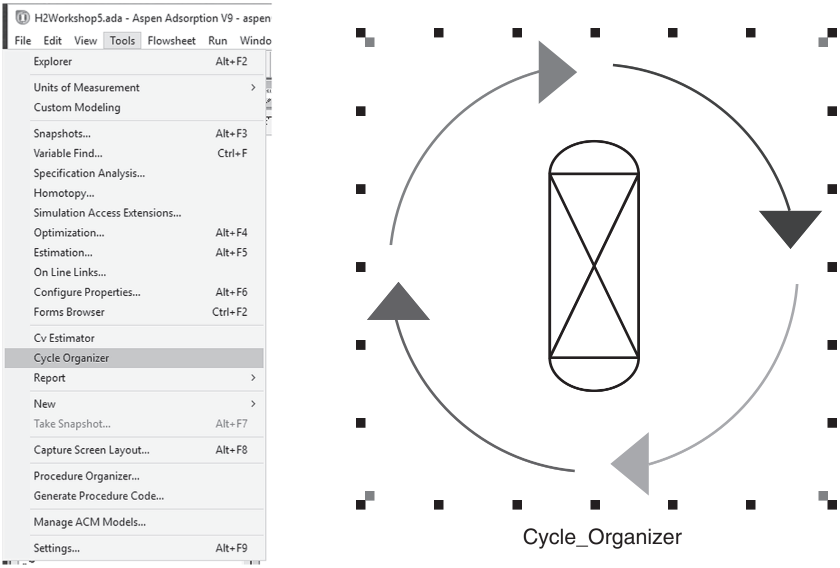


Figure 1.114 Adding a Cycle Organizer.

This is a special block, and only one is allowed per flowsheet. It presents an easy interface for scheduling changes (e.g. valve opening and closing) during a simulation.

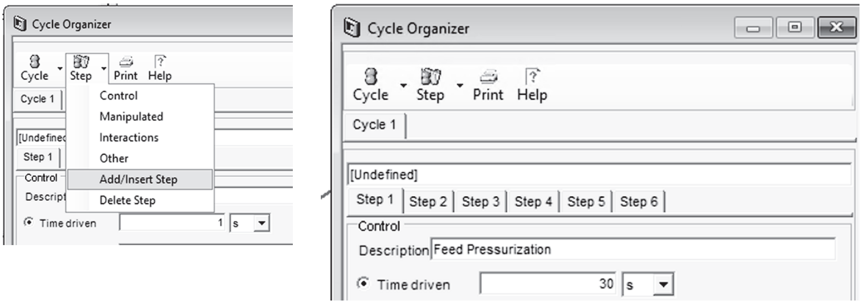
Step 24: Specify the Cycle Organizer

Each cycle tracked by the Cycle Organizer comprises steps. These steps have three major components.

- Control: Manages when the step triggers
- Manipulated: Manages what variables the step changes

- Interactions: When using a gas_interaction bed, the interactions define how information is shared between the gas_interaction block and other parts of the flowsheet.

To begin with, we will define six steps and set their Control options. To add a new step, use the button indicated in Figure 1.115. Ensure that there are a total of six steps.

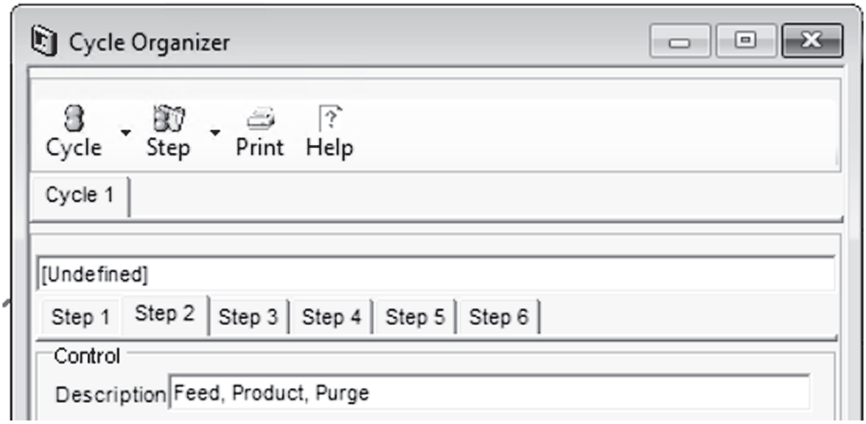


Description: Feed Pressurization

Time driven: 30 s

Figure 1.115 Add step 1 – feed pressurization.

We now set the control options for all six steps in figures. Step-dependency is a way to assert that one step will take exactly the same amount of time as the second step (Figures 1.116–1.120).

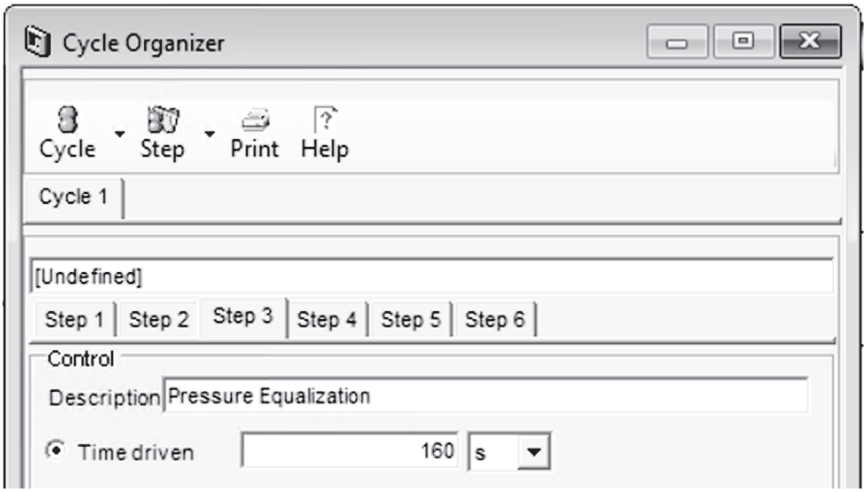


Description: Feed, Product, Purge

Figure 1.116 Step 2 – feed adsorption.

How do we specify steps 5–6 with the help of the gas_interaction block? We use the gas_interaction model as part of the single-bed modeling approach, to record the profile of material received, and later replay this profile to simulate the returned material. The model records: (1) molar flow rate, (2) mole fraction composition, (3) temperature, (4) upstream bed pressure, and (5) specific enthalpy.

We need to open their Interaction settings. Do this with the button highlighted in Figure 1.121.

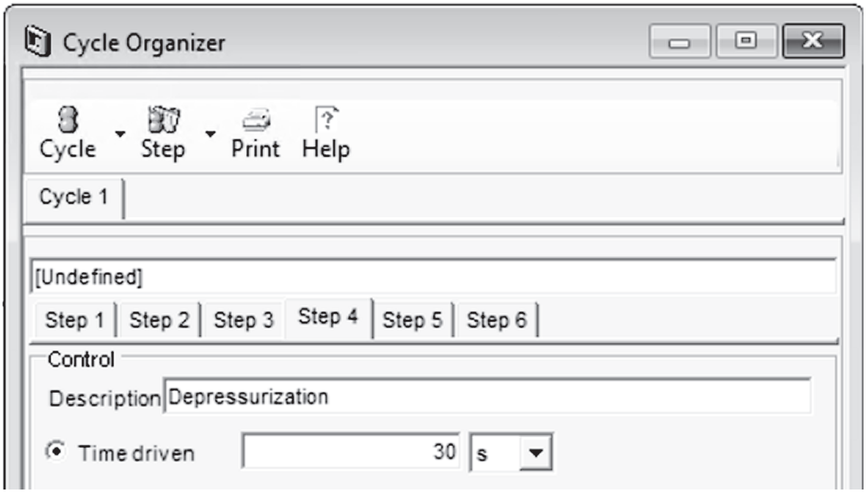


[Undefined]

Description: Pressure Equalization

● Time driven 160 s

Figure 1.117 Step 3 – pressure equalization.



[Undefined]

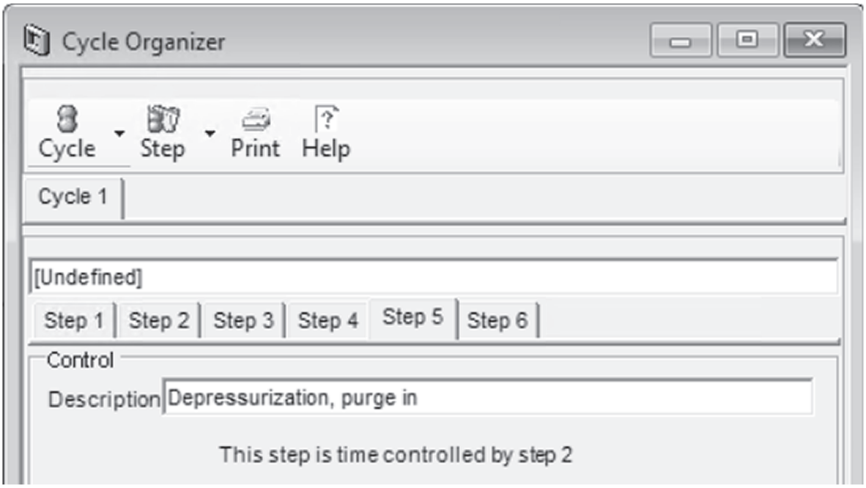
Description: Depressurization

● Time driven 30 s

Figure 1.118 Step 4 – depressurization.

In the step interaction window, use the drop downs shown in Figure 1.121 to specify the interactions depicted in Figure 1.122. According to both Figures 1.7 and 1.111, step 5 and step 2, as well as step 6 and step 2, are closely related in a forward–reverse mode operationally (Figure 1.123).

Next, we move on to the manipulated variables. This is where we specify the variables that will change between each step of the cycle (Figures 1.124–1.129).

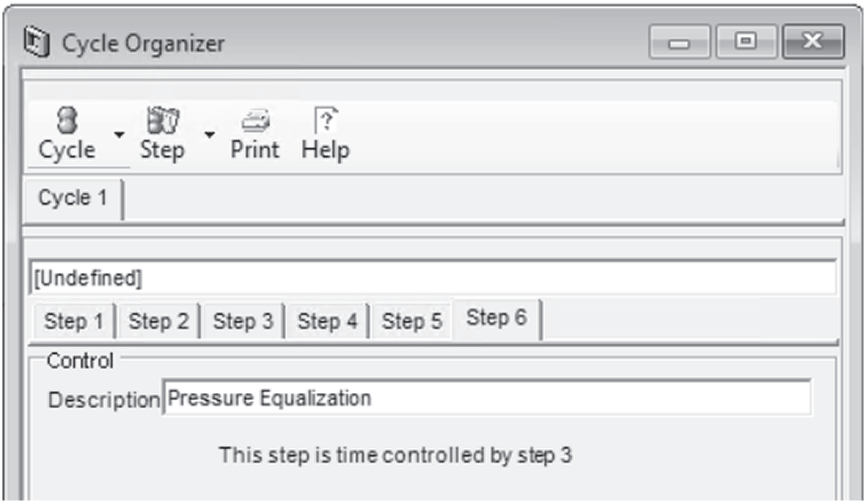


[Undefined]

Description: Depressurization, purge in

This step is time controlled by step 2

Figure 1.119 Step 5 – bed purging and depressurization.



[Undefined]

Description: Pressure Equalization

This step is time controlled by step 3

Figure 1.120 Step 6 – pressure equalization.

Step 25: Generate the cycle

Merely specifying the Cycle Organizer is not enough. We also must "Activate" it. Figure 1.130 illustrates this process.

We can also check to ensure that the cycle is active by looking in the Explorer. A block called Cycle1 with a lightning bolt indicates that the Cycle Organizer is ready to go. See Figure 1.131.

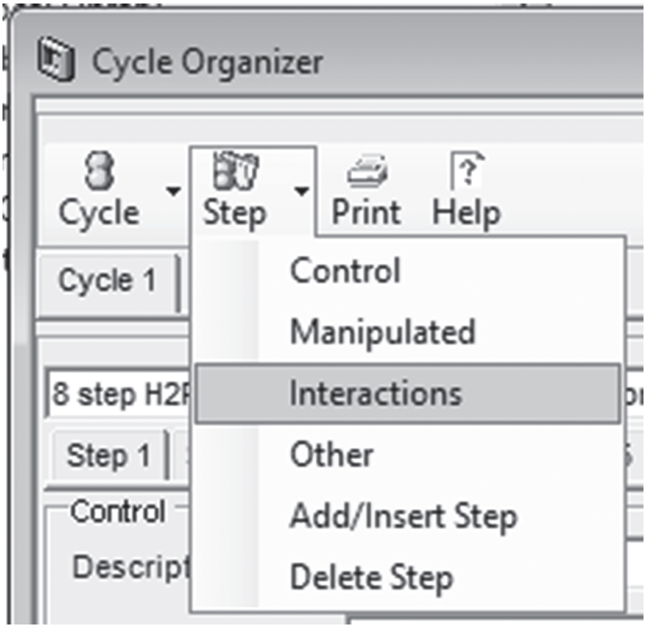
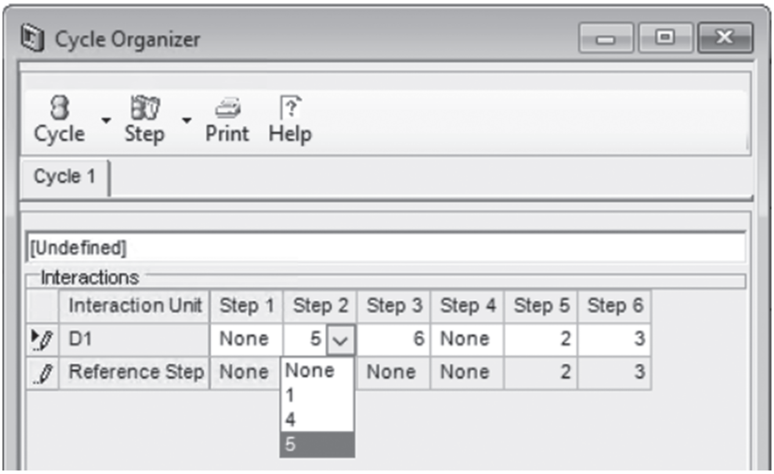


Figure 1.121 Step interactions.



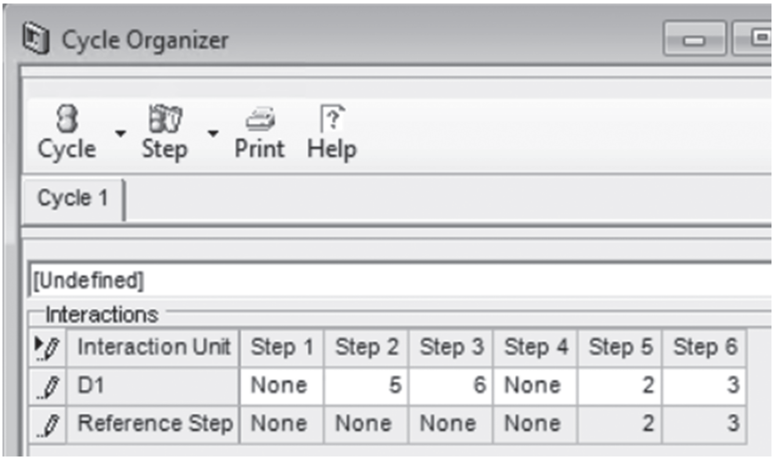
[Undefined]

Interaction Unit	Step 1	Step 2	Step 3	Step 4	Step 5	Step 6
D1	None	5	6	None	2	3
Reference Step	None	None	None	None	2	3

Figure 1.122 The step interaction setting.

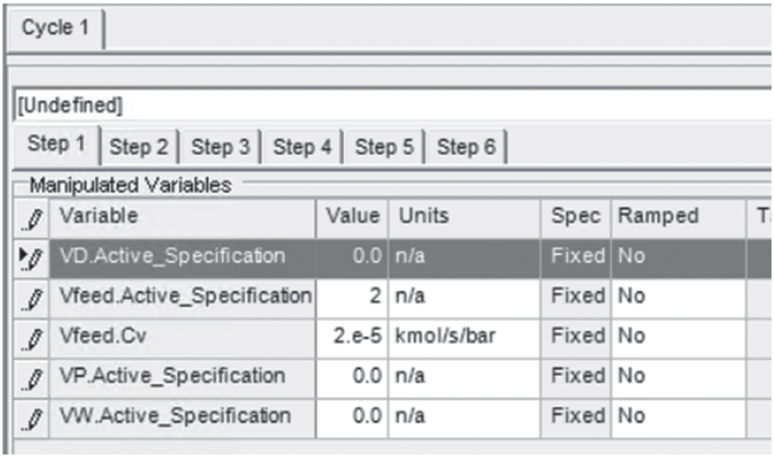
Step 26: Run the simulation

Once again, use the “Check and Initial” to resolve the underspecified problem. The Initialization scripts check to see if a Cycle Organizer is present, and initialize the flowsheet differently, if it is. Set the Cycle Organizer to run for five cycles. See Figure 1.132.



Interaction Unit	Step 1	Step 2	Step 3	Step 4	Step 5	Step 6
D1	None	5	6	None	2	3
Reference Step	None	None	None	None	2	3

Figure 1.123 The completed interactions.



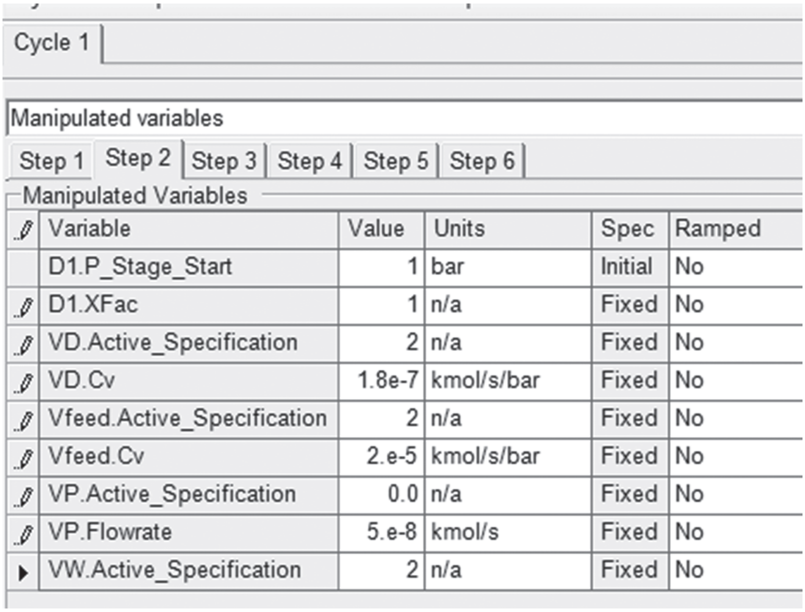
Variable	Value	Units	Spec	Ramped
VD.Active_Specification	0.0	n/a	Fixed	No
Vfeed.Active_Specification	2	n/a	Fixed	No
Vfeed.Cv	2.e-5	kmol/s/bar	Fixed	No
VP.Active_Specification	0.0	n/a	Fixed	No
VW.Active_Specification	0.0	n/a	Fixed	No

Figure 1.124 Step 1 – feed pressurization.

Afterward, run the simulation and look at the breakthrough plot we made earlier (Figure 1.133).

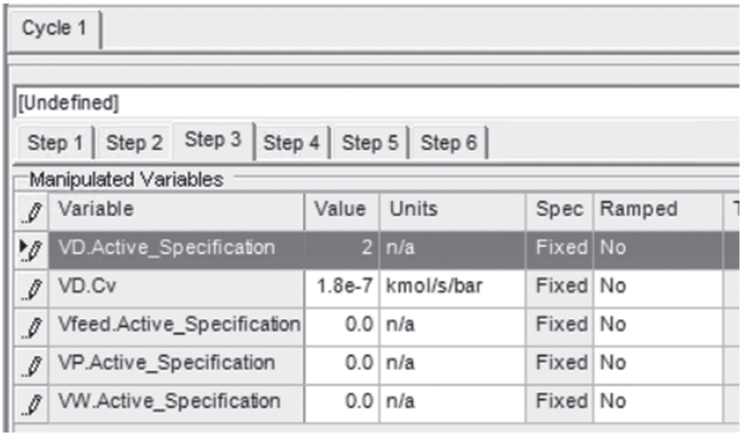
Save the finished simulation as **`H2Workshop7.ada`**.

As you can see, the H2 concentration (in red) is slowly increasing each cycle. After many cycles, the separation unit will reach a steady state at approximately 95% hydrogen. If you have a powerful computer, try running the simulation for 15 cycles.



Variable	Value	Units	Spec	Ramped
D1.P_Stage_Start	1	bar	Initial	No
D1.XFac	1	n/a	Fixed	No
VD.Active_Specification	2	n/a	Fixed	No
VD.Cv	1.8e-7	kmol/s/bar	Fixed	No
Vfeed.Active_Specification	2	n/a	Fixed	No
Vfeed.Cv	2.e-5	kmol/s/bar	Fixed	No
VP.Active_Specification	0.0	n/a	Fixed	No
VP.Flowrate	5.e-8	kmol/s	Fixed	No
VW.Active_Specification	2	n/a	Fixed	No

Figure 1.125 Step 2 – feed adsoprtion.

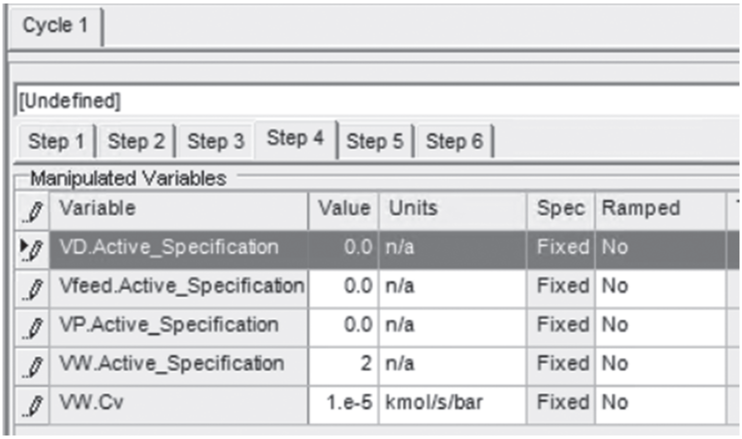


Variable	Value	Units	Spec	Ramped
VD.Active_Specification	2	n/a	Fixed	No
VD.Cv	1.8e-7	kmol/s/bar	Fixed	No
Vfeed.Active_Specification	0.0	n/a	Fixed	No
VP.Active_Specification	0.0	n/a	Fixed	No
VW.Active_Specification	0.0	n/a	Fixed	No

Figure 1.126 Step 3 – pressure equalization.

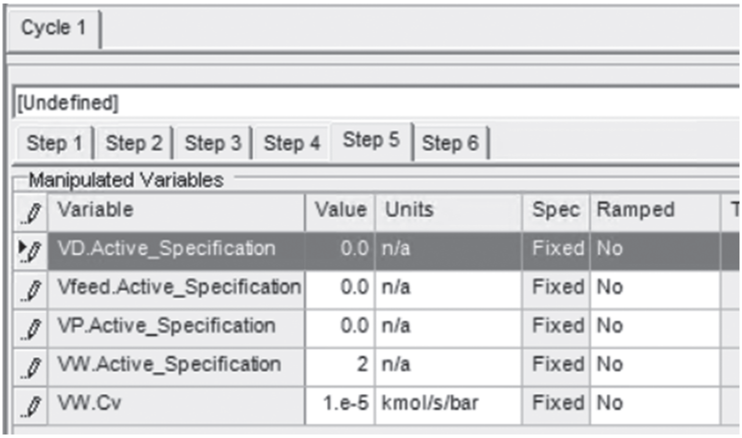
1.9 PSA Workshop: Modeling Hydrogen Separation using gCSS

In the previous workshop, we used the "one bed" approach to model hydrogen separation. It allows for faster simulations, but Aspen is certainly capable of



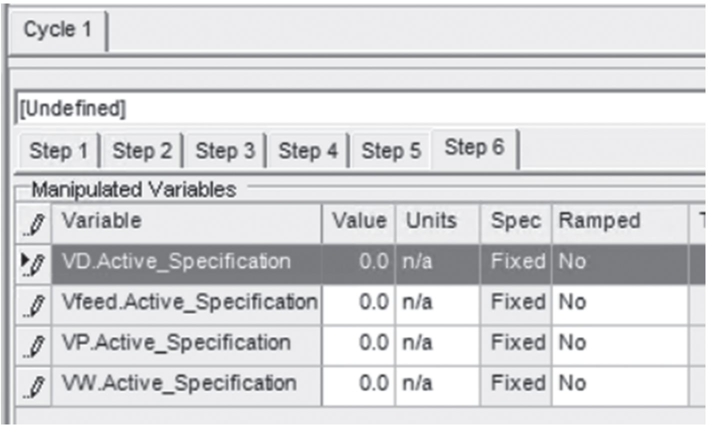
Variable	Value	Units	Spec	Ramped
VD.Active_Specification	0.0	n/a	Fixed	No
Vfeed.Active_Specification	0.0	n/a	Fixed	No
VP.Active_Specification	0.0	n/a	Fixed	No
VW.Active_Specification	2	n/a	Fixed	No
VW.Cv	1.e-5	kmol/s/bar	Fixed	No

Figure 1.127 Step 4 – depressurization.



Variable	Value	Units	Spec	Ramped
VD.Active_Specification	0.0	n/a	Fixed	No
Vfeed.Active_Specification	0.0	n/a	Fixed	No
VP.Active_Specification	0.0	n/a	Fixed	No
VW.Active_Specification	2	n/a	Fixed	No
VW.Cv	1.e-5	kmol/s/bar	Fixed	No

Figure 1.128 Step 5 – bed purging and depressurization.



Variable	Value	Units	Spec	Ramped
VD.Active_Specification	0.0	n/a	Fixed	No
Vfeed.Active_Specification	0.0	n/a	Fixed	No
VP.Active_Specification	0.0	n/a	Fixed	No
VW.Active_Specification	0.0	n/a	Fixed	No

Figure 1.129 Step 6 – pressure equalization.

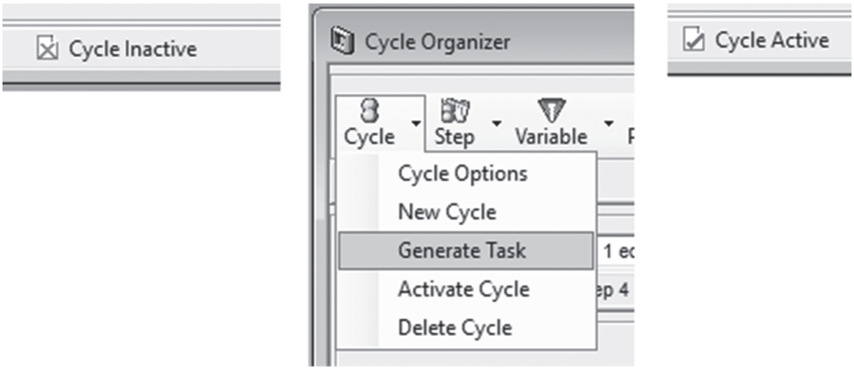
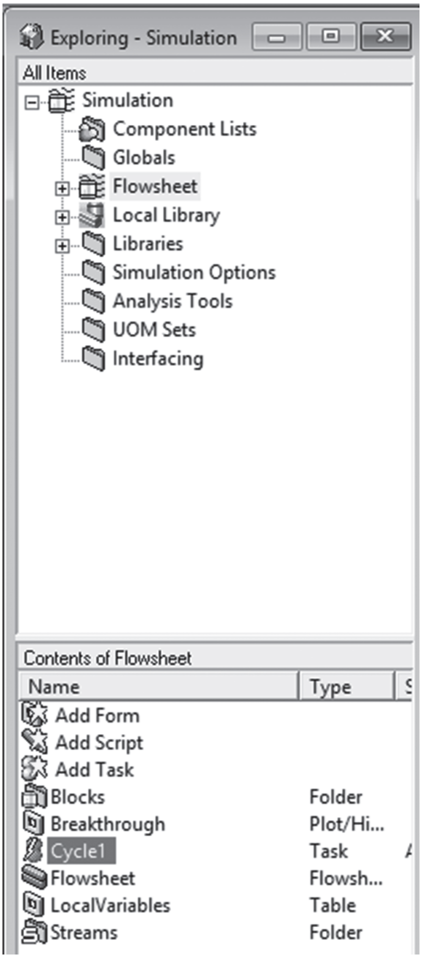
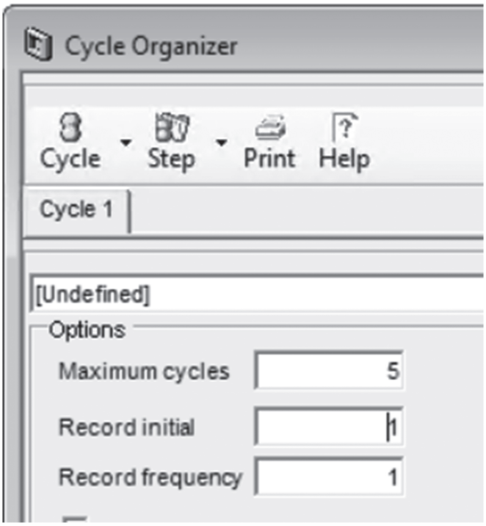


Figure 1.130 Activating a deactivated cycle.



Name	Type
Add Form	
Add Script	
Add Task	
Blocks	Folder
Breakthrough	Plot/Hi...
Cycle1	Task
Flowsheet	Flowsh...
LocalVariables	Table
Streams	Folder

Figure 1.131 Contents of flowsheet showing that cycle1 is ready to go.



Maximum cycles 5

Record initial 1

Record frequency 1

Figure 1.132 Setting the maximum cycles.

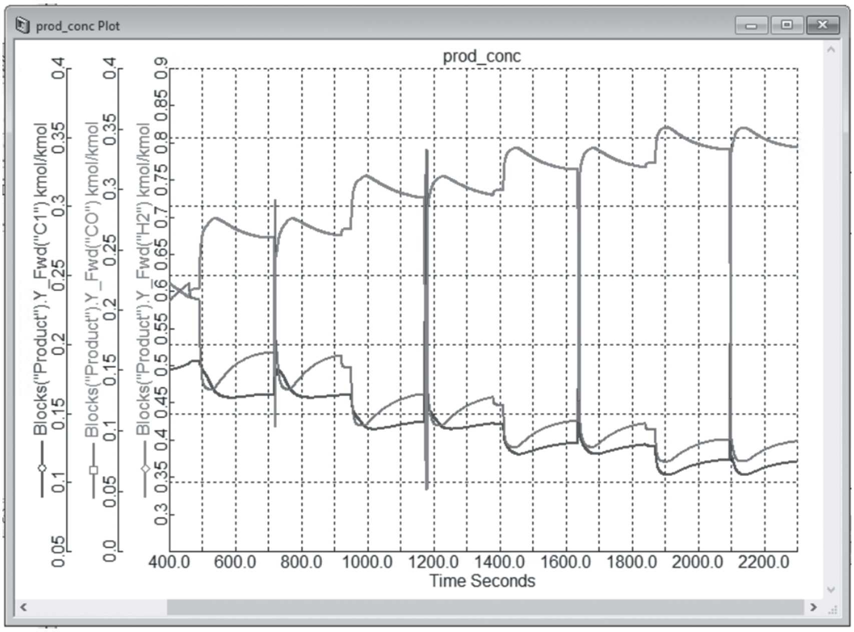


Figure 1.133 Product composition.

modeling multiple beds. In this workshop, we revisit the hydrogen separation, using the two-bed model described in Figure 1.134. We will also replace the “dynamic” blocks with gas cyclic steady state (gCSS) blocks.

The gCSS models enable the direct determination of the cyclic steady state, without carrying out a dynamic simulation over a large number of cycles. gCSS models result from complete discretization of both time and space, and present a periodic adsorption process as a steady-state problem. They offer an extremely

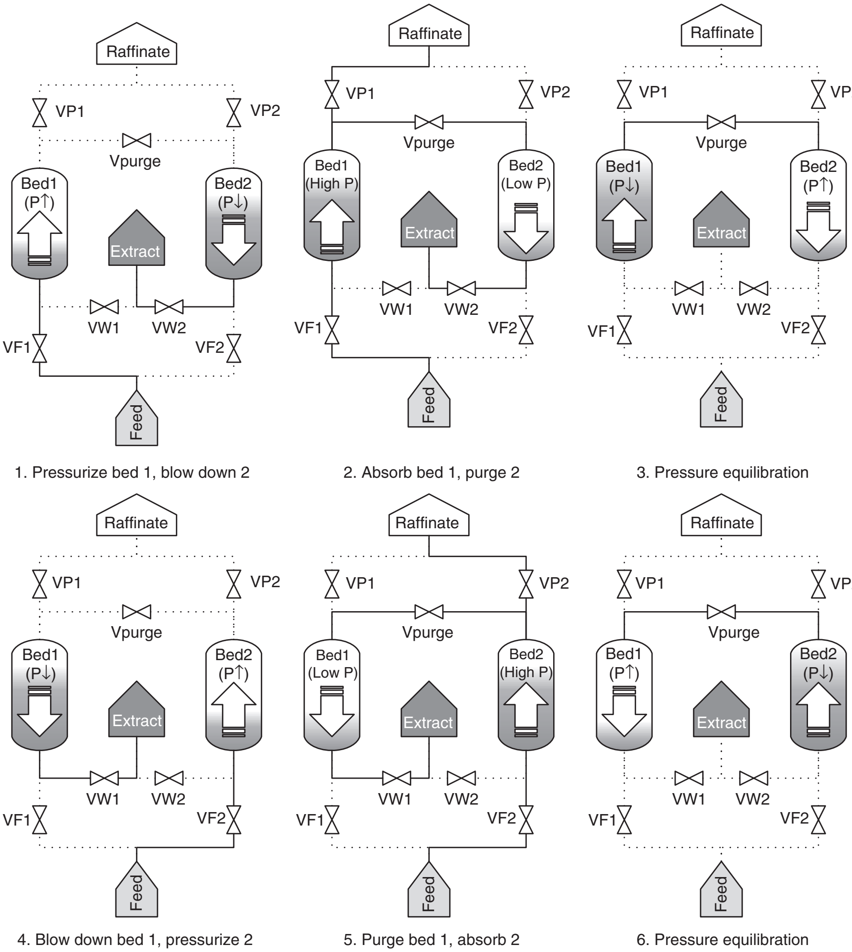


Figure 1.134 The configuration for hydrogen separation.

efficient design tool to optimize the design and operating conditions for an adsorption process. gCSS blocks must be configured differently than dynamic blocks, and so it is important that we know how to work with them.

1.9.1 Define the Components and Property Models

Step 1: Open Aspen

To start with, open a blank Aspen Adsorption document, and show the model libraries using the procedure described in workshop 1 (Figure 1.135). Save the file as **Workshop3a.ada.**

Step 2: Components

Just as before, we start creating our simulation by defining the components that will be present in the simulation. To do this, double-click on the "Default" component list (Figure 1.136) to bring up the "Physical Properties Configuration"

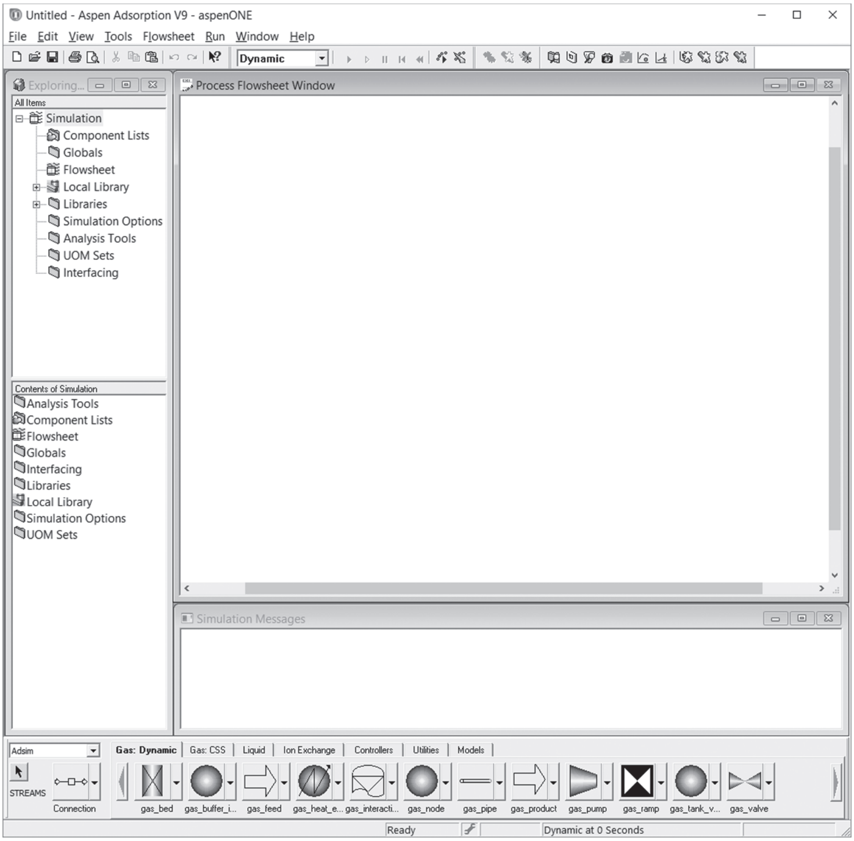


Figure 1.135 A blank adsorption flowsheet.

dialog (Figure 1.137). Configure Aspen Adsorption to use Aspen Properties, which will allow our simulation to calculate important physical properties at a variety of temperatures and conditions.

We need to request data for all of the components in the separation, so we enter all 5 components. Fortunately, we can easily find the simple components we are working with. All we need to do is to enter their names in the “Component ID” column, and Aspen will automatically retrieve the data (Figure 1.138).

After selecting the components, we choose the method for estimating their physical properties. For this separation, the Peng–Robinson method is appropriate (Figure 1.139). Set this value either by clicking on the “specifications” entry in the “Methods” folder on the left, or by clicking on the “Next” button in the ribbon.

Once this step is completed, we are ready to generate the property file that will be used by Aspen Adsorption. To do this, we click on the “Run” button in the ribbon. If the run button is inactive, it is likely that some parameters were not automatically retrieved from the databank. The simplest way to retrieve the parameters is to click on the “Next” button. It will automatically take you

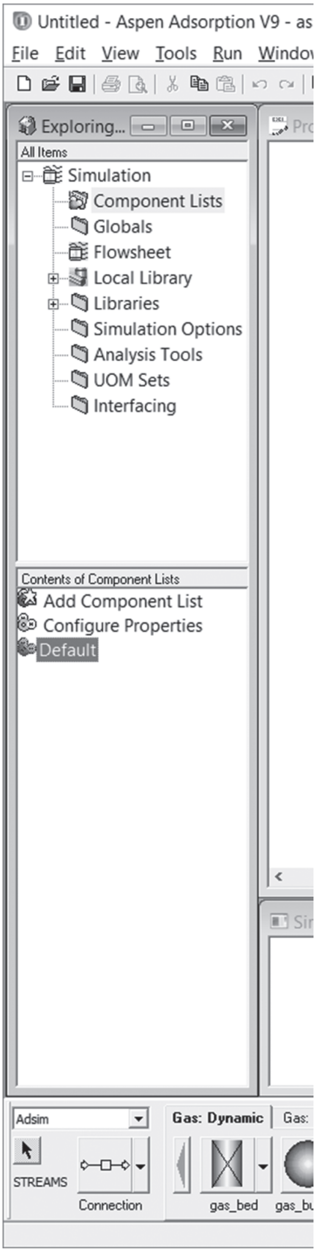
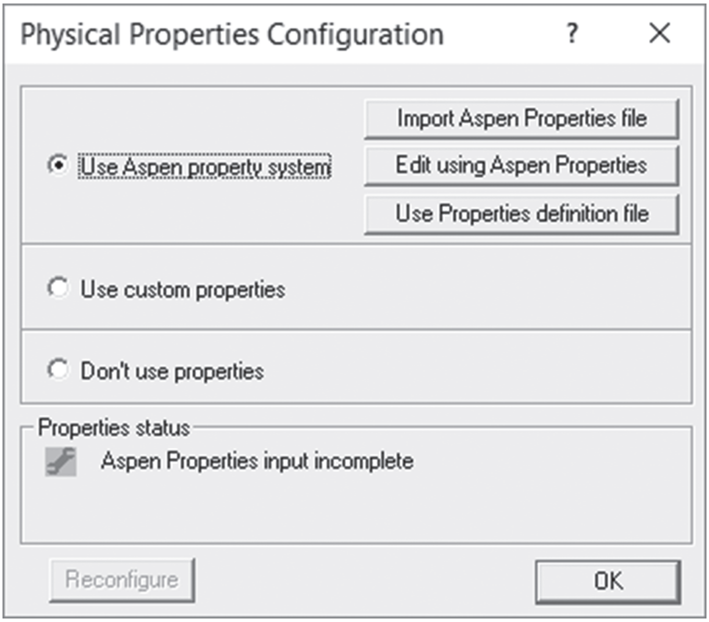


Figure 1.136 Selecting the component list in the explorer window.

to the parameter page, and any parameters that were not previously retrieved will be updated. Once they have been filled in, you may then either click the run button, or "Next" button to run the "Property Analysis/Setup" as shown in Figures 1.140 and 1.141.

Once the property analysis is complete, close the Aspen Properties window, and save the document as **PropsPlus.aprbkp** file when prompted



● Use Aspen property system

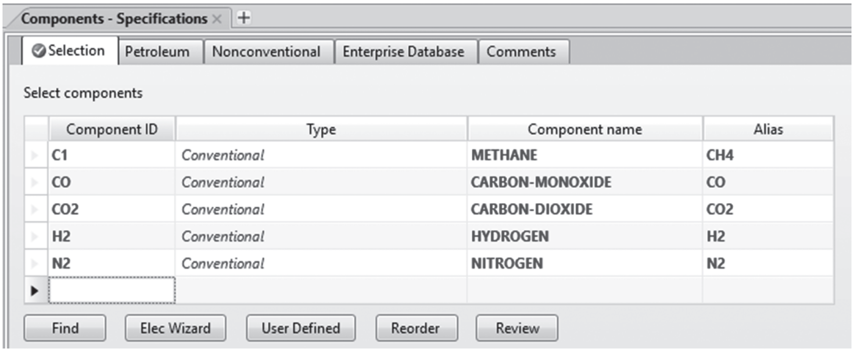
○ Use custom properties

○ Don't use properties

Properties status

Aspen Properties input incomplete

Figure 1.137 Configure the Aspen property system.



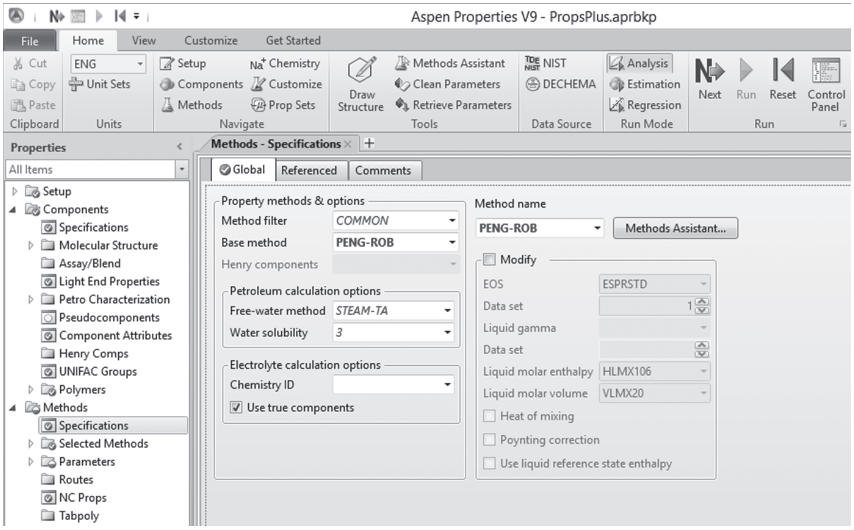
Select components

Component ID	Type	Component name	Alias
C1	Conventional	METHANE	CH4
CO	Conventional	CARBON-MONOXIDE	CO
CO2	Conventional	CARBON-DIOXIDE	CO2
H2	Conventional	HYDROGEN	H2
N2	Conventional	NITROGEN	N2

Figure 1.138 Retrieving components from the property databank.

(Figure 1.142). You may save the file as an Aspen Properties Document format (*.aprop file) if you want to, but we recommend that you select "no" and ask Aspen to not show the message again (Figure 1.143).

If the property file was saved correctly, Aspen Adsorption will report that the Physical Properties have been configured. Click "OK" (Figure 1.144) and then move all of the components from the "available" section to the right-hand column so that they will appear in the simulation (Figure 1.145). Save the file as **Workshop3b.ada**.



Property methods & options

Method filter: COMMON

Base method: PENG-ROB

Henry components:

Petroleum calculation options

Free-water method: STEAM-TA

Water solubility: 3

Electrolyte calculation options

Chemistry ID:

☑ Use true components

Method name: PENG-ROB

☐ Modify

EOS: ESPRSTD

Data set: 1

Liquid gamma:

Data set:

Liquid molar enthalpy: HLMX106

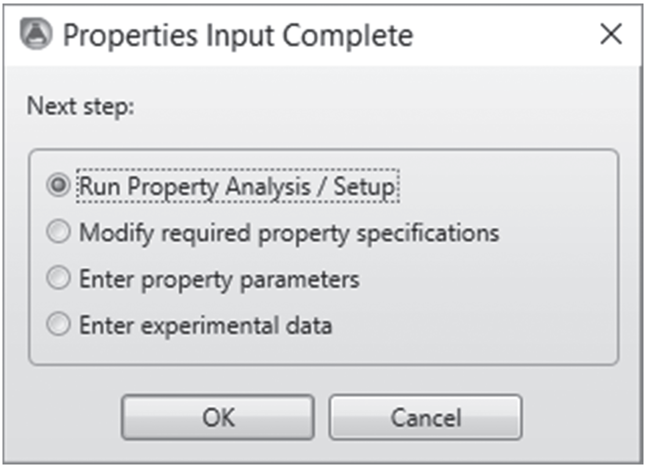
Liquid molar volume: VLMX20

☐ Heat of mixing

☐ Poynting correction

☐ Use liquid reference state enthalpy

Figure 1.139 Selecting the property method.


Properties Input Complete

Next step:

● Run Property Analysis / Setup

○ Modify required property specifications

○ Enter property parameters

○ Enter experimental data

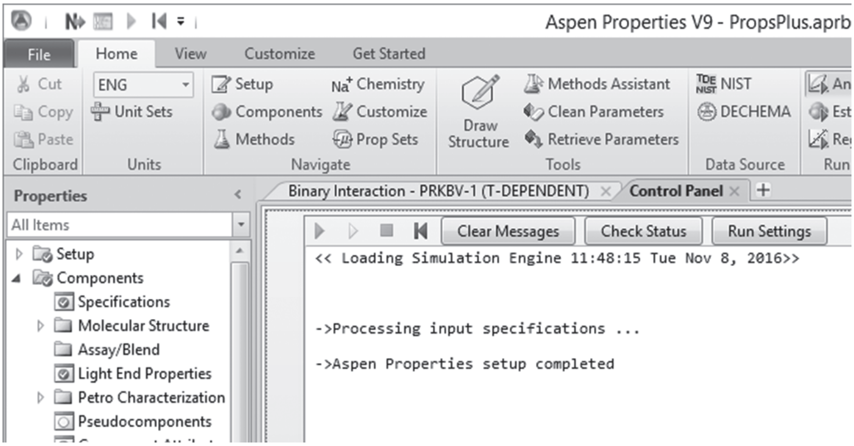
Figure 1.140 Running the Property Analysis.

1.9.2 Working with Model Libraries: Advanced Flowsheet Options

Step 3: Configure CSS_Info and add Cycle Organizer

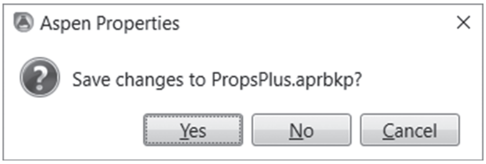
Now that we have completed the component setup, we need to prepare the flowsheet. Because we use gCSS blocks in this simulation, there are some important steps we need to complete before we begin adding the blocks. The first new step is to create an instance of the CSS_Info structure (Figure 1.146). This object contains settings essential to gCSS operation, including:

- The step time
- The number of step time nodes in CSS simulations



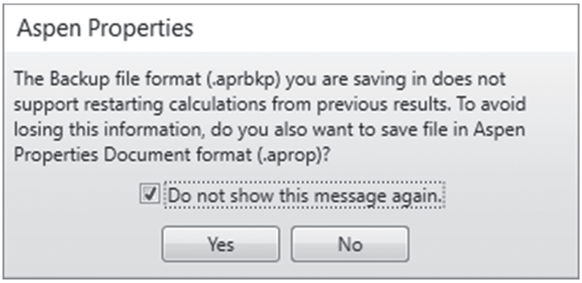
```
<< Loading Simulation Engine 11:48:15 Tue Nov 8, 2016>>


->Processing input specifications ...

->Aspen Properties setup completed
```

Figure 1.141 Control Panel reporting that the Property Analysis was successful.



Save changes to PropsPlus.aprbkp?

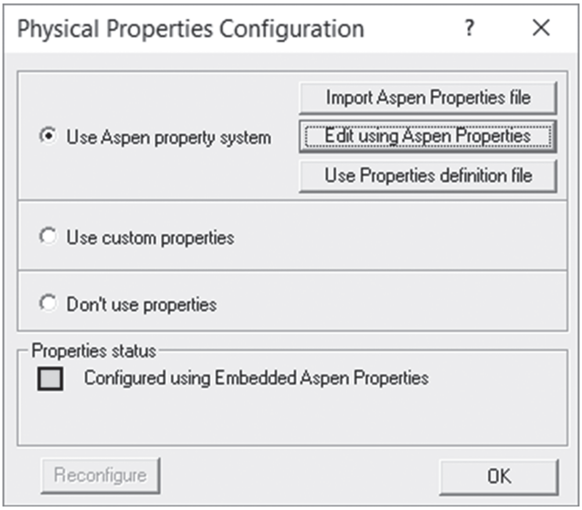
Figure 1.142 Saving the properties for use in Adsorption.



The Backup file format (.aprbkp) you are saving in does not support restarting calculations from previous results. To avoid losing this information, do you also want to save file in Aspen Properties Document format (.aprop)?

☑ Do not show this message again.

Figure 1.143 Additional saving options.



● Use Aspen property system

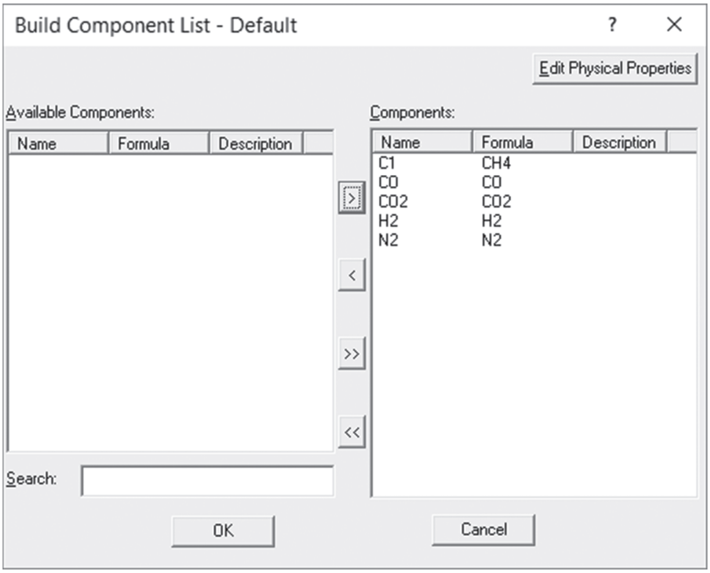
○ Use custom properties

○ Don't use properties

Properties status

☐ Configured using Embedded Aspen Properties

Figure 1.144 The property file is recognized.



Components:

Name	Formula	Description
C1	CH4	
CO	CO	
CO2	CO2	
H2	H2	
N2	N2	

Figure 1.145 Adding all of the components to the simulation.

- Global tearing values
- Whether all gCSS blocks are isothermal or nonisothermal.

Note that it is mandatory to create this object ***before*** placing any blocks on the flowsheet. If you place blocks on the flowsheet before a **CSS_Info** object (Figures 1.147 and 1.148) exists, they will not be able to get the values they need, even if you add a CSS_Info object later. Also note that the name of the CSS_Info block matters. Most of the gCSS blocks we add later are correctly coded to be able to use a CSS_Info block of any name, but some, such as the gCSS_Tank, assume that the CSS_Info block will be named "**CSSInfo**" and will not work if you supply any other name.

Once we have added the structure, we also add a Cycle Organizer (Figure 1.149). At this time, we are not adding any information to the Cycle Organizer, so simply close the Cycle Organizer window that pops up. If you are presented with a "Store Data" dialog, click "yes" (Figure 1.150).

With this, we have performed all the necessary set-up steps, and may now begin laying out the H2 separation. Save as the file as **Workshop3b.ada**.

Step 4: Build flowsheet

We lay out the flowsheet in a very similar way to the air separation workshop, except we use blocks from the Gas: CSS tab in the model library. To begin with, add two gCSS_Adsorber blocks, using any of the icons you wish. We can see icon options by clicking on the small arrow in Figure 1.151.

At this point, the precise placement of the adsorber blocks (Figure 1.152) is not too important, we can align them more carefully once everything is in place.

Now add the void volumes for our simulation. We may use several different icons to help indicate the role of each tank. For example, we can place the

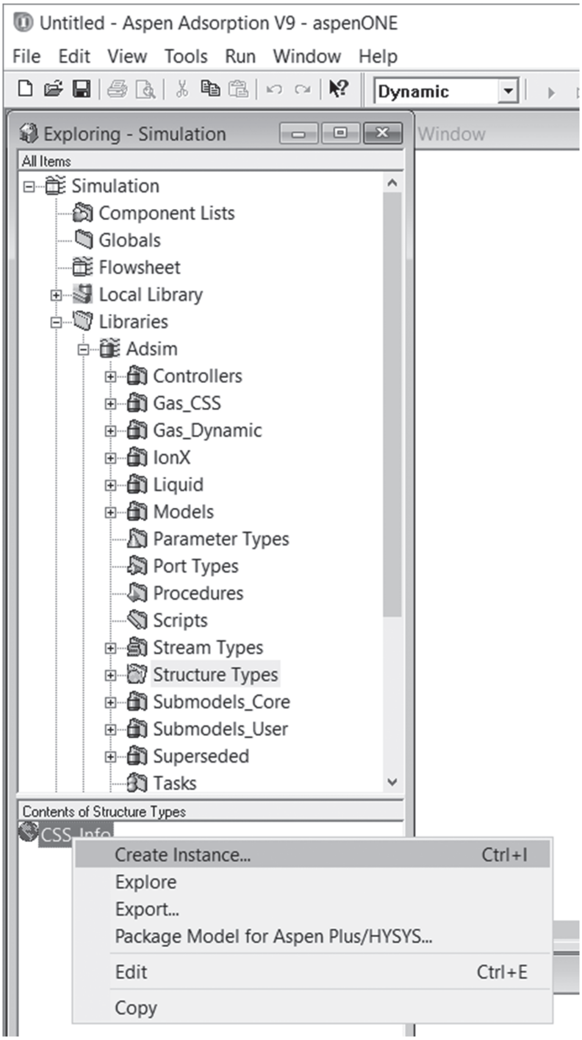
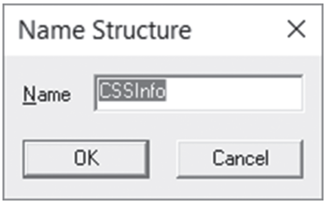


Figure 1.146 Creating an instance of the CSS_Info object.



Name: CSSInfo

Figure 1.147 Naming the CSS_Info structure. This name will work correctly with the gCSS_Tank block.

top and bottom cap icons to indicate that the tanks represent voids at the top and bottom of the adsorption bed, respectively (Figures 1.153 and 1.154). As described previously in Step 8, Section 1.7.2, these gas_tank_void blocks also serve as **essential pressure setters** for the flowsheet.

Figure 1.148 The CSS_Info structure has been successfully added to the flowsheet.

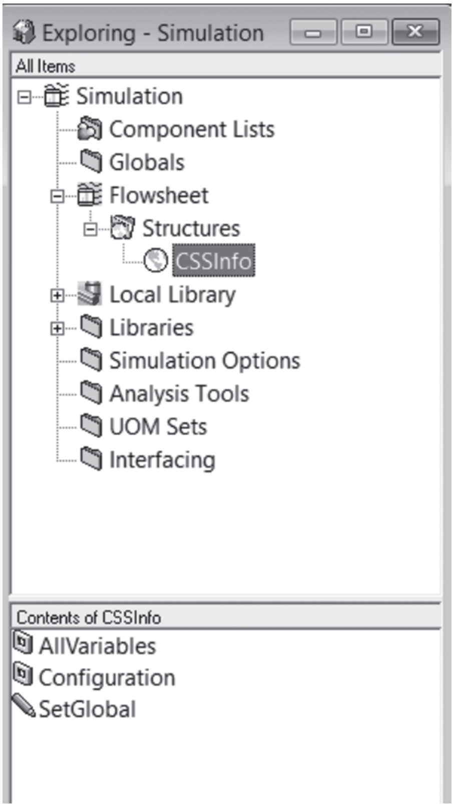
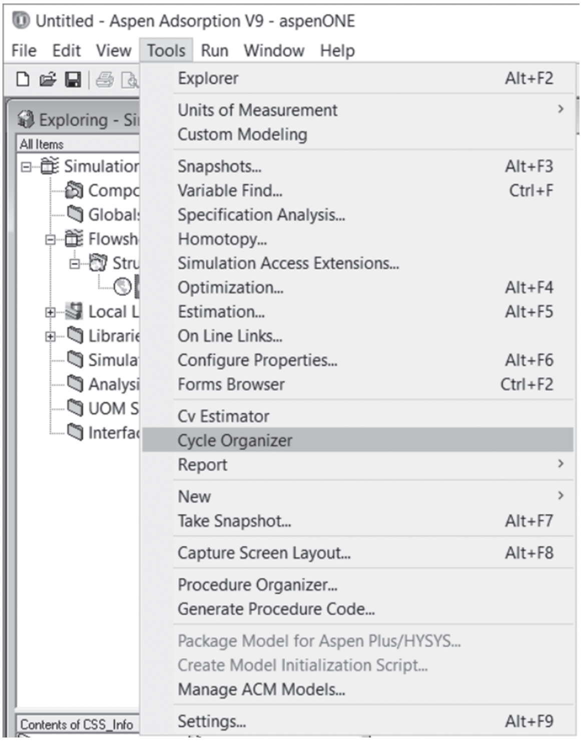
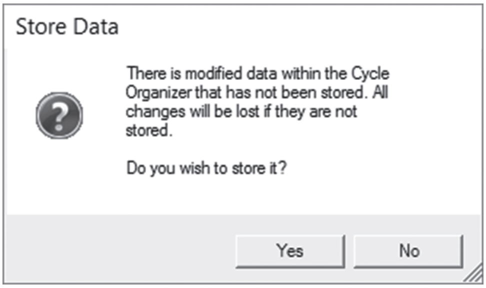


Figure 1.149 Adding the Cycle Organizer.





Store Data

There is modified data within the Cycle Organizer that has not been stored. All changes will be lost if they are not stored.

Do you wish to store it?

Figure 1.150 Always click "yes" when you see this dialog.

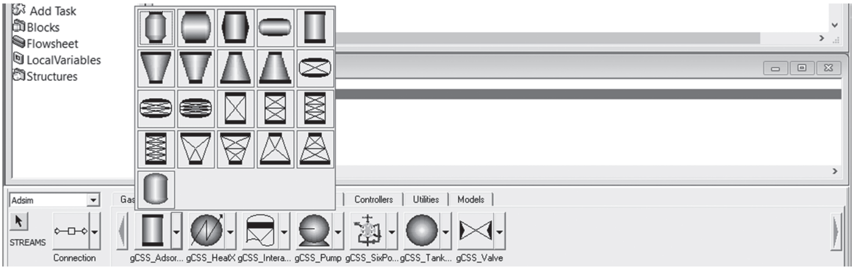


Figure 1.151 Selecting an icon for the gCSS_Adsorber.

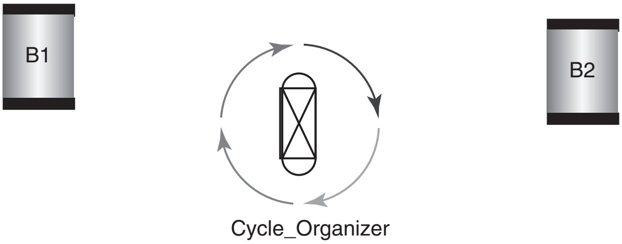
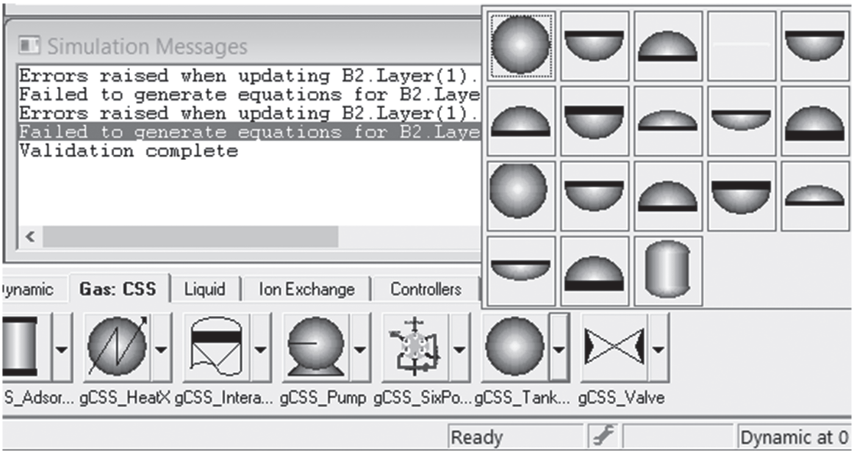


Figure 1.152 gCSS_Adsorber placement.



Simulation Messages

```
Errors raised when updating B2.Layer(1).
Failed to generate equations for B2.Laye
Errors raised when updating B2.Layer(1).
Failed to generate equations for B2.Laye
Validation complete
```

Figure 1.153 Selecting icons for the gCSS_TankVoid block.

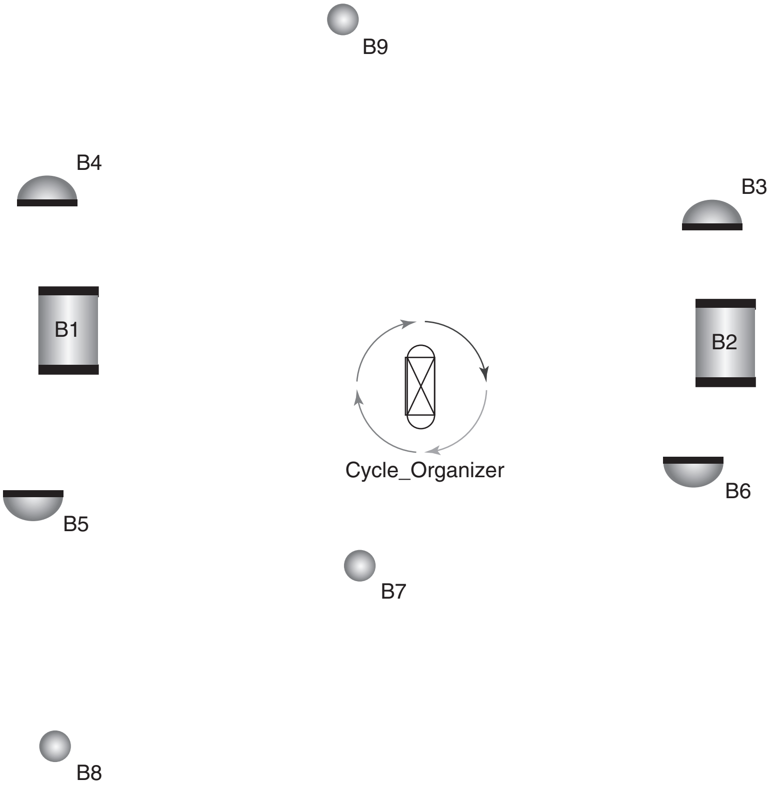
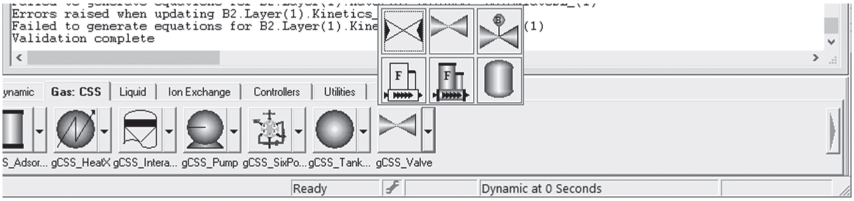


Figure 1.154 Placing tanks on the flowsheet, using three different icons.

Once again, do not spend too much time aligning blocks at this stage, the goal is to get the correct blocks into the flowsheet.

Finally, we add the 10 valves (Figures 1.155 and 1.156).



```
Errors raised when updating B2.Layer(1).Kinetics_
Failed to generate equations for B2.Layer(1).Kine        (1)
Validation complete
```

Figure 1.155 Valve icon selection.

Once again, there is no need for precise placement.

Now, in order to get ready for the connecting streams, let us rotate the valves on either side of the adsorbent beds. To do that, make sure that the Process Flowsheet ToolBar is visible. It can be toggled by right-clicking on the flowsheet and clicking on the Process Flowsheet ToolBar entry (Figure 1.157).

Now once the rotation icons are visible, rotate the four valves that are selected in Figure 1.158 to the left.

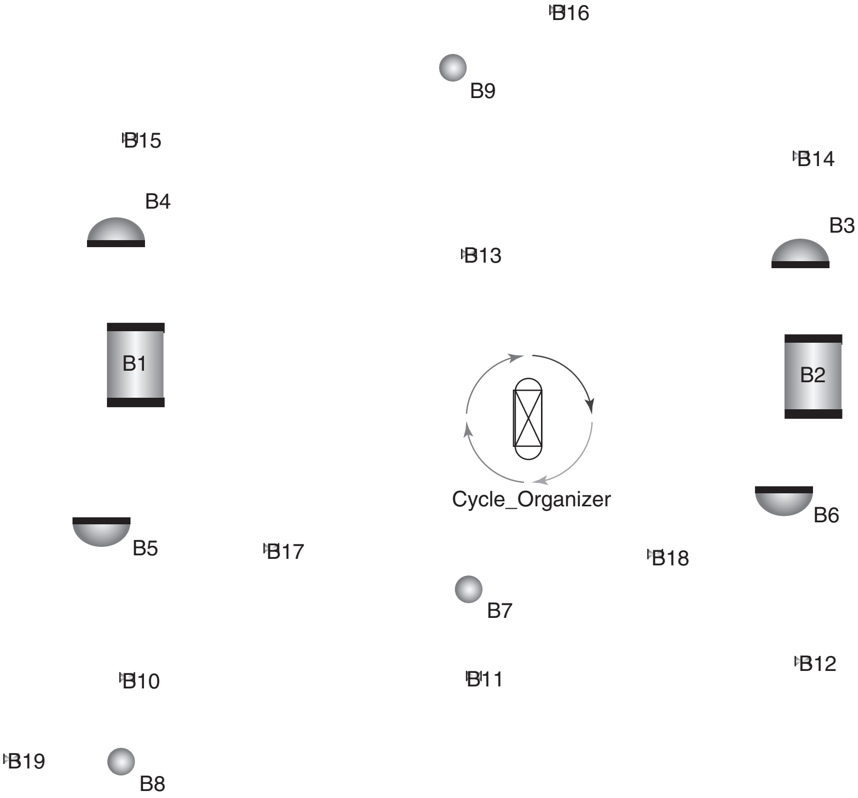


Figure 1.156 Valve placement.

Figure 1.157 Toggling the Process Flowsheet ToolBar.

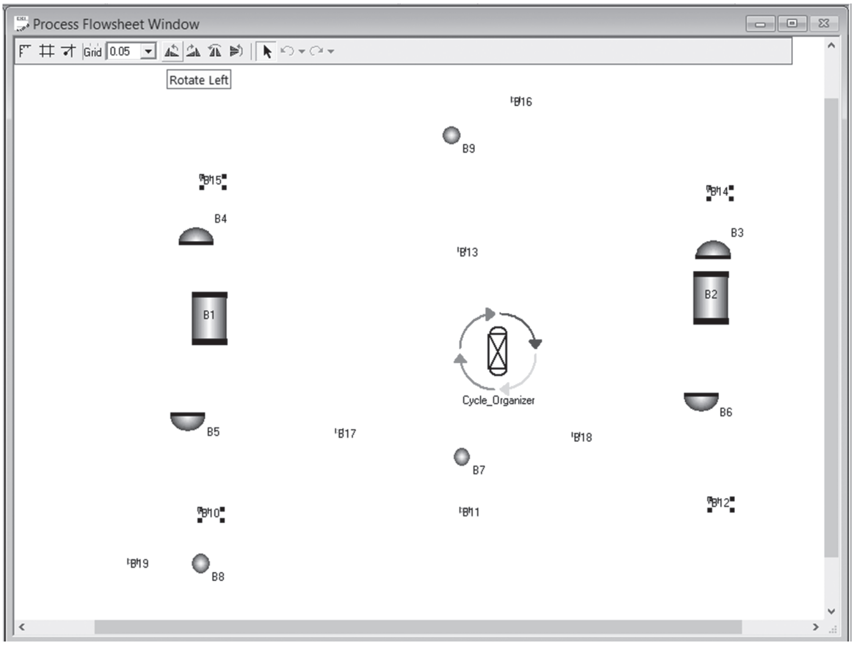
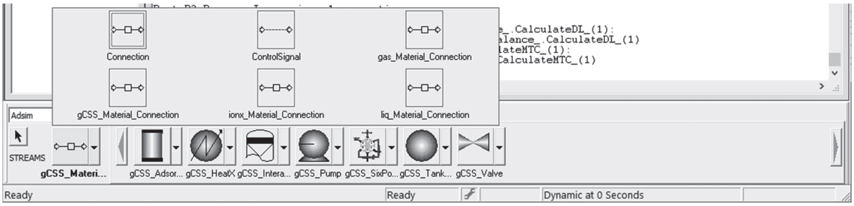


Figure 1.158 Rotating the adsorbent bed valves.

After rotating the valves, we begin connecting the blocks together. Because we are using gCSS blocks, we must select the gCSS_material_connection before connecting the blocks (Figure 1.159).



```
_.CalculateDL_(1):
alance_.CalculateDL_(1)
lateMTC_(1):
CalculateMTC_(1)
```

Figure 1.159 Selecting the gCSS_material_connection in order to define flowsheet connections.

Once we have selected the gCSS_material_connection, the connectivity arrows will appear on the flowsheet (Figure 1.160). Connect the streams as usual, and double-check that the streams are connected in the correct directions.

Once the connection streams have been laid out, we save the flowsheet. Also consider flipping the valve on the right-hand side so that the connections will be more linear (Figure 1.161).

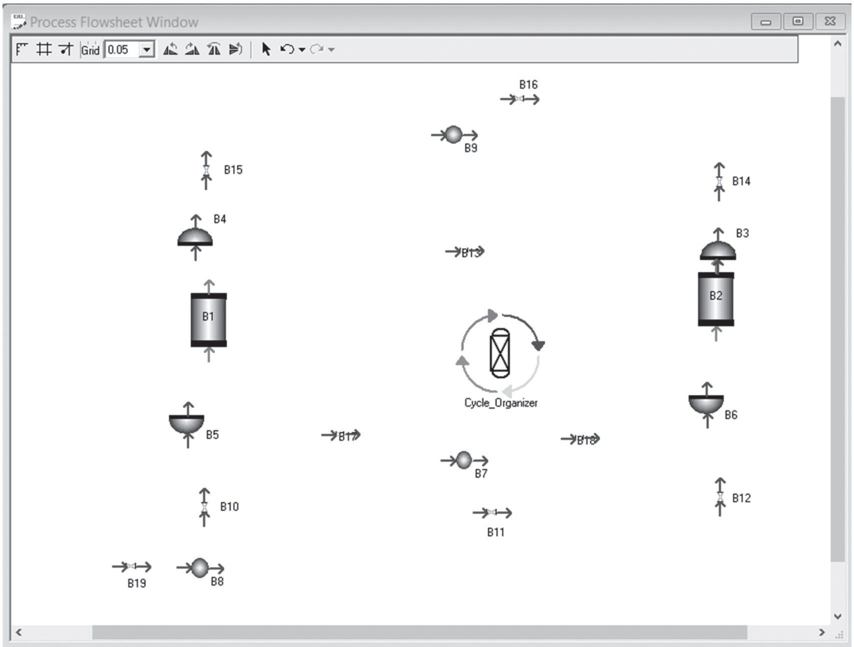


Figure 1.160 Flowsheet connection arrows.

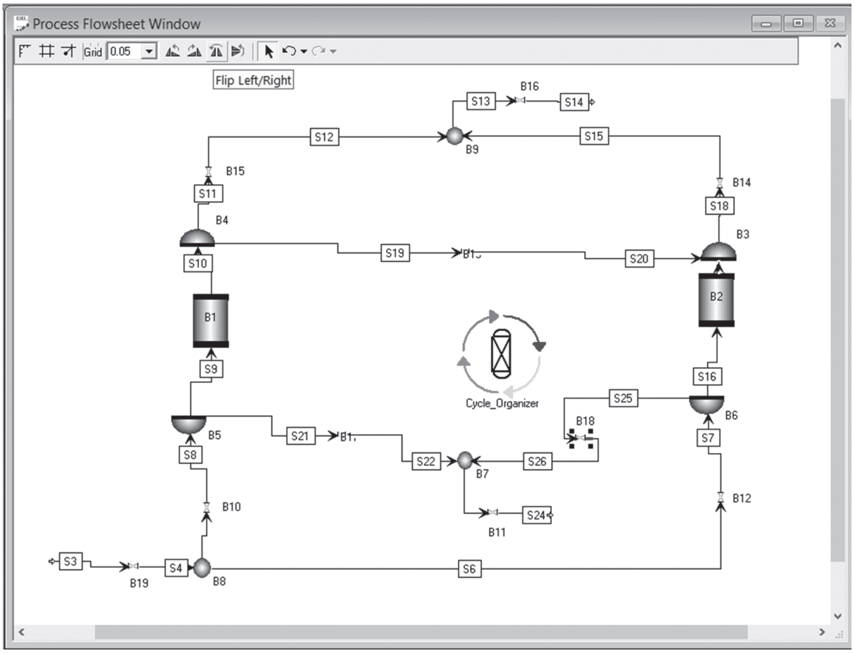
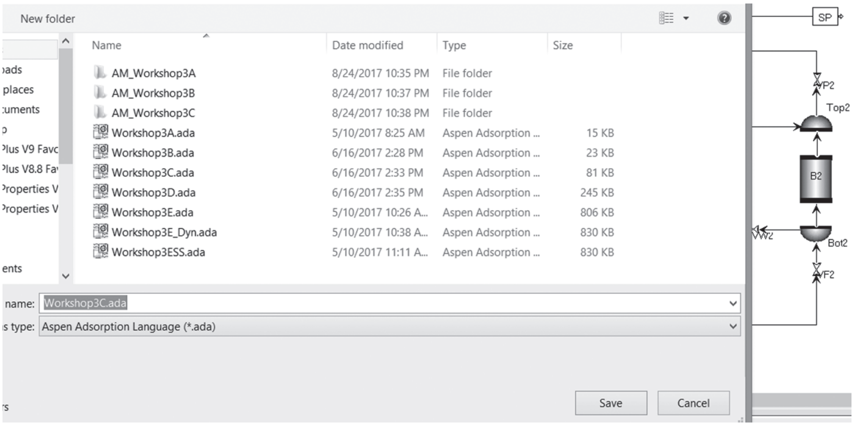


Figure 1.161 Flipping the B18 block left-to-right.

Step 5: Save the file as *Workshop3c.ada* (Figure 1.162)



Name	Date modified	Type	Size
AM_Workshop3A	8/24/2017 10:35 PM	File folder	
AM_Workshop3B	8/24/2017 10:37 PM	File folder	
AM_Workshop3C	8/24/2017 10:38 PM	File folder	
Workshop3A.ada	5/10/2017 8:25 AM	Aspen Adsorption ...	15 KB
Workshop3B.ada	6/16/2017 2:28 PM	Aspen Adsorption ...	23 KB
Workshop3C.ada	6/16/2017 2:33 PM	Aspen Adsorption ...	81 KB
Workshop3D.ada	6/16/2017 2:35 PM	Aspen Adsorption ...	245 KB
Workshop3E.ada	5/10/2017 10:26 A...	Aspen Adsorption ...	806 KB
Workshop3E_Dyn.ada	5/10/2017 10:38 A...	Aspen Adsorption ...	830 KB
Workshop3ESS.ada	5/10/2017 11:11 A...	Aspen Adsorption ...	830 KB

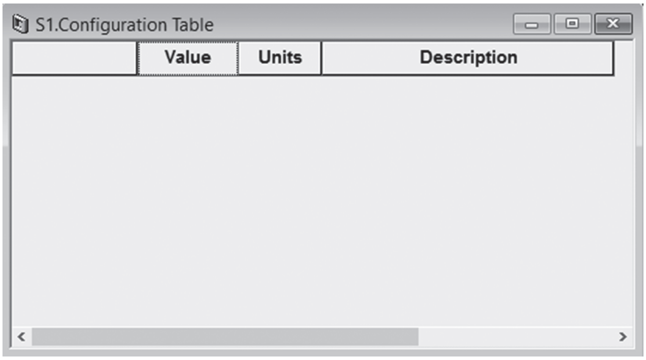
name: Workshop3C.ada

s type: Aspen Adsorption Language (*.ada)

Figure 1.162 Save the document using the default file type as **Workshop3c.ada**.

Step 6: Clean up

Before we finalize the flowsheet, it is useful to check if the blocks and streams are correctly recognizing the CSS_Info structure that we created in step 1. A simple way to do this is to double-click on the feed stream, and look at the form which comes up. If the form has no variables (Figure 1.163), then the streams cannot locate the CSS_Info structure. The simplest fix for this miscommunication is to cut all the blocks out of the flowsheet, then paste them back in.



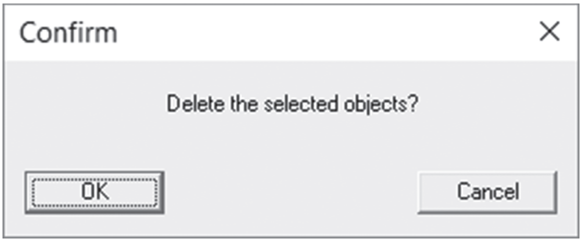
	Value	Units	Description

Figure 1.163 A stream that cannot communicate with the CSS_Info structure.

When you cut the objects, you will be presented with a delete dialog, and you must pick “OK” (Figure 1.164).

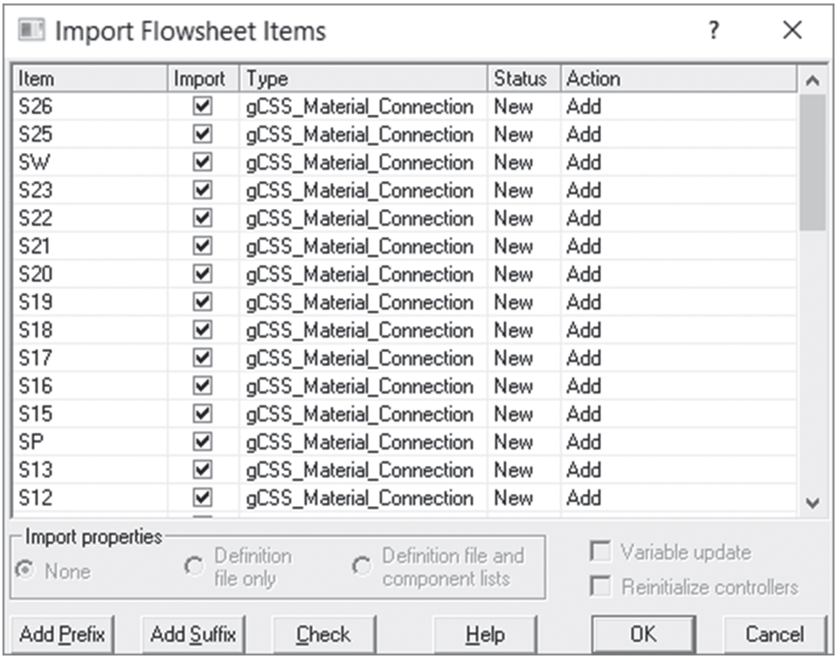
When you paste the objects, you will be presented with a dialog that allows you to specify which objects you wish to paste, and make changes to their names if you wish (Figure 1.165).

Once we have ensured that all the blocks are correctly communicating with the CSS_Info Structure, we can do some housekeeping. The simplest



Delete the selected objects?

Figure 1.164 Cutting objects from the flowsheet.



Item	Import	Type	Status	Action
S26	☑	gCSS_Material_Connection	New	Add
S25	☑	gCSS_Material_Connection	New	Add
SW	☑	gCSS_Material_Connection	New	Add
S23	☑	gCSS_Material_Connection	New	Add
S22	☑	gCSS_Material_Connection	New	Add
S21	☑	gCSS_Material_Connection	New	Add
S20	☑	gCSS_Material_Connection	New	Add
S19	☑	gCSS_Material_Connection	New	Add
S18	☑	gCSS_Material_Connection	New	Add
S17	☑	gCSS_Material_Connection	New	Add
S16	☑	gCSS_Material_Connection	New	Add
S15	☑	gCSS_Material_Connection	New	Add
SP	☑	gCSS_Material_Connection	New	Add
S13	☑	gCSS_Material_Connection	New	Add
S12	☑	gCSS_Material_Connection	New	Add

Import properties: ● None ○ Definition file only ○ Definition file and component lists

☐ Variable update

☐ Reinitialize controllers

Figure 1.165 Pasting objects back into the flowsheet.

way to make a well-organized flowsheet is to use the “Align Blocks” and “Redraw streams” tools. This flowsheet is simple enough that we can do these operations on all the streams at once. Use the **ctrl+A** shortcut to select all the objects in the flowsheet, then press **ctrl+B** to align the blocks, and **ctrl+J** to update the path of the streams. You may repeat the **ctrl+B** and **ctrl+J** process a few times to make sure that everything is fully aligned (Figure 1.166). If your flowsheet is well laid out to begin with, you will quickly end up with a neat and organized final result. If your flowsheet is too disorganized to begin with, you may have to manually move blocks and streams around before you can get a good end-product.

Now that everything is organized, we can declutter the flowsheet by hiding the names of some streams. In this flowsheet, we do not need to know the names of any streams, except those of the feed and product streams, so we can hide everything else. Use ctrl+click to select all of the process streams, except the feed and products, then use ctrl+H to hide the labels containing the stream names (Figure 1.167).

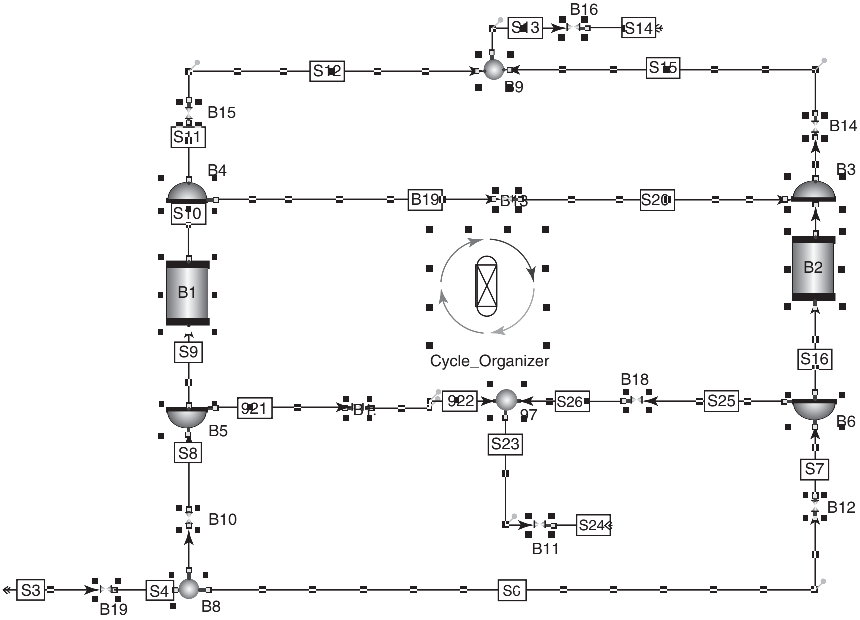


Figure 1.166 Flowsheet with all streams selected and aligned.

Finally, we can give more descriptive names to the blocks and streams in the flowsheet. To do this, click on the block you wish to rename, then press

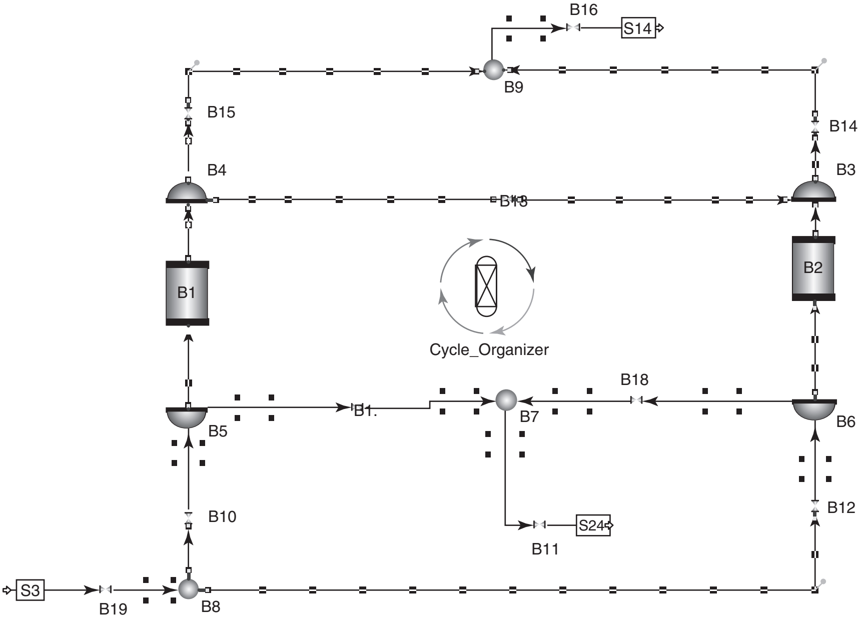
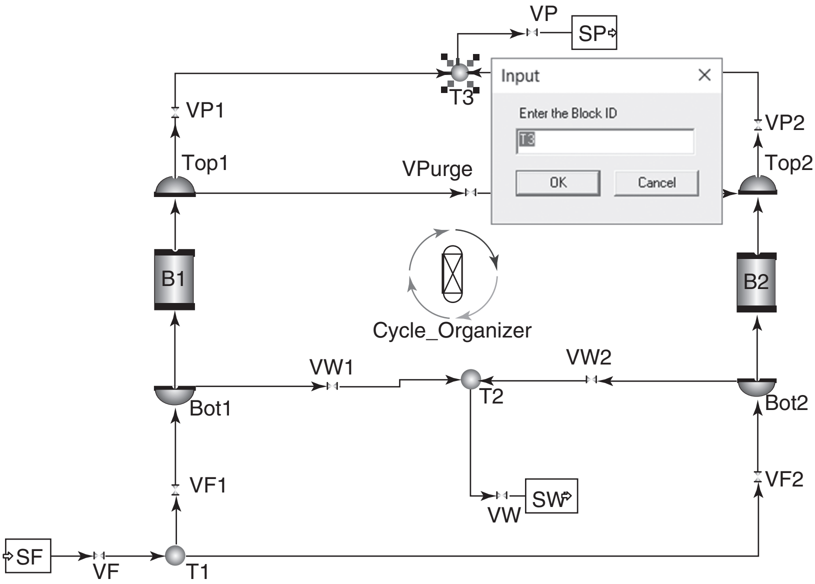


Figure 1.167 Flowsheet with stream names hidden.

ctrl+M to rename it. There are some restrictions on the names you may use, and Aspen will give you a helpful message if you accidentally enter a disallowed name. Rename all the tanks and valves in the flowsheet with helpful names, as shown in Figure 1.168.



Enter the Block ID

T3

Figure 1.168 Renaming the tanks, valves, and streams.

Step 7: Specify Feed Streams

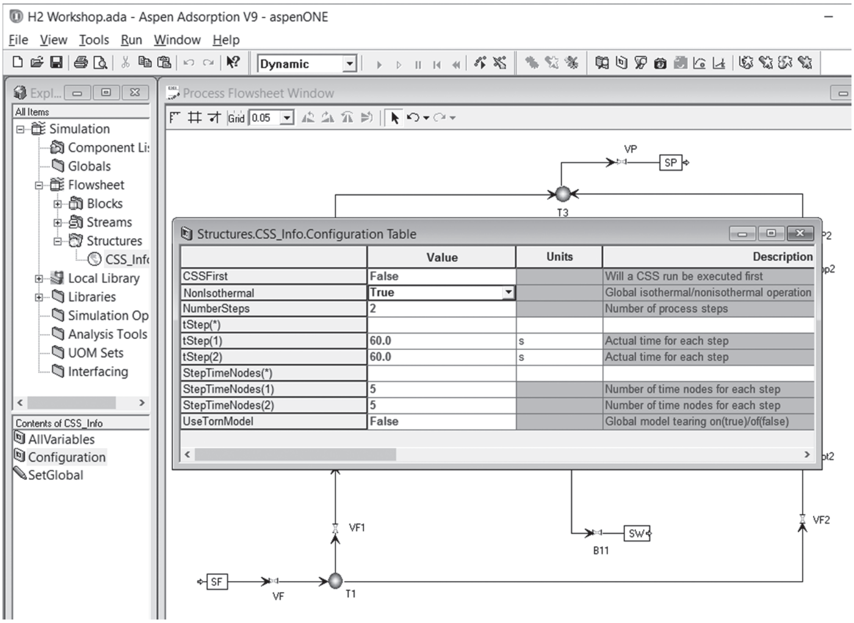
The first step to specifying the feed blocks is to make sure that the feed blocks will have all the variables we wish to specify. By default, the gCSS blocks are considered to be isothermal, which we do not want. To change this, we must edit the CSS_Info structure we created in step 3. Open the "Configuration" form from the Explorer, and set the "NonIsothermal" variable to "True" (Figure 1.169). This will update all the gCSS streams, tanks, and valves to have additional temperature-related options and variables.

Now we can specify the concentrations and temperatures of our feed, product, and waste streams (Figures 1.170–1.172). To do this, double-click on the stream whose values you wish to set. Be careful not to click close to the end of a stream, or you may end up moving the location of the end.

1.9.3 Introduction to Scripting: Set Repeated Values and Initialize Blocks

Step 8: Set all tanks to be nonadiabatic

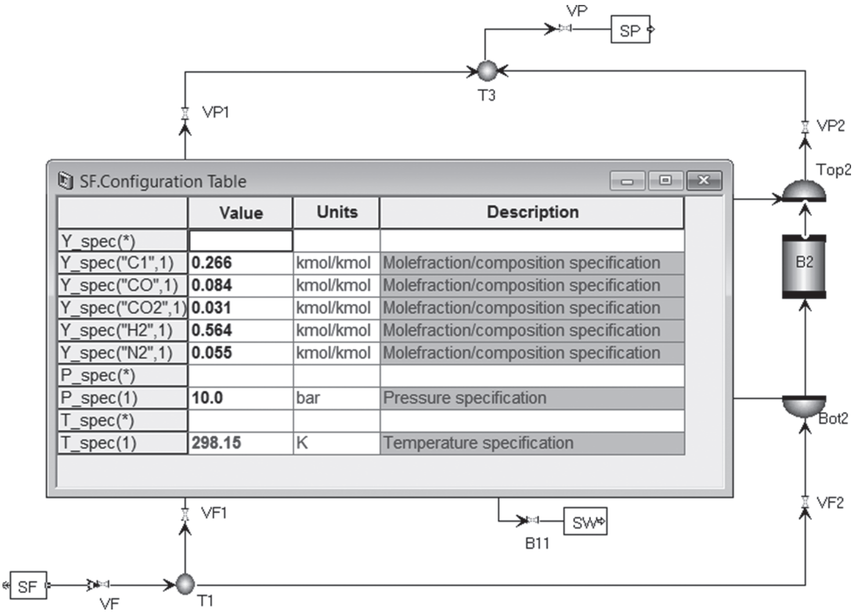
Double-click on each tank to open their configuration form. Set the "NonAdiabaticTankVolume" to "True" (Figure 1.173). Doing this manually can be slow, but there is an alternative!



Structures.CSS_Info.Configuration Table

	Value	Units	Description
CSSFirst	False		Will a CSS run be executed first
NonIsothermal	True		Global isothermal/nonisothermal operation
NumberSteps	2		Number of process steps
tStep(*)			
tStep(1)	60.0	s	Actual time for each step
tStep(2)	60.0	s	Actual time for each step
StepTimeNodes(*)			
StepTimeNodes(1)	5		Number of time nodes for each step
StepTimeNodes(2)	5		Number of time nodes for each step
UseTornModel	False		Global model tearing on(true)/of(false)

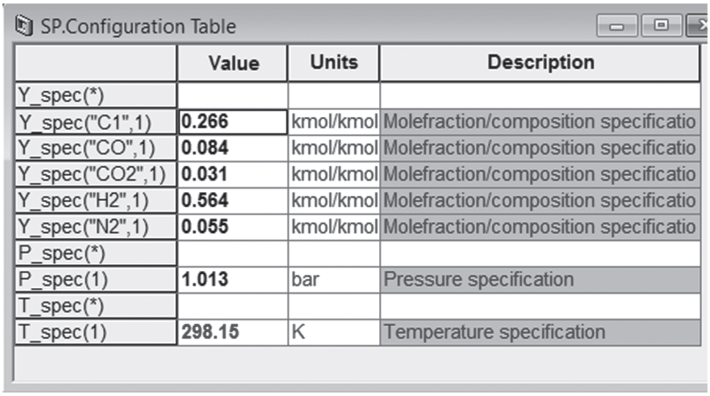
Figure 1.169 Configuring the CSSInfo structure to be nonisothermal.



SF.Configuration Table

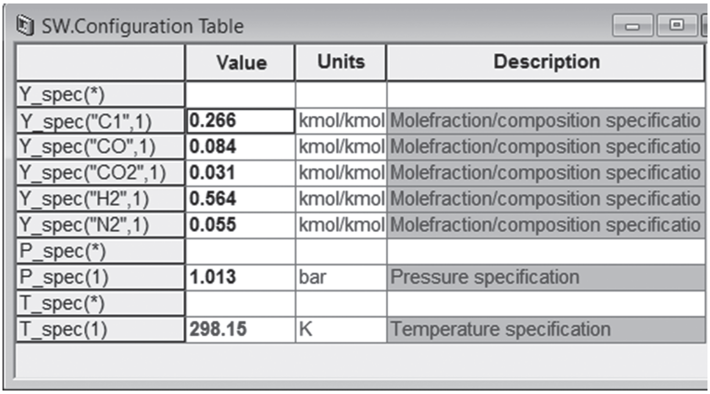
	Value	Units	Description
Y_spec(*)			
Y_spec("C1",1)	0.266	kmol/kmol	Molefraction/composition specification
Y_spec("CO",1)	0.084	kmol/kmol	Molefraction/composition specification
Y_spec("CO2",1)	0.031	kmol/kmol	Molefraction/composition specification
Y_spec("H2",1)	0.564	kmol/kmol	Molefraction/composition specification
Y_spec("N2",1)	0.055	kmol/kmol	Molefraction/composition specification
P_spec(*)			
P_spec(1)	10.0	bar	Pressure specification
T_spec(*)			
T_spec(1)	298.15	K	Temperature specification

Figure 1.170 Specifying the Feed Stream.


SP.Configuration Table

	Value	Units	Description
Y_spec(*)			
Y_spec("C1",1)	0.266	kmol/kmol	Molefraction/composition specificatio
Y_spec("CO",1)	0.084	kmol/kmol	Molefraction/composition specificatio
Y_spec("CO2",1)	0.031	kmol/kmol	Molefraction/composition specificatio
Y_spec("H2",1)	0.564	kmol/kmol	Molefraction/composition specificatio
Y_spec("N2",1)	0.055	kmol/kmol	Molefraction/composition specificatio
P_spec(*)			
P_spec(1)	1.013	bar	Pressure specification
T_spec(*)			
T_spec(1)	298.15	K	Temperature specification

Figure 1.171 Specify the Product Stream.


SW.Configuration Table

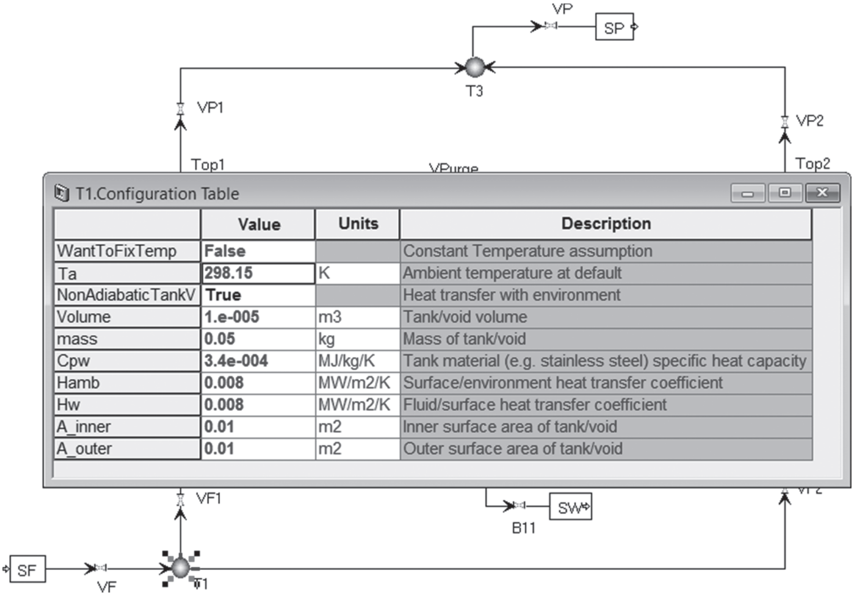
	Value	Units	Description
Y_spec(*)			
Y_spec("C1",1)	0.266	kmol/kmol	Molefraction/composition specificatio
Y_spec("CO",1)	0.084	kmol/kmol	Molefraction/composition specificatio
Y_spec("CO2",1)	0.031	kmol/kmol	Molefraction/composition specificatio
Y_spec("H2",1)	0.564	kmol/kmol	Molefraction/composition specificatio
Y_spec("N2",1)	0.055	kmol/kmol	Molefraction/composition specificatio
P_spec(*)			
P_spec(1)	1.013	bar	Pressure specification
T_spec(*)			
T_spec(1)	298.15	K	Temperature specification

Figure 1.172 The Waste Stream.

If we wish, instead of manually setting all the values, we can create a *script* to automate the process. In the "Flowsheet" section of the Explorer window, click on "Add Script" and name it UtilityScript. Inside the script, add the lines of code specified in Figure 1.174.

This script not only sets the NonAdiabatic variable that we care about, it also sets an initial value for the gas composition inside the tank. By default, Aspen assumes that all the components are present in equal quantities, so for our five-component system, Aspen assumes a value of 0.2 for the mole fraction of each component. This script gives us a nice way to change that assumption in all the tanks at once.

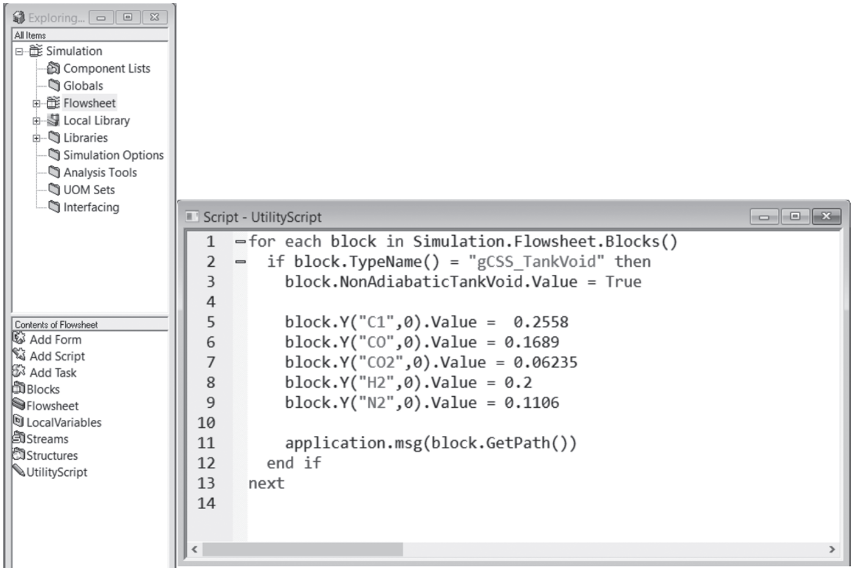
To execute this script, you can either press ctrl+shift+I while the script is open, or simply double-click the UtilityScript object in the explorer window. Once you do that, you should see the following messages in the message window to confirm that the script set the values in each of the seven tanks (Figure 1.175).



T1.Configuration Table

	Value	Units	Description
WantToFixTemp	False		Constant Temperature assumption
Ta	298.15	K	Ambient temperature at default
NonAdiabaticTankV	True		Heat transfer with environment
Volume	1.e-005	m3	Tank/void volume
mass	0.05	kg	Mass of tank/void
Cpw	3.4e-004	MJ/kg/K	Tank material (e.g. stainless steel) specific heat capacity
Hamb	0.008	MW/m2/K	Surface/environment heat transfer coefficient
Hw	0.008	MW/m2/K	Fluid/surface heat transfer coefficient
A_inner	0.01	m2	Inner surface area of tank/void
A_outer	0.01	m2	Outer surface area of tank/void

Figure 1.173 Specifying the tank to be nonadiabatic.



```
for each block in Simulation.Flowsheet.Blocks()
  if block.TypeName() = "gCSS_TankVoid" then
    block.NonAdiabaticTankVoid.Value = True

    block.Y("C1",0).Value =  0.2558
    block.Y("CO",0).Value = 0.1689
    block.Y("CO2",0).Value = 0.06235
    block.Y("H2",0).Value = 0.2
    block.Y("N2",0).Value = 0.1106

    application.msg(block.GetPath())
  end if
next
```

Figure 1.174 Creating the UtilityScript.

Step 9: Specify valves

We use the same strategy as the air separation workshop. VF, VP, VW, and Vpurge will all be implemented as control valves that have their flow rate set by the pressure drop across them, while the bed-specific valves (VF1, VF2, VP1, VP2, VW1, and VW2) will be either completely open or completely closed. As

```
Top2
Top1
Bot1
Bot2
T2
T1
T3
```

Figure 1.175 The output of our utility script.

with the tanks, the names of the variables and their presentation is different between the "dynamic" and gCSS valves.

Set the values shown in Table 1.11. If you are paying attention, you may notice that the Use_Spec(1) variables will simply be overwritten by the Cycle Organizer, once we implement it. However, in this workshop, setting the values does actually serve a purpose, which will be explained once the simulation is ready to be run.

Table 1.11 Valve specifications for workshop 3.

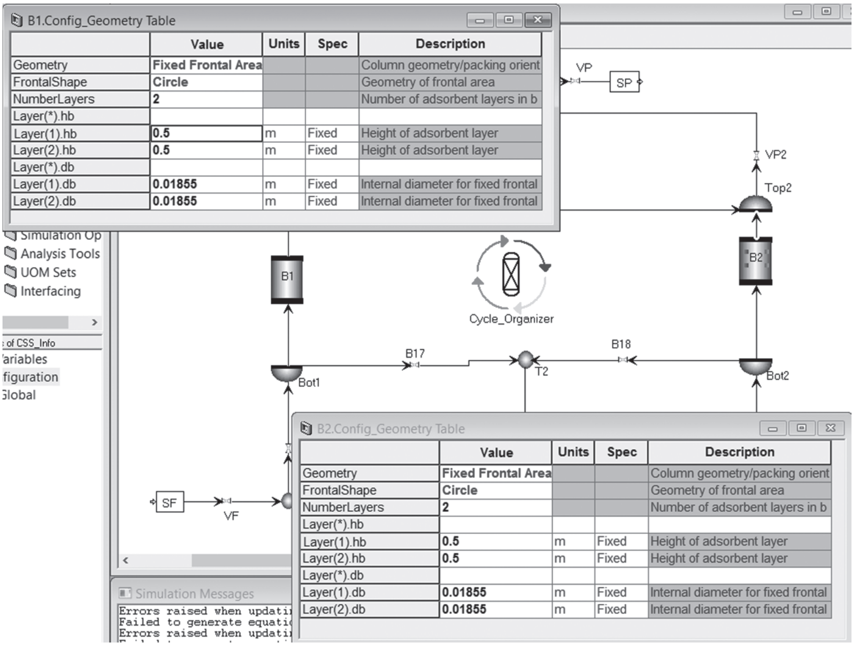
Valve variable	#	Valve variable	kmol/(s bar^{-1})
VF1.Use_spec(1)	1	VF.Cv_spec(1)	2.00e−05
VF2.Use_spec(1)	1	VP.Cv_spec(1)	5.60e−09
VF.Use_spec(1)	2	Vpurge.Cv_spec(1)	1.80e−07
VP1.Use_spec(1)	1	VW.Cv_spec(1)	1.00e−05
VP2.Use_spec(1)	1		
VP.Use_spec(1)	2		
Vpurge.Use_spec(1)	0		
VW1.Use_spec(1)	1		
VW2.Use_spec(1)	1		
VW.Use_spec(1)	2		

1.9.4 Inspecting Blocks: Advanced Operating Conditions

Step 10: Specify separators

We have now set up the flowsheet, but we have two remaining tasks before we can run the simulation. First, we need to specify the properties of the adsorbent bed. Following this, we schedule the valve timings. To start with, simply double-click on each bed to open the geometry form. Specify that the adsorbent bed has two layers, and have the sizes specified in Figure 1.176.

Unlike with the "Gas: Dynamic" blocks, the gCSS blocks do not provide a nice user interface for specifying the rest of the property values. We have to find



B1.Config_Geometry Table

	Value	Units	Spec	Description
Geometry	**Fixed Frontal Area**			Column geometry/packing orient
FrontalShape	**Circle**			Geometry of frontal area
NumberLayers	**2**			Number of adsorbent layers in b
Layer(*).hb				
Layer(1).hb	**0.5**	m	Fixed	Height of adsorbent layer
Layer(2).hb	**0.5**	m	Fixed	Height of adsorbent layer
Layer(*).db				
Layer(1).db	**0.01855**	m	Fixed	Internal diameter for fixed frontal
Layer(2).db	**0.01855**	m	Fixed	Internal diameter for fixed frontal

B2.Config_Geometry Table

	Value	Units	Spec	Description
Geometry	**Fixed Frontal Area**			Column geometry/packing orient
FrontalShape	**Circle**			Geometry of frontal area
NumberLayers	**2**			Number of adsorbent layers in b
Layer(*).hb				
Layer(1).hb	**0.5**	m	Fixed	Height of adsorbent layer
Layer(2).hb	**0.5**	m	Fixed	Height of adsorbent layer
Layer(*).db				
Layer(1).db	**0.01855**	m	Fixed	Internal diameter for fixed frontal
Layer(2).db	**0.01855**	m	Fixed	Internal diameter for fixed frontal

```
Errors raised when updati
Failed to generate equati
Errors raised when updati
```

Figure 1.176 Identical bed geometries.

and specify the values manually. To begin, explore the first bed by right-clicking on it (Figure 1.177).

Once the explorer is open, we see a long list of “Config” forms, as shown in the left-hand window in Figure 1.178.

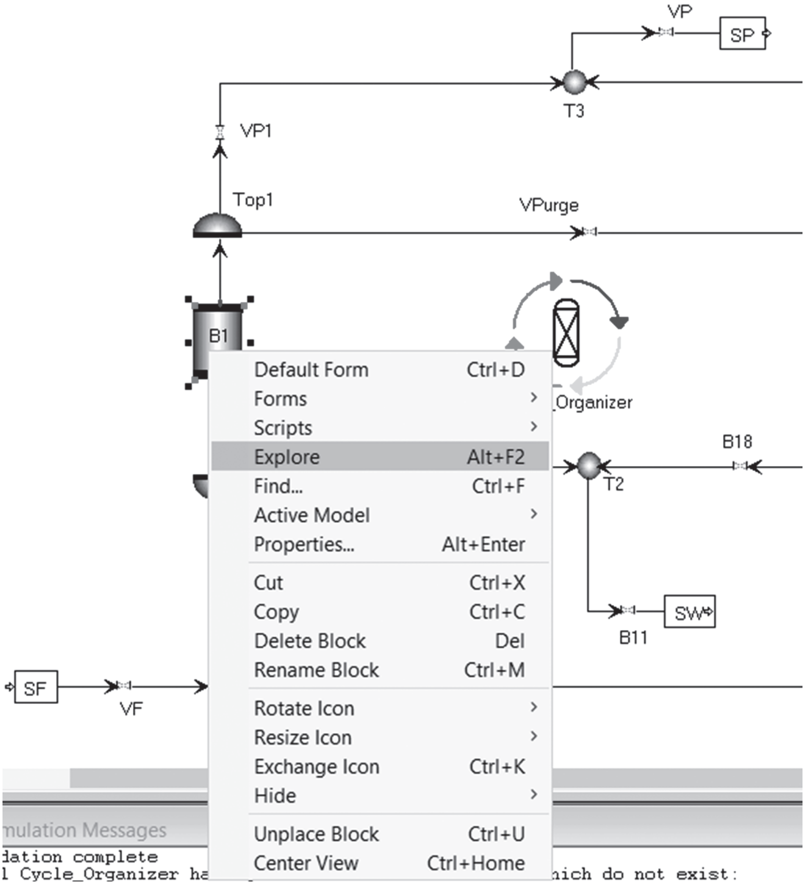
Step 11: Specify the adsorbent properties

Once the “Config” forms are visible, begin opening them one at a time in order to specify the adsorbent bed’s properties. To begin with, open the Adsorbent Property form.

Note that each variable has two entries, because our adsorber has two layers. Remember that we are modeling an adsorber that uses two different adsorbents, so this is precisely the behavior we need, provided we have the data for both adsorbents.

Step 12: Make assumptions about heat transfer and specify energy balance values

Since we have specified that our gCSS simulation is nonisothermal, we need to provide information about the energy balances in the adsorber. Fortunately, the options in this block are well named, so it is easy to tell what options are available to you. Note that the exact mathematical forms of these assumptions are available in the help files, and in most cases, are identical to the Gas: Dynamic blocks from the first workshop.

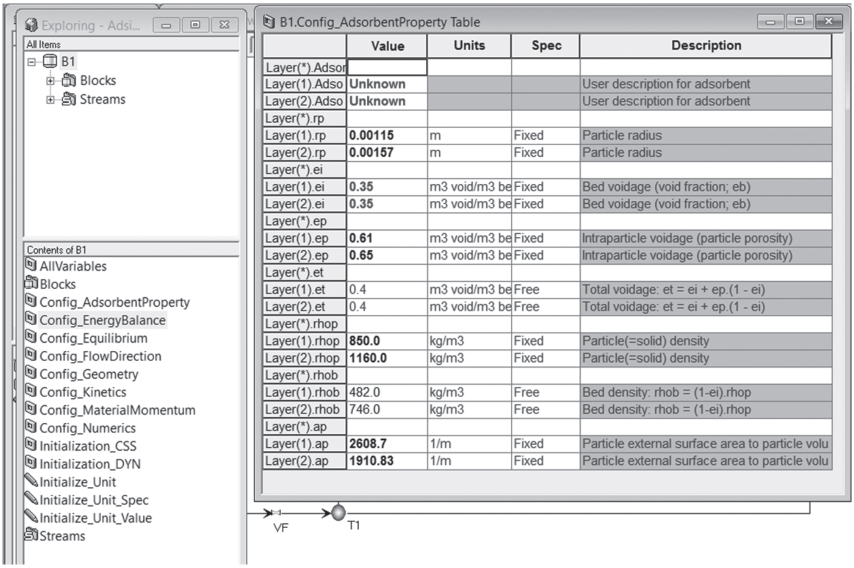


```
lation complete
l Cycle_Organizer ha                                   hich do not exist:
```

Figure 1.177 Opening the Explorer at the first bed.

The general form of the energy balance used here, when no reaction is present, is given in Eq. (1.16):

$$\overbrace{-k_{\mathrm{ga}}\varepsilon_i\frac{\partial^2 T_{\mathrm{g}}}{\partial z^2}}^{\text{Conduction}} + \overbrace{C_{\mathrm{vg}}v_{\mathrm{g}}\rho_{\mathrm{g}}\frac{\partial T}{\partial z}}^{\text{Convention}} + \overbrace{\varepsilon_{\mathrm{b}}C_{\mathrm{vg}}\rho_{\mathrm{g}}\frac{\partial T_{\mathrm{g}}}{\partial t}}^{\text{Accumulation}} + \overbrace{P\frac{\partial v_{\mathrm{g}}}{\partial z}}^{\text{Compression}} + \overbrace{\mathrm{HTC}\ a_{\mathrm{p}}(T_{\mathrm{g}} - T_{\mathrm{s}})}^{\text{Gas–Solid Transfer}} + \overbrace{\frac{4H_{\mathrm{w}}}{D_{\mathrm{B}}}(T_{\mathrm{g}} - T_{\mathrm{W}})}^{\text{Gas–Wall Transfer}} = 0. \tag{1.16}$$



B1.Config_AdsorbentProperty Table

	Value	Units	Spec	Description
Layer(*).Adsor				
Layer(1).Adso	**Unknown**			User description for adsorbent
Layer(2).Adso	**Unknown**			User description for adsorbent
Layer(*).rp				
Layer(1).rp	**0.00115**	m	Fixed	Particle radius
Layer(2).rp	**0.00157**	m	Fixed	Particle radius
Layer(*).ei				
Layer(1).ei	**0.35**	m3 void/m3 be	Fixed	Bed voidage (void fraction; eb)
Layer(2).ei	**0.35**	m3 void/m3 be	Fixed	Bed voidage (void fraction; eb)
Layer(*).ep				
Layer(1).ep	**0.61**	m3 void/m3 be	Fixed	Intraparticle voidage (particle porosity)
Layer(2).ep	**0.65**	m3 void/m3 be	Fixed	Intraparticle voidage (particle porosity)
Layer(*).et				
Layer(1).et	0.4	m3 void/m3 be	Free	Total voidage: et = ei + ep.(1 - ei)
Layer(2).et	0.4	m3 void/m3 be	Free	Total voidage: et = ei + ep.(1 - ei)
Layer(*).rhop				
Layer(1).rhop	**850.0**	kg/m3	Fixed	Particle(=solid) density
Layer(2).rhop	**1160.0**	kg/m3	Fixed	Particle(=solid) density
Layer(*).rhob				
Layer(1).rhob	482.0	kg/m3	Free	Bed density: rhob = (1-ei).rhop
Layer(2).rhob	746.0	kg/m3	Free	Bed density: rhob = (1-ei).rhop
Layer(*).ap				
Layer(1).ap	**2608.7**	1/m	Fixed	Particle external surface area to particle volu
Layer(2).ap	**1910.83**	1/m	Fixed	Particle external surface area to particle volu

Figure 1.178 Using the explorer window to open the Adsorbent Properties form.

When we enable the rigorous wall balance, Aspen Adsorption calculates the change in wall temperatures according to Eq. (1.17):

$$\overbrace{-k_{\mathrm{w}}\frac{\partial^2 T_{\mathrm{w}}}{\partial z^2}}^{\text{Conduction}} + \overbrace{\rho_{\mathrm{w}} C_{\mathrm{pw}}\frac{\partial T_{\mathrm{w}}}{\partial t}}^{\text{Accumulation}} - \overbrace{H_{\mathrm{w}}\frac{4D_{\mathrm{B}}}{(D_{\mathrm{B}}+W_{\mathrm{T}})^2 - D_{\mathrm{B}}^2}(T_{\mathrm{g}}-T_{\mathrm{w}})}^{\text{Bed–Wall Transfer}} + \overbrace{H_{\mathrm{amb}}\frac{4(D_{\mathrm{B}}+W_{\mathrm{T}})^2}{(D_{\mathrm{B}}+W_{\mathrm{T}})^2 - D_{\mathrm{B}}^2}(T_{\mathrm{w}}-T_{\mathrm{amb}})}^{\text{Wall–Ambient Transfer}} = 0. \tag{1.17}$$

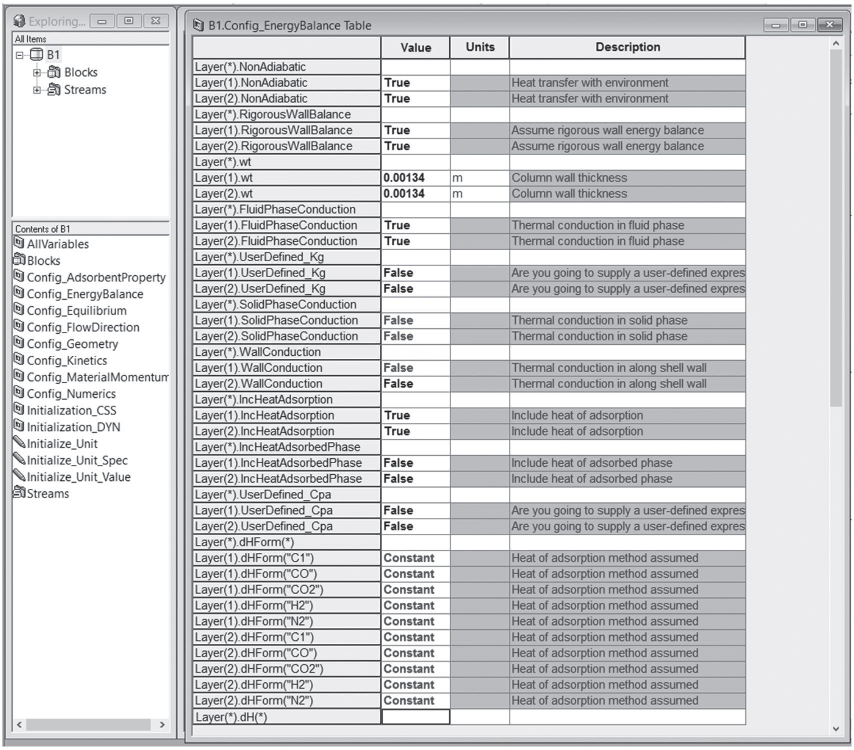
And finally, since we are assuming that the adsorption is nonisothermal, Aspen will use Eq. (1.18) to calculate the temperature of the adsorbent:

$$\overbrace{\rho_{\mathrm{s}} C_{\mathrm{ps}}\frac{\partial T_{\mathrm{s}}}{\partial t}}^{\text{Accumulation}} + \overbrace{\rho_{\mathrm{s}}\sum_{i=1}^{n}\Delta H_i\frac{\partial w_i}{\partial t}}^{\text{Heat of Adsorption}} + \overbrace{\mathrm{HTC}\; a_{\mathrm{p}}\,(T_{\mathrm{g}}-T_{\mathrm{s}})}^{\text{Gas–Solid Transfer}} = 0. \tag{1.18}$$

That means, by enabling the nonadiabatic and rigorous wall balances, we need to specify a large number of property parameters to describe these heating effects. Specifically, we need:

- Gas-phase thermal conductivity, k_{ga}.
- Thermal conductivity of the wall, k_{w}.
- Specific gas-phase heat capacity (constant volume) C_{vg}.
- Specific heat capacity of the wall, c_{pw}.
- Specific heat capacity of the adsorbent, c_{ps}.
- Heat transfer coefficient between gas and solid phase, HTC.
- Heat transfer coefficient between the gas phase and wall, H_{w}.
- Heat transfer coefficient between the wall and ambient conditions, H_{amb}.
- Wall thickness, W_{T}.
- Wall density, ρ_{W}.
- The heat of adsorption for component i, ΔH_{i}.

See Figures 1.179 and 1.180 for specifying the energy balance properties. Note that we do not need information about gas density, compressibility, and velocity because Aspen Properties will be able to calculate these properties for us.

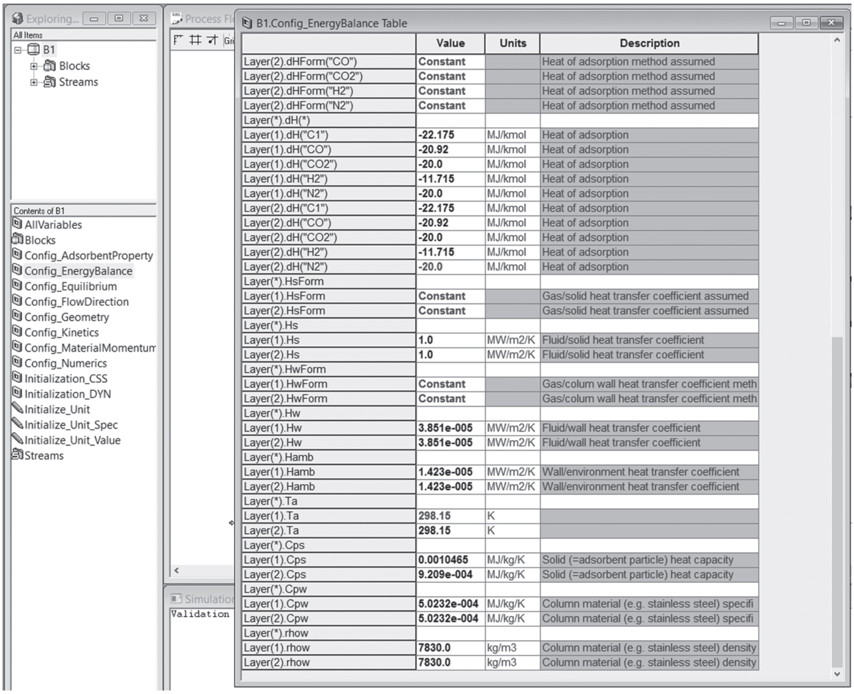


	Value	Units	Description
Layer(*).NonAdiabatic			
Layer(1).NonAdiabatic	True		Heat transfer with environment
Layer(2).NonAdiabatic	True		Heat transfer with environment
Layer(*).RigorousWallBalance			
Layer(1).RigorousWallBalance	True		Assume rigorous wall energy balance
Layer(2).RigorousWallBalance	True		Assume rigorous wall energy balance
Layer(*).wt			
Layer(1).wt	0.00134	m	Column wall thickness
Layer(2).wt	0.00134	m	Column wall thickness
Layer(*).FluidPhaseConduction			
Layer(1).FluidPhaseConduction	True		Thermal conduction in fluid phase
Layer(2).FluidPhaseConduction	True		Thermal conduction in fluid phase
Layer(*).UserDefined_Kg			
Layer(1).UserDefined_Kg	False		Are you going to supply a user-defined expres
Layer(2).UserDefined_Kg	False		Are you going to supply a user-defined expres
Layer(*).SolidPhaseConduction			
Layer(1).SolidPhaseConduction	False		Thermal conduction in solid phase
Layer(2).SolidPhaseConduction	False		Thermal conduction in solid phase
Layer(*).WallConduction			
Layer(1).WallConduction	False		Thermal conduction in along shell wall
Layer(2).WallConduction	False		Thermal conduction in along shell wall
Layer(*).IncHeatAdsorption			
Layer(1).IncHeatAdsorption	True		Include heat of adsorption
Layer(2).IncHeatAdsorption	True		Include heat of adsorption
Layer(*).IncHeatAdsorbedPhase			
Layer(1).IncHeatAdsorbedPhase	False		Include heat of adsorbed phase
Layer(2).IncHeatAdsorbedPhase	False		Include heat of adsorbed phase
Layer(*).UserDefined_Cpa			
Layer(1).UserDefined_Cpa	False		Are you going to supply a user-defined expres
Layer(2).UserDefined_Cpa	False		Are you going to supply a user-defined expres
Layer(*).dHForm(*)			
Layer(1).dHForm("C1")	Constant		Heat of adsorption method assumed
Layer(1).dHForm("CO")	Constant		Heat of adsorption method assumed
Layer(1).dHForm("CO2")	Constant		Heat of adsorption method assumed
Layer(1).dHForm("H2")	Constant		Heat of adsorption method assumed
Layer(1).dHForm("N2")	Constant		Heat of adsorption method assumed
Layer(2).dHForm("C1")	Constant		Heat of adsorption method assumed
Layer(2).dHForm("CO")	Constant		Heat of adsorption method assumed
Layer(2).dHForm("CO2")	Constant		Heat of adsorption method assumed
Layer(2).dHForm("H2")	Constant		Heat of adsorption method assumed
Layer(2).dHForm("N2")	Constant		Heat of adsorption method assumed
Layer(*).dH(*)			

Figure 1.179 Using the explorer window to open the Energy Balance Properties form.

Step 13: Define the equilibrium behavior of the system

The next configuration form is the equilibrium behavior of the adsorption. We specify what form of the isotherm we use first, under “Equilibrium Model.” There are a large number of options, and we can find their details in the help



B1.Config_EnergyBalance Table

	Value	Units	Description
Layer(2).dHForm("CO")	Constant		Heat of adsorption method assumed
Layer(2).dHForm("CO2")	Constant		Heat of adsorption method assumed
Layer(2).dHForm("H2")	Constant		Heat of adsorption method assumed
Layer(2).dHForm("N2")	Constant		Heat of adsorption method assumed
Layer(*).dH(*)			
Layer(1).dH("C1")	-22.175	MJ/kmol	Heat of adsorption
Layer(1).dH("CO")	-20.92	MJ/kmol	Heat of adsorption
Layer(1).dH("CO2")	-20.0	MJ/kmol	Heat of adsorption
Layer(1).dH("H2")	-11.715	MJ/kmol	Heat of adsorption
Layer(1).dH("N2")	-20.0	MJ/kmol	Heat of adsorption
Layer(2).dH("C1")	-22.175	MJ/kmol	Heat of adsorption
Layer(2).dH("CO")	-20.92	MJ/kmol	Heat of adsorption
Layer(2).dH("CO2")	-20.0	MJ/kmol	Heat of adsorption
Layer(2).dH("H2")	-11.715	MJ/kmol	Heat of adsorption
Layer(2).dH("N2")	-20.0	MJ/kmol	Heat of adsorption
Layer(*).HsForm			
Layer(1).HsForm	Constant		Gas/solid heat transfer coefficient assumed
Layer(2).HsForm	Constant		Gas/solid heat transfer coefficient assumed
Layer(*).Hs			
Layer(1).Hs	1.0	MW/m2/K	Fluid/solid heat transfer coefficient
Layer(2).Hs	1.0	MW/m2/K	Fluid/solid heat transfer coefficient
Layer(*).HwForm			
Layer(1).HwForm	Constant		Gas/colum wall heat transfer coefficient meth
Layer(2).HwForm	Constant		Gas/colum wall heat transfer coefficient meth
Layer(*).Hw			
Layer(1).Hw	3.851e-005	MW/m2/K	Fluid/wall heat transfer coefficient
Layer(2).Hw	3.851e-005	MW/m2/K	Fluid/wall heat transfer coefficient
Layer(*).Hamb			
Layer(1).Hamb	1.423e-005	MW/m2/K	Wall/environment heat transfer coefficient
Layer(2).Hamb	1.423e-005	MW/m2/K	Wall/environment heat transfer coefficient
Layer(*).Ta			
Layer(1).Ta	298.15	K	
Layer(2).Ta	298.15	K	
Layer(*).Cps			
Layer(1).Cps	0.0010465	MJ/kg/K	Solid (=adsorbent particle) heat capacity
Layer(2).Cps	9.209e-004	MJ/kg/K	Solid (=adsorbent particle) heat capacity
Layer(*).Cpw			
Layer(1).Cpw	5.0232e-004	MJ/kg/K	Column material (e.g. stainless steel) specifi
Layer(2).Cpw	5.0232e-004	MJ/kg/K	Column material (e.g. stainless steel) specifi
Layer(*).rhow			
Layer(1).rhow	7830.0	kg/m3	Column material (e.g. stainless steel) density
Layer(2).rhow	7830.0	kg/m3	Column material (e.g. stainless steel) density

Figure 1.180 Specifying the rest of the Energy Balance Properties.

files. Once the isotherms form are selected, you must supply all the equilibrium property parameters (Figures 1.181 and 1.182).

To find out what isotherm form is assumed by "Loading Ratio Correlation 3" seen in Figure 1.183, we can look it up in the help files. Open "Aspen Adsorption Contents" under the help menu, then search for "loading ratio correlation" (Figures 1.183 and 1.184).

By clicking on the correct entry, we can find the full equilibrium equation assumed (Figure 1.184).

Step 14: Specify the flow direction options

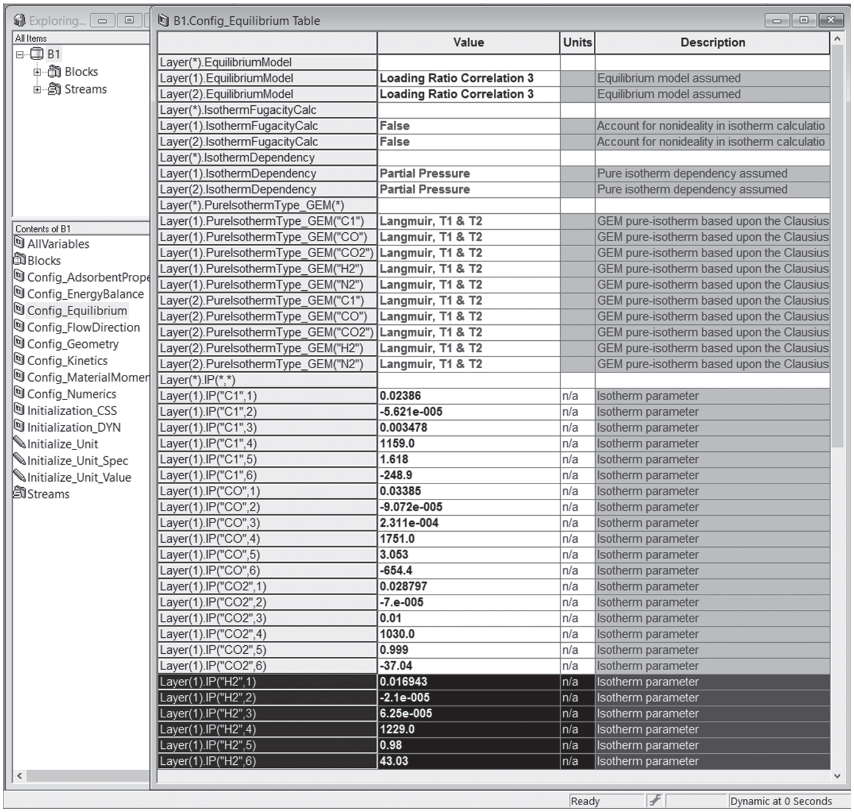
If gas will only flow in one direction through a bed, calculations can be slightly more efficient. However, we let the pressure gradients determine the flow direction for us (Figure 1.185).

Step 15: Choose the mass transfer models to use

These options are identical to those mentioned in workshop 1. The most common model is lumped LDF, Eq. (1.15), since other models can add significant computational overhead, with very little improvement in accuracy. See Figure 1.186.

Step 16: Specify the momentum balance assumptions

In the momentum balance table, we may leave all values at their defaults. These options allow us to adjust how the adsorption bed calculates gas pressures drops and velocities. The well-known Ergun equation, Eq. (1.11), is suitable for most conditions (Figure 1.187), since it combines the equations useful at



	Value	Units	Description
Layer(*).EquilibriumModel			
Layer(1).EquilibriumModel	Loading Ratio Correlation 3		Equilibrium model assumed
Layer(2).EquilibriumModel	Loading Ratio Correlation 3		Equilibrium model assumed
Layer(*).IsothermFugacityCalc			
Layer(1).IsothermFugacityCalc	False		Account for nonideality in isotherm calculatio
Layer(2).IsothermFugacityCalc	False		Account for nonideality in isotherm calculatio
Layer(*).IsothermDependency			
Layer(1).IsothermDependency	Partial Pressure		Pure isotherm dependency assumed
Layer(2).IsothermDependency	Partial Pressure		Pure isotherm dependency assumed
Layer(*).PureIsothermType_GEM(*)			
Layer(1).PureIsothermType_GEM("C1")	Langmuir, T1 & T2		GEM pure-isotherm based upon the Clausius
Layer(1).PureIsothermType_GEM("CO")	Langmuir, T1 & T2		GEM pure-isotherm based upon the Clausius
Layer(1).PureIsothermType_GEM("CO2")	Langmuir, T1 & T2		GEM pure-isotherm based upon the Clausius
Layer(1).PureIsothermType_GEM("H2")	Langmuir, T1 & T2		GEM pure-isotherm based upon the Clausius
Layer(1).PureIsothermType_GEM("N2")	Langmuir, T1 & T2		GEM pure-isotherm based upon the Clausius
Layer(2).PureIsothermType_GEM("C1")	Langmuir, T1 & T2		GEM pure-isotherm based upon the Clausius
Layer(2).PureIsothermType_GEM("CO")	Langmuir, T1 & T2		GEM pure-isotherm based upon the Clausius
Layer(2).PureIsothermType_GEM("CO2")	Langmuir, T1 & T2		GEM pure-isotherm based upon the Clausius
Layer(2).PureIsothermType_GEM("H2")	Langmuir, T1 & T2		GEM pure-isotherm based upon the Clausius
Layer(2).PureIsothermType_GEM("N2")	Langmuir, T1 & T2		GEM pure-isotherm based upon the Clausius
Layer(*).IP(*,*)			
Layer(1).IP("C1",1)	0.02386	n/a	Isotherm parameter
Layer(1).IP("C1",2)	-5.621e-005	n/a	Isotherm parameter
Layer(1).IP("C1",3)	0.003478	n/a	Isotherm parameter
Layer(1).IP("C1",4)	1159.0	n/a	Isotherm parameter
Layer(1).IP("C1",5)	1.618	n/a	Isotherm parameter
Layer(1).IP("C1",6)	-248.9	n/a	Isotherm parameter
Layer(1).IP("CO",1)	0.03385	n/a	Isotherm parameter
Layer(1).IP("CO",2)	-9.072e-005	n/a	Isotherm parameter
Layer(1).IP("CO",3)	2.311e-004	n/a	Isotherm parameter
Layer(1).IP("CO",4)	1751.0	n/a	Isotherm parameter
Layer(1).IP("CO",5)	3.053	n/a	Isotherm parameter
Layer(1).IP("CO",6)	-654.4	n/a	Isotherm parameter
Layer(1).IP("CO2",1)	0.028797	n/a	Isotherm parameter
Layer(1).IP("CO2",2)	-7.e-005	n/a	Isotherm parameter
Layer(1).IP("CO2",3)	0.01	n/a	Isotherm parameter
Layer(1).IP("CO2",4)	1030.0	n/a	Isotherm parameter
Layer(1).IP("CO2",5)	0.999	n/a	Isotherm parameter
Layer(1).IP("CO2",6)	-37.04	n/a	Isotherm parameter
Layer(1).IP("H2",1)	0.016943	n/a	Isotherm parameter
Layer(1).IP("H2",2)	-2.1e-005	n/a	Isotherm parameter
Layer(1).IP("H2",3)	6.25e-005	n/a	Isotherm parameter
Layer(1).IP("H2",4)	1229.0	n/a	Isotherm parameter
Layer(1).IP("H2",5)	0.98	n/a	Isotherm parameter
Layer(1).IP("H2",6)	43.03	n/a	Isotherm parameter

Figure 1.181 Using the explorer window to open the Equilibrium Properties form.

laminar conditions (Carman–Kozeny) with the equations for turbulent flow (Burke–Plummer).

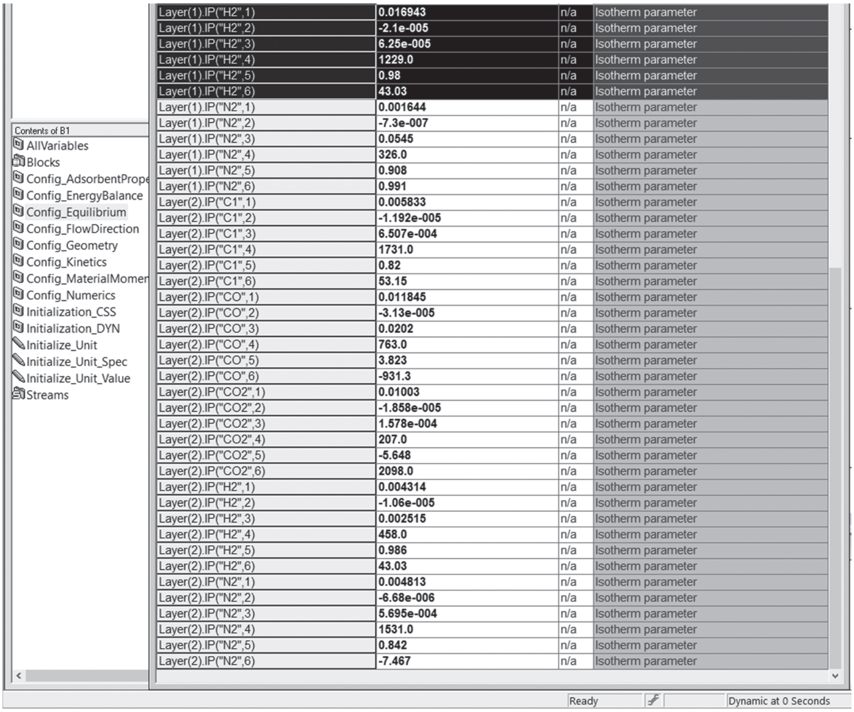
Step 17: Choose the numerical discretization options

In this form, we may select the methods used for finite element discretization and estimation. The options are identical to those discussed in the first workshop. In this case, we use a second-order Central Finite Difference (CFD2) approximation with 16 nodes in each bed (Figure 1.188). This is adequate, and has good computational performance; for brand new simulations, it is generally a good idea to begin with a simulation using an Orthogonal Collocation Finite Element (OCFE) method. Once a solution is found with OCFE, the finite difference method can be compared to the more accurate result in terms of computation speed and accuracy.

With this, the adsorbent beds have been completely specified.

Step 18: Perform gCSS initializations

After completing all these steps, the simulation will still not be runnable. The reason is found at the very bottom of the Aspen window. The green box with red triangle indicates that our flowsheet is overspecified: there are negative degrees of freedom (Figure 1.189). The reason for this is that several variables



Layer(1).IP("H2",1)	0.016943	n/a	Isotherm parameter
Layer(1).IP("H2",2)	-2.1e-005	n/a	Isotherm parameter
Layer(1).IP("H2",3)	6.25e-005	n/a	Isotherm parameter
Layer(1).IP("H2",4)	1229.0	n/a	Isotherm parameter
Layer(1).IP("H2",5)	0.98	n/a	Isotherm parameter
Layer(1).IP("H2",6)	43.03	n/a	Isotherm parameter
Layer(1).IP("N2",1)	0.001644	n/a	Isotherm parameter
Layer(1).IP("N2",2)	-7.3e-007	n/a	Isotherm parameter
Layer(1).IP("N2",3)	0.0545	n/a	Isotherm parameter
Layer(1).IP("N2",4)	326.0	n/a	Isotherm parameter
Layer(1).IP("N2",5)	0.908	n/a	Isotherm parameter
Layer(1).IP("N2",6)	0.991	n/a	Isotherm parameter
Layer(2).IP("C1",1)	0.005833	n/a	Isotherm parameter
Layer(2).IP("C1",2)	-1.192e-005	n/a	Isotherm parameter
Layer(2).IP("C1",3)	6.507e-004	n/a	Isotherm parameter
Layer(2).IP("C1",4)	1731.0	n/a	Isotherm parameter
Layer(2).IP("C1",5)	0.82	n/a	Isotherm parameter
Layer(2).IP("C1",6)	53.15	n/a	Isotherm parameter
Layer(2).IP("CO",1)	0.011845	n/a	Isotherm parameter
Layer(2).IP("CO",2)	-3.13e-005	n/a	Isotherm parameter
Layer(2).IP("CO",3)	0.0202	n/a	Isotherm parameter
Layer(2).IP("CO",4)	763.0	n/a	Isotherm parameter
Layer(2).IP("CO",5)	3.823	n/a	Isotherm parameter
Layer(2).IP("CO",6)	-931.3	n/a	Isotherm parameter
Layer(2).IP("CO2",1)	0.01003	n/a	Isotherm parameter
Layer(2).IP("CO2",2)	-1.858e-005	n/a	Isotherm parameter
Layer(2).IP("CO2",3)	1.578e-004	n/a	Isotherm parameter
Layer(2).IP("CO2",4)	207.0	n/a	Isotherm parameter
Layer(2).IP("CO2",5)	-5.648	n/a	Isotherm parameter
Layer(2).IP("CO2",6)	2098.0	n/a	Isotherm parameter
Layer(2).IP("H2",1)	0.004314	n/a	Isotherm parameter
Layer(2).IP("H2",2)	-1.06e-005	n/a	Isotherm parameter
Layer(2).IP("H2",3)	0.002515	n/a	Isotherm parameter
Layer(2).IP("H2",4)	458.0	n/a	Isotherm parameter
Layer(2).IP("H2",5)	0.986	n/a	Isotherm parameter
Layer(2).IP("H2",6)	43.03	n/a	Isotherm parameter
Layer(2).IP("N2",1)	0.004813	n/a	Isotherm parameter
Layer(2).IP("N2",2)	-6.68e-006	n/a	Isotherm parameter
Layer(2).IP("N2",3)	5.695e-004	n/a	Isotherm parameter
Layer(2).IP("N2",4)	1531.0	n/a	Isotherm parameter
Layer(2).IP("N2",5)	0.842	n/a	Isotherm parameter
Layer(2).IP("N2",6)	-7.467	n/a	Isotherm parameter

Figure 1.182 Specifying the rest of the Equilibrium Properties.

in the gCSS blocks (specifically, tanks and beds) are set to be fixed, when in a dynamic run, they should only represent initial conditions.

Fortunately, the gCSS blocks contain initialization scripts which fix this for us. To run the initialization script on a block, right-click the block, mouse over script, then click on Initialize_Unit (Figure 1.190). Save the file as **Workshop3d.ada**.

Once you do this, you should notice that the simulation will only be overspecified by six variables. You can manually run each initialization script, or we can once again run the flowsheet > "Check and initial."

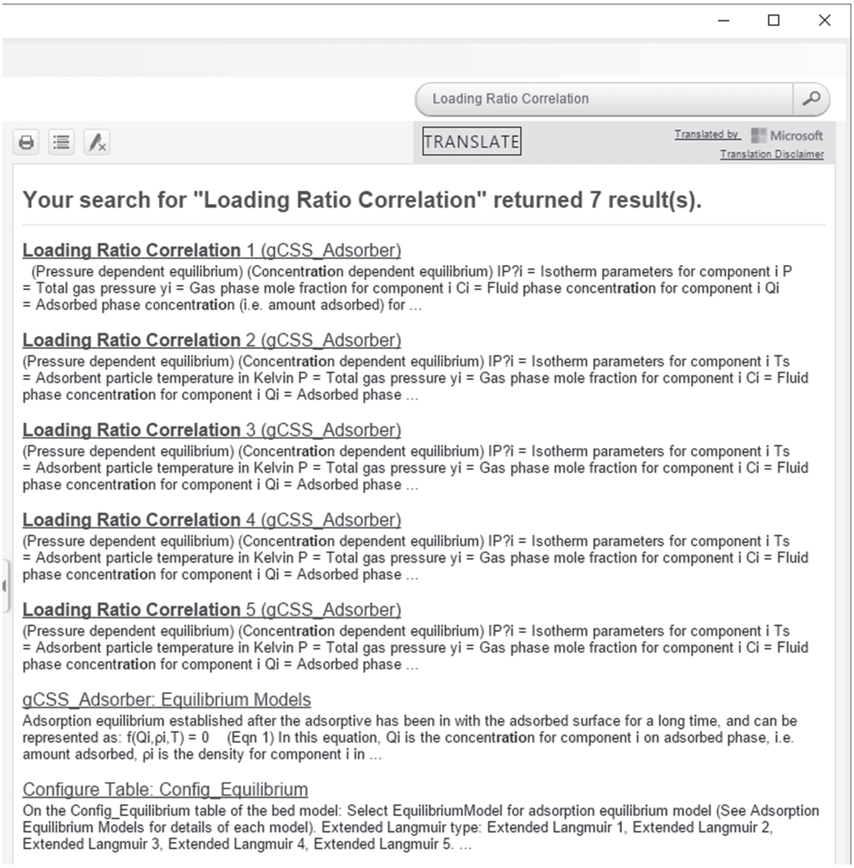
1.9.5 Defining the Cycle Organizer

Step 19: Add the Cycle Organizer

Use the "Tools" menu to add the cycle organizer to the flowsheet.

Step 20: Define the cycle steps

As we saw previously, the gCSS valves use different variable names than the dynamic valves. To toggle the valves open and closed, we need to assign values to the "Use_Spec(1)" variable. Add the Use_Spec variables for the seven valves that change over time to step 1, then create six cycle steps containing a copy of those variables. Following this, assign the values according to Table 1.12. Refer to Table 1.5 in connection with Figure 1.7 for the meanings of valve ASs of 0–2.



Your search for "Loading Ratio Correlation" returned 7 result(s).

Loading Ratio Correlation 1 (gCSS_Adsorber)
(Pressure dependent equilibrium) (Concentration dependent equilibrium) IP?i = Isotherm parameters for component i P = Total gas pressure yi = Gas phase mole fraction for component i Ci = Fluid phase concentration for component i Qi = Adsorbed phase concentration (i.e. amount adsorbed) for ...

Loading Ratio Correlation 2 (gCSS_Adsorber)
(Pressure dependent equilibrium) (Concentration dependent equilibrium) IP?i = Isotherm parameters for component i Ts = Adsorbent particle temperature in Kelvin P = Total gas pressure yi = Gas phase mole fraction for component i Ci = Fluid phase concentration for component i Qi = Adsorbed phase ...

Loading Ratio Correlation 3 (gCSS_Adsorber)
(Pressure dependent equilibrium) (Concentration dependent equilibrium) IP?i = Isotherm parameters for component i Ts = Adsorbent particle temperature in Kelvin P = Total gas pressure yi = Gas phase mole fraction for component i Ci = Fluid phase concentration for component i Qi = Adsorbed phase ...

Loading Ratio Correlation 4 (gCSS_Adsorber)
(Pressure dependent equilibrium) (Concentration dependent equilibrium) IP?i = Isotherm parameters for component i Ts = Adsorbent particle temperature in Kelvin P = Total gas pressure yi = Gas phase mole fraction for component i Ci = Fluid phase concentration for component i Qi = Adsorbed phase ...

Loading Ratio Correlation 5 (gCSS_Adsorber)
(Pressure dependent equilibrium) (Concentration dependent equilibrium) IP?i = Isotherm parameters for component i Ts = Adsorbent particle temperature in Kelvin P = Total gas pressure yi = Gas phase mole fraction for component i Ci = Fluid phase concentration for component i Qi = Adsorbed phase ...

gCSS_Adsorber: Equilibrium Models
Adsorption equilibrium established after the adsorptive has been in with the adsorbed surface for a long time, and can be represented as: f(Qi,ρi,T) = 0 (Eqn 1) In this equation, Qi is the concentration for component i on adsorbed phase, i.e. amount adsorbed, ρi is the density for component i in ...

Configure Table: Config_Equilibrium
On the Config_Equilibrium table of the bed model: Select EquilibriumModel for adsorption equilibrium model (See Adsorption Equilibrium Models for details of each model). Extended Langmuir type: Extended Langmuir 1, Extended Langmuir 2, Extended Langmuir 3, Extended Langmuir 4, Extended Langmuir 5. ...

Figure 1.183 Searching for the isotherm equation.

Step 21: Wait! Do not generate the Cycle Task!

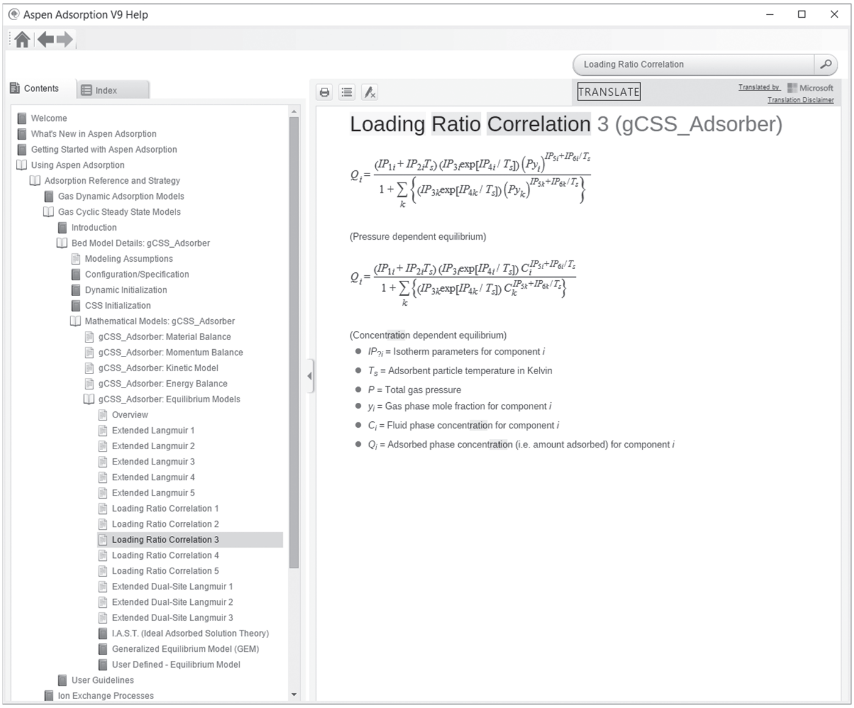
This simulation is more complex than our previous air separation example. Not only are there more components, but our adsorption beds have two layers, and we are using a more complex isotherm. All these factors can make it difficult for Aspen to “get things started.” That is to say, the first few seconds of a dynamic simulation can be the hardest on the Aspen solver. To avoid having to repeatedly wait for this difficult solver step, we will perform a trick.

Step 22: Set the simulation to pause at one second

Use the “Run Control” button shown in Figure 1.191.

Step 23: Set the Solver Integration options

The Solver Options provide advanced control over the mathematical solution methods used in Aspen. For the vast majority of cases, the default values work very well. In this case, we will change how the numerical integration takes place. Specifically, we are going to set the initial time-integration step to be smaller, so that the changes in the various process variables will change by smaller amounts and be less likely to take on extreme values. Click on the “Solver” options button (Figure 1.191), and then select the Integrator tab and



Loading Ratio Correlation 3 (gCSS_Adsorber)

$$Q_i = \frac{(IP_{1i} + IP_{2i}T_s)\,(IP_{3i}\exp[IP_{4i}/T_s])\left(Py_i\right)^{IP_{5i}+IP_{6i}/T_s}}{1 + \sum_k \left\{(IP_{3k}\exp[IP_{4k}/T_s])\left(Py_k\right)^{IP_{5k}+IP_{6k}/T_s}\right\}}$$

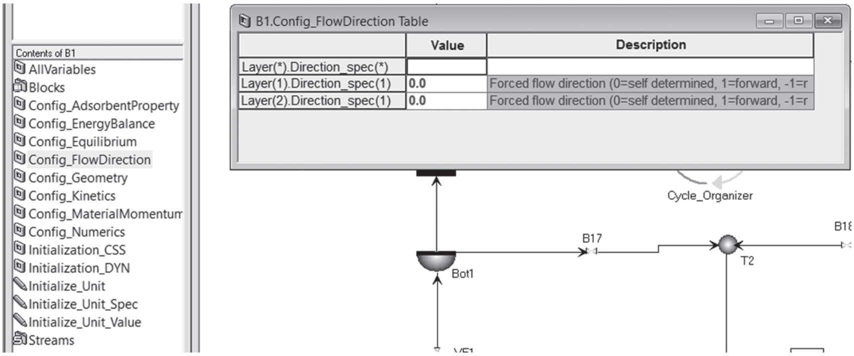
(Pressure dependent equilibrium)

$$Q_i = \frac{(IP_{1i} + IP_{2i}T_s)\,(IP_{3i}\exp[IP_{4i}/T_s])\,C_i^{IP_{5i}+IP_{6i}/T_s}}{1 + \sum_k \left\{(IP_{3k}\exp[IP_{4k}/T_s])\,C_k^{IP_{5k}+IP_{6k}/T_s}\right\}}$$

(Concentration dependent equilibrium)

- $IP_{?i}$ = Isotherm parameters for component i
- T_s = Adsorbent particle temperature in Kelvin
- P = Total gas pressure
- y_i = Gas phase mole fraction for component i
- C_i = Fluid phase concentration for component i
- Q_i = Adsorbed phase concentration (i.e. amount adsorbed) for component i

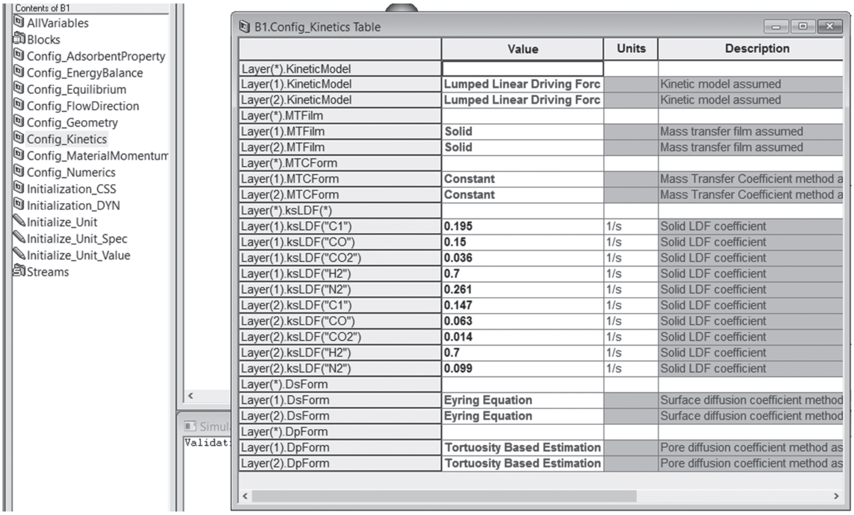
Figure 1.184 Viewing the full form of the Loading Ratio Correlation 3.



B1.Config_FlowDirection Table

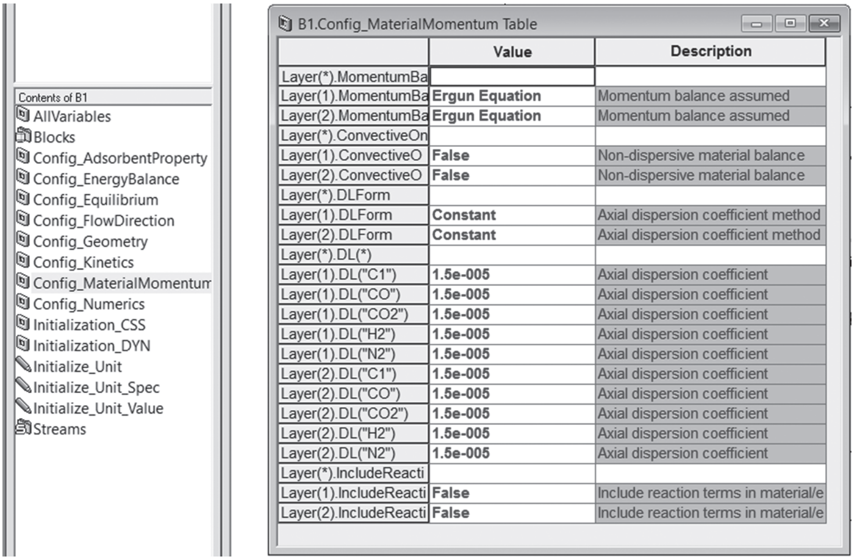
	Value	Description
Layer(*).Direction_spec(*)		
Layer(1).Direction_spec(1)	0.0	Forced flow direction (0=self determined, 1=forward, -1=r
Layer(2).Direction_spec(1)	0.0	Forced flow direction (0=self determined, 1=forward, -1=r

Figure 1.185 Set Aspen to automatically determine the gas flow direction in the adsorbent beds.



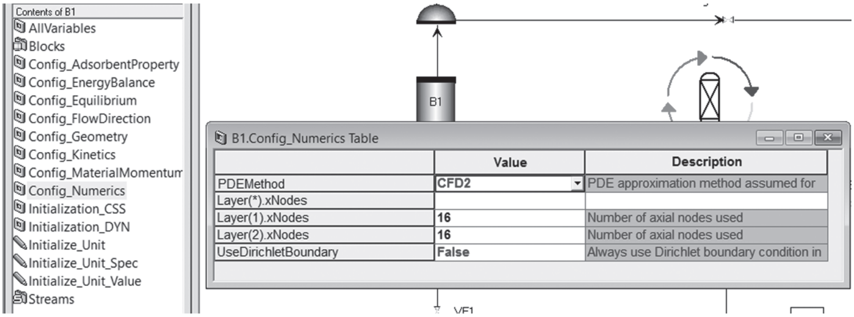
	Value	Units	Description
Layer(*).KineticModel			
Layer(1).KineticModel	Lumped Linear Driving Forc		Kinetic model assumed
Layer(2).KineticModel	Lumped Linear Driving Forc		Kinetic model assumed
Layer(*).MTFilm			
Layer(1).MTFilm	Solid		Mass transfer film assumed
Layer(2).MTFilm	Solid		Mass transfer film assumed
Layer(*).MTCForm			
Layer(1).MTCForm	Constant		Mass Transfer Coefficient method a
Layer(2).MTCForm	Constant		Mass Transfer Coefficient method a
Layer(*).ksLDF(*)			
Layer(1).ksLDF("C1")	0.195	1/s	Solid LDF coefficient
Layer(1).ksLDF("CO")	0.15	1/s	Solid LDF coefficient
Layer(1).ksLDF("CO2")	0.036	1/s	Solid LDF coefficient
Layer(1).ksLDF("H2")	0.7	1/s	Solid LDF coefficient
Layer(1).ksLDF("N2")	0.261	1/s	Solid LDF coefficient
Layer(2).ksLDF("C1")	0.147	1/s	Solid LDF coefficient
Layer(2).ksLDF("CO")	0.063	1/s	Solid LDF coefficient
Layer(2).ksLDF("CO2")	0.014	1/s	Solid LDF coefficient
Layer(2).ksLDF("H2")	0.7	1/s	Solid LDF coefficient
Layer(2).ksLDF("N2")	0.099	1/s	Solid LDF coefficient
Layer(*).DsForm			
Layer(1).DsForm	Eyring Equation		Surface diffusion coefficient method
Layer(2).DsForm	Eyring Equation		Surface diffusion coefficient method
Layer(*).DpForm			
Layer(1).DpForm	Tortuosity Based Estimation		Pore diffusion coefficient method as
Layer(2).DpForm	Tortuosity Based Estimation		Pore diffusion coefficient method as

Figure 1.186 Specifying the kinetic properties of our adsorbent bed.



	Value	Description
Layer(*).MomentumBa		
Layer(1).MomentumBa	Ergun Equation	Momentum balance assumed
Layer(2).MomentumBa	Ergun Equation	Momentum balance assumed
Layer(*).ConvectiveOn		
Layer(1).ConvectiveO	False	Non-dispersive material balance
Layer(2).ConvectiveO	False	Non-dispersive material balance
Layer(*).DLForm		
Layer(1).DLForm	Constant	Axial dispersion coefficient method
Layer(2).DLForm	Constant	Axial dispersion coefficient method
Layer(*).DL(*)		
Layer(1).DL("C1")	1.5e-005	Axial dispersion coefficient
Layer(1).DL("CO")	1.5e-005	Axial dispersion coefficient
Layer(1).DL("CO2")	1.5e-005	Axial dispersion coefficient
Layer(1).DL("H2")	1.5e-005	Axial dispersion coefficient
Layer(1).DL("N2")	1.5e-005	Axial dispersion coefficient
Layer(2).DL("C1")	1.5e-005	Axial dispersion coefficient
Layer(2).DL("CO")	1.5e-005	Axial dispersion coefficient
Layer(2).DL("CO2")	1.5e-005	Axial dispersion coefficient
Layer(2).DL("H2")	1.5e-005	Axial dispersion coefficient
Layer(2).DL("N2")	1.5e-005	Axial dispersion coefficient
Layer(*).IncludeReacti		
Layer(1).IncludeReacti	False	Include reaction terms in material/e
Layer(2).IncludeReacti	False	Include reaction terms in material/e

Figure 1.187 Choose the coefficients for the Ergun model in our momentum balance.



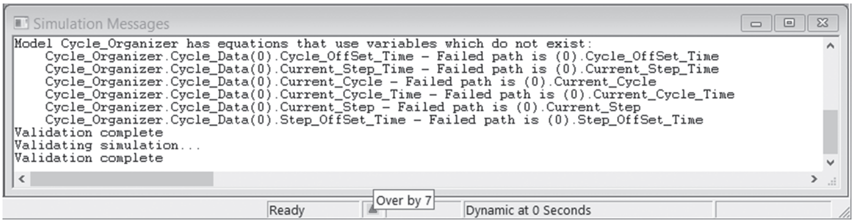
Contents of B1

- AllVariables
- Blocks
- Config_AdsorbentProperty
- Config_EnergyBalance
- Config_Equilibrium
- Config_FlowDirection
- Config_Geometry
- Config_Kinetics
- Config_MaterialMomentum
- Config_Numerics
- Initialization_CSS
- Initialization_DYN
- Initialize_Unit
- Initialize_Unit_Spec
- Initialize_Unit_Value
- Streams

B1.Config_Numerics Table

	Value	Description
PDEMethod	CFD2	PDE approximation method assumed for
Layer(*).xNodes		
Layer(1).xNodes	16	Number of axial nodes used
Layer(2).xNodes	16	Number of axial nodes used
UseDirichletBoundary	False	Always use Dirichlet boundary condition in

Figure 1.188 Choose the numerical PDE solution options.



Simulation Messages

```
Model Cycle_Organizer has equations that use variables which do not exist:
    Cycle_Organizer.Cycle_Data(0).Cycle_OffSet_Time - Failed path is (0).Cycle_OffSet_Time
    Cycle_Organizer.Cycle_Data(0).Current_Step_Time - Failed path is (0).Current_Step_Time
    Cycle_Organizer.Cycle_Data(0).Current_Cycle - Failed path is (0).Current_Cycle
    Cycle_Organizer.Cycle_Data(0).Current_Cycle_Time - Failed path is (0).Current_Cycle_Time
    Cycle_Organizer.Cycle_Data(0).Current_Step - Failed path is (0).Current_Step
    Cycle_Organizer.Cycle_Data(0).Step_OffSet_Time - Failed path is (0).Step_OffSet_Time
Validation complete
Validating simulation...
Validation complete
```

Ready | Over by 7 | Dynamic at 0 Seconds

Figure 1.189 An overspecified flowsheet.

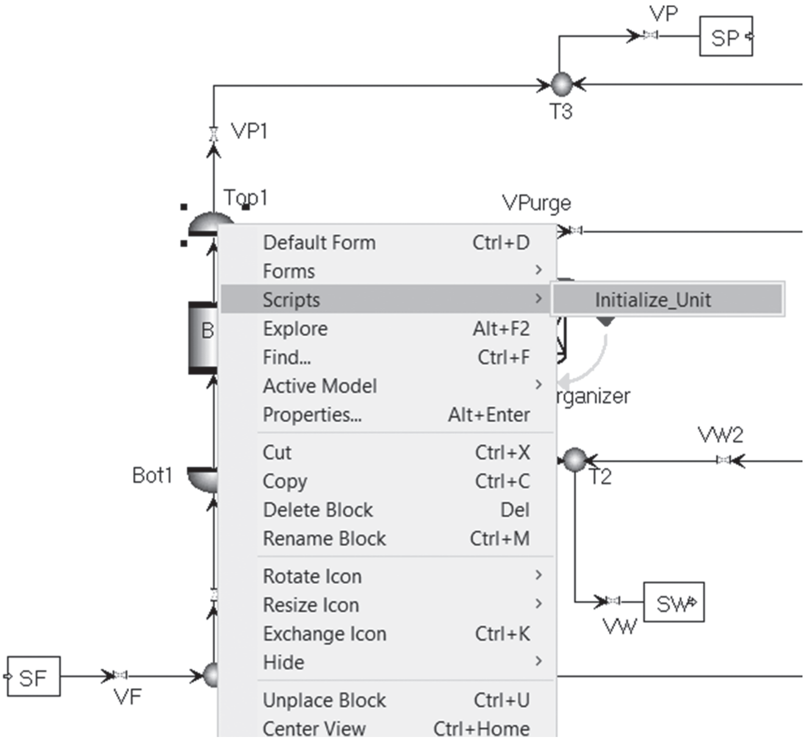
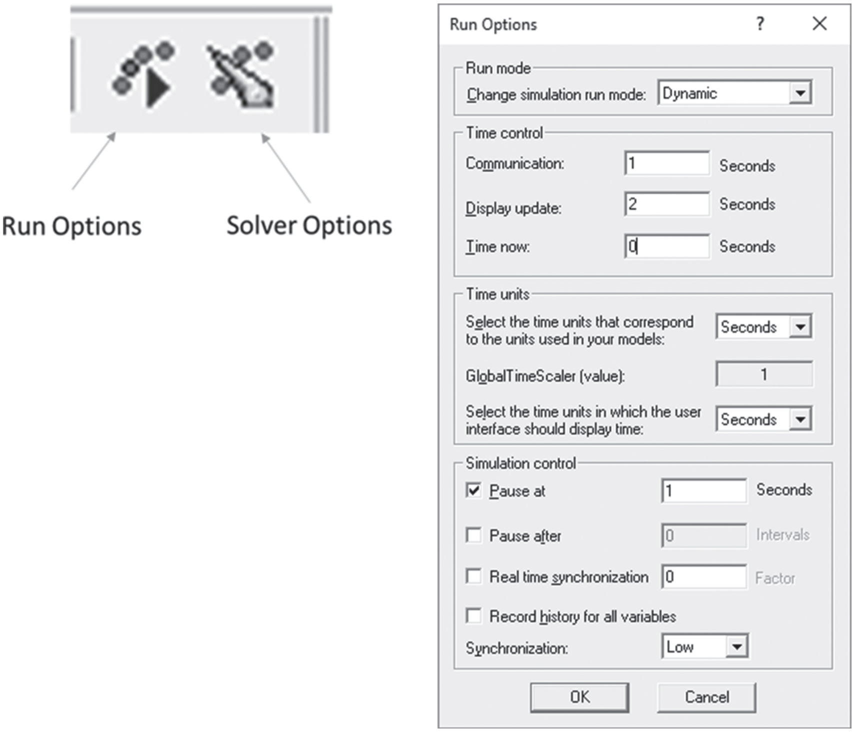


Figure 1.190 Initializing a gCSS block with an initialization script.

Table 1.12 Hydrogen PSA cycle and valve "Use_Specs."

Cycle	Step 1	Step 2	Step 3	Step 4	Step 5	Step 6
Role	Pressurize bed 1, depressurize bed 2	Adsorption bed 1, purge bed 2	Pressure equilibration	Pressurize bed 2, depressurize bed 1	Adsorption bed 2, purge bed 1	Pressure equilibration
Duration (s)	30	40	140	30	40	140
VF1	1	1	0	0	0	0
VF2	0	0	0	1	1	0
VP1	0	1	0	0	0	0
VP2	0	0	0	0	1	0
VPurge	0	2	2	0	2	2
VW1	0	0	0	1	1	0
VW2	1	1	0	0	0	0



Run mode
Change simulation run mode: Dynamic

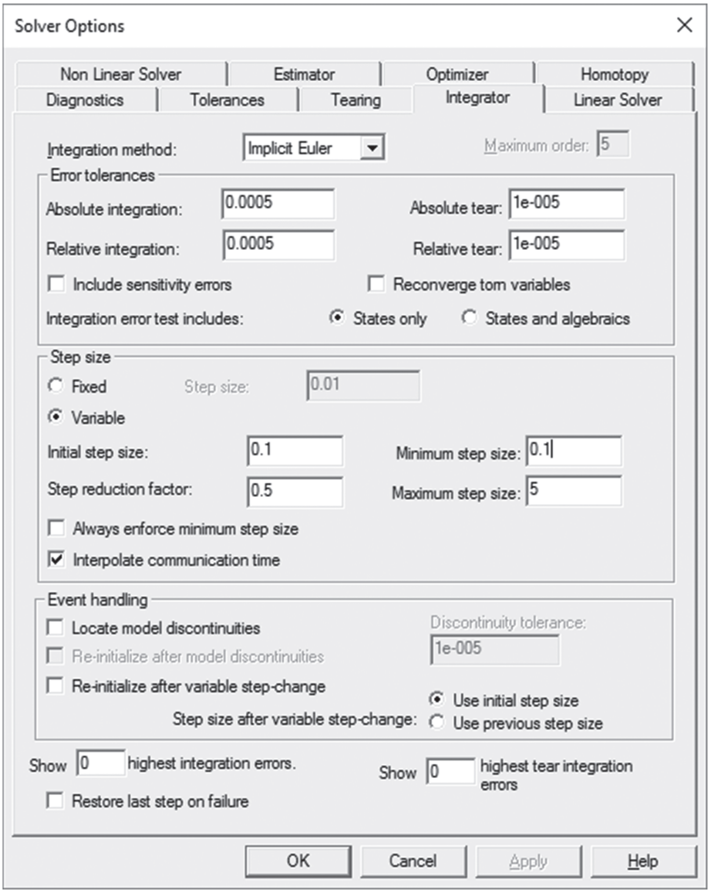
Time control
Communication: 1 Seconds
Display update: 2 Seconds
Time now: 0 Seconds

Time units
Select the time units that correspond to the units used in your models: Seconds
GlobalTimeScaler (value): 1
Select the time units in which the user interface should display time: Seconds

Simulation control
☑ Pause at 1 Seconds
☐ Pause after 0 Intervals
☐ Real time synchronization 0 Factor
☐ Record history for all variables
Synchronization: Low

Figure 1.191 The run control button, and the run control panel.

change the “Initial step size” and “Minimum step size” to 0.1 (Figure 1.192). Save the file as **Workshop3e.ada**.



Solver Options

Integration method: Implicit Euler

Maximum order: 5

Error tolerances

Absolute integration: 0.0005

Absolute tear: 1e-005

Relative integration: 0.0005

Relative tear: 1e-005

☐ Include sensitivity errors

☐ Reconverge torn variables

Integration error test includes: ● States only ○ States and algebraics

Step size

○ Fixed Step size: 0.01

● Variable

Initial step size: 0.1

Minimum step size: 0.1

Step reduction factor: 0.5

Maximum step size: 5

☐ Always enforce minimum step size

☑ Interpolate communication time

Event handling

☐ Locate model discontinuities

☐ Re-initialize after model discontinuities

Discontinuity tolerance: 1e-005

☐ Re-initialize after variable step-change

Step size after variable step-change: ● Use initial step size ○ Use previous step size

Show 0 highest integration errors.

Show 0 highest tear integration errors

☐ Restore last step on failure

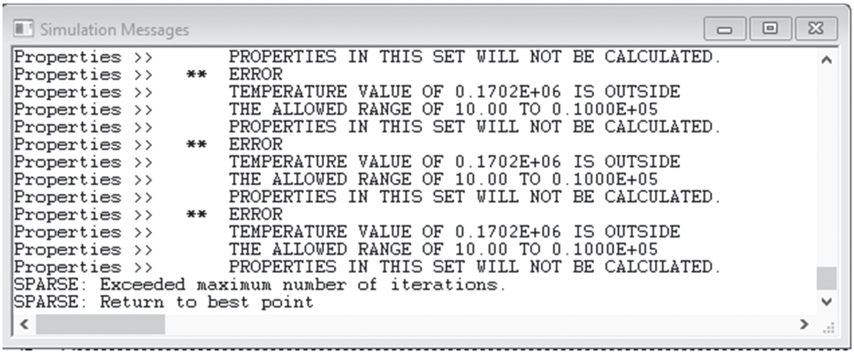
Figure 1.192 The Solver Options – Integrator tab.

Step 24: Run simulation

After confirming that the cycle *has not been generated*, and that the run mode is “Dynamic,” click on the “Run” button to begin the simulation. This will begin the dynamic run (Figure 1.193), and it will automatically end after 1 s. This may take some time, and there may be errors during the initial integration steps.

Figure 1.193 Run the dynamic simulation.

Examples of the types of errors that arise during the first few integration steps are shown in Figure 1.194. In this case, the solver has chosen a temperature



```
Properties >>       PROPERTIES IN THIS SET WILL NOT BE CALCULATED.
Properties >>   **  ERROR
Properties >>       TEMPERATURE VALUE OF 0.1702E+06 IS OUTSIDE
Properties >>       THE ALLOWED RANGE OF 10.00 TO 0.1000E+05
Properties >>       PROPERTIES IN THIS SET WILL NOT BE CALCULATED.
Properties >>   **  ERROR
Properties >>       TEMPERATURE VALUE OF 0.1702E+06 IS OUTSIDE
Properties >>       THE ALLOWED RANGE OF 10.00 TO 0.1000E+05
Properties >>       PROPERTIES IN THIS SET WILL NOT BE CALCULATED.
Properties >>   **  ERROR
Properties >>       TEMPERATURE VALUE OF 0.1702E+06 IS OUTSIDE
Properties >>       THE ALLOWED RANGE OF 10.00 TO 0.1000E+05
Properties >>       PROPERTIES IN THIS SET WILL NOT BE CALCULATED.
SPARSE: Exceeded maximum number of iterations.
SPARSE: Return to best point
```

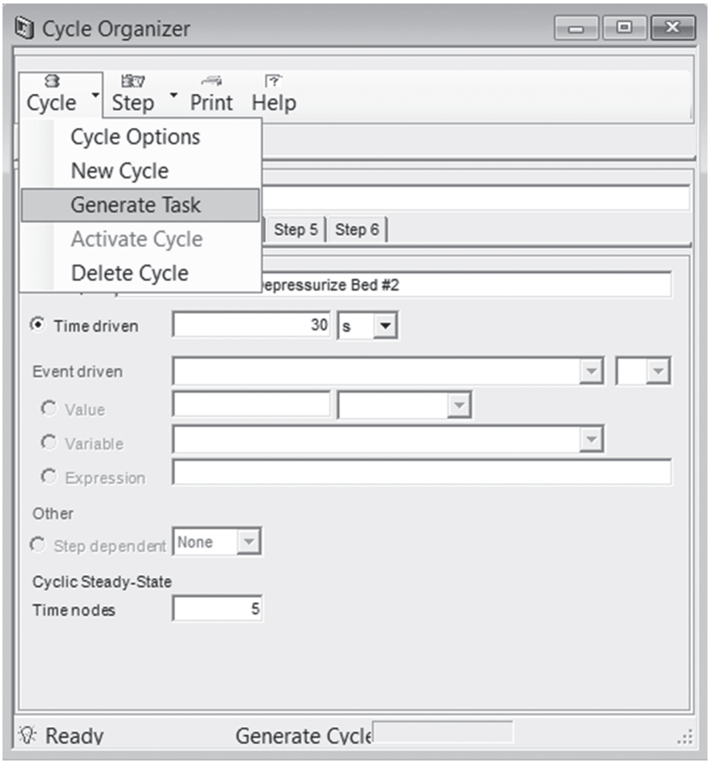
Figure 1.194 Initial simulation step example.

that is outside the range of what the property method (Peng–Rob) is capable of dealing with.

After a while, Aspen will calculate appropriate temperatures and pressures, and these messages will be resolved. Once the simulation has run for 1 s, it will pause. At this point, reopen the run control options (Figure 1.191) and enter a 0 for current time (“time now”), then uncheck the “pause at” box.

Step 25: Generate the cycle task

At this point, we can finally generate the cycle task. Set the cycle to run for 10 cycles, then generate the task as shown in Figure 1.195.



epressurize Bed #2

● Time driven 30 s

○ Step dependent None

Time nodes 5

Figure 1.195 Generating the Cycle Organizer task.

Step 26: Run simulation

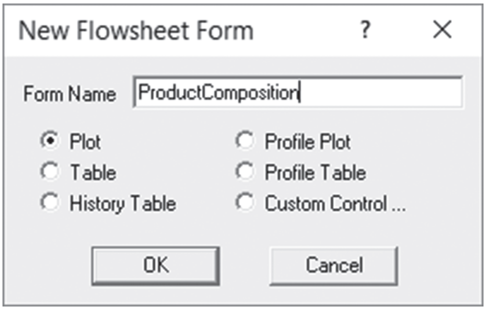
After confirming that the flowsheet is correct, and that the run mode is "Dynamic," click on the "Run" button to begin the simulation. This will begin the dynamic run, and it will automatically end after 10 cycles. See Figure 1.196.

Figure 1.196 Run the dynamic simulation.

1.9.6 Viewing Results

Step 27: Plot results

Once the simulation completes successfully, we would want to view the separation results in plot form. To do this, click on the "New form" button in the Explorer window, and add a new plot (Figure 1.197).



Form Name ProductComposition

● Plot
○ Table
○ History Table
○ Profile Plot
○ Profile Table
○ Custom Control ...

Figure 1.197 Creating a new plot.

To retrieve the variables we want to plot, right-click on the product tank, T3. By mousing over "Forms," we can see several predefined forms for the Tank blocks. For example, we could look at the Result_Plot_DYN to see one representation of the results (Figure 1.198). However, we plot the mole fraction of the various components, so we need to open the "AllVariables" form.

Once the AllVariables table is open, select all the mole fraction variables and drag them onto the y-axis of the plot (Figure 1.199). You can also drag them one at a time.

After adding the variables, right-click on the plot and "Zoom Full" to see the entire history (Figure 1.200).

When the full history is visible, the result should look like Figure 1.201. The product should be >99.7% pure hydrogen.

If your result matches, you have completed the workshop! Save the file as **Workshop3e_dyn.ada**.

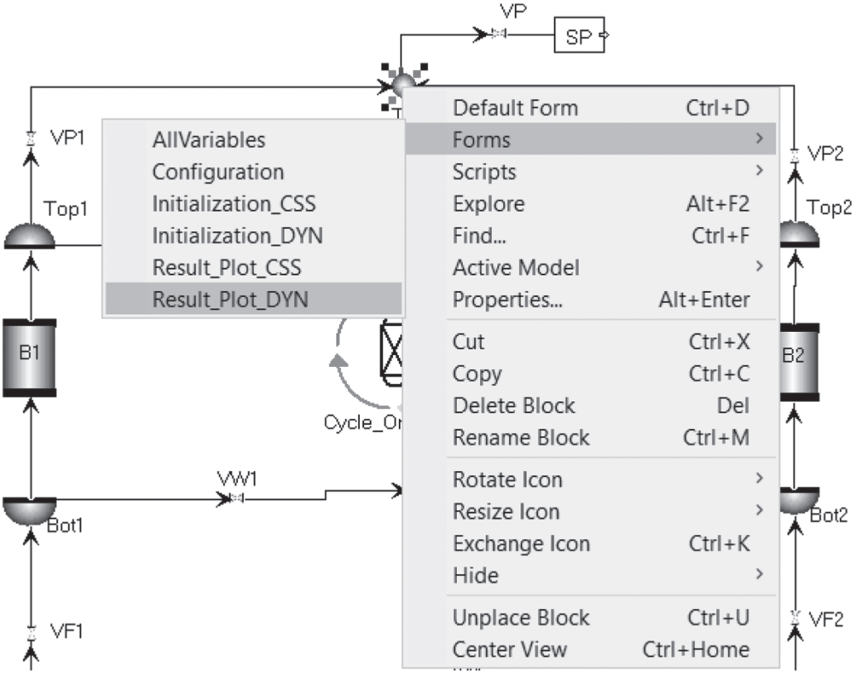


Figure 1.198 Locating variables to plot. Result_Plot_DYN contains a premade graph, but we want variables from AllVariables.

1.10 TSA Workshop: Temperature Swing Adsorption for Air Drying

Another major application of adsorption technology is air drying. Unlike the previous examples, this process typically involves TSA, as opposed to pressure swing. Let us consider a small process designed to dry air by passing moist air over an alumina adsorbent.

Step 1: Draw the flowsheet

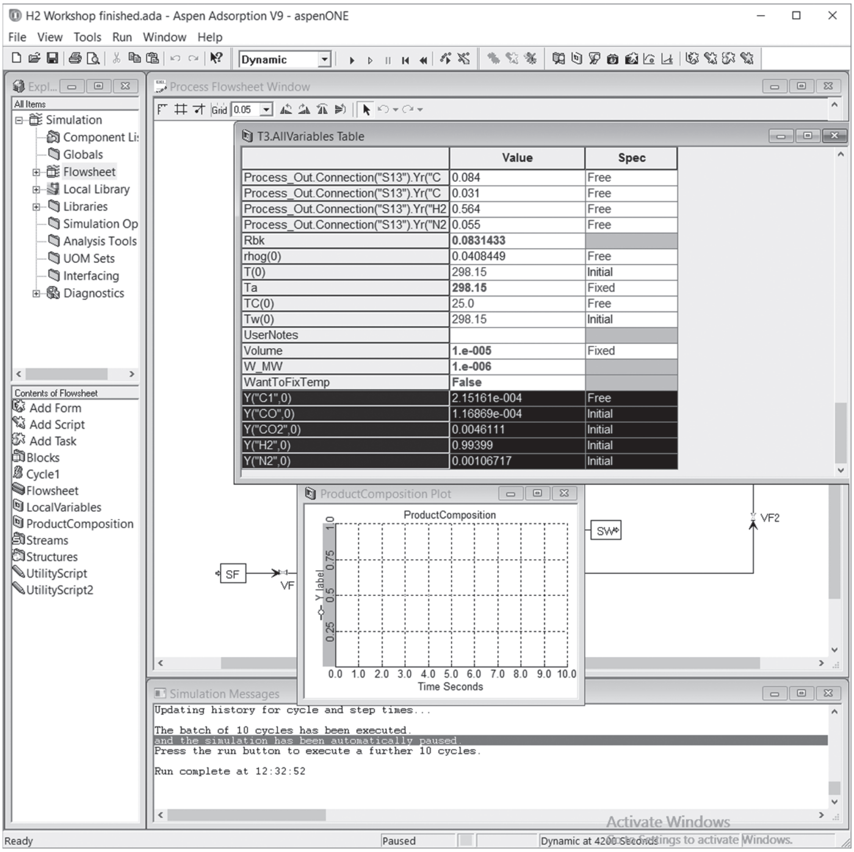
Using the techniques learned in the first three workshops, create the flowsheet shown in Figure 1.202. Start with a new Aspen file called `Workshop4a.ada`. The components for the system are "Air" and "H_2O," both of which can be found in the Aspen Properties Databanks. In this process, we use the models in the gas_dynamic folder, rather than the gCSS folder.

The flowsheet shown in Figure 1.202 allows us to implement the cyclic procedure described in Figure 1.203. Not that this is very similar to the PSA case, but temperature changes as well.

Step 2: Enter the process data

Add the following information to the flowsheet as Figures 1.204 and 1.205 using the same techniques as in the PSA Workshop, Figures 1.45 and 1.46.

We also need to specify the pressure at the outlets to this process (Figures 1.206 and 1.207).



	Value	Spec
Process_Out.Connection("S13").Yr("C	0.084	Free
Process_Out.Connection("S13").Yr("C	0.031	Free
Process_Out.Connection("S13").Yr("H2	0.564	Free
Process_Out.Connection("S13").Yr("N2	0.055	Free
Rbk	**0.0831433**	
rhog(0)	0.0408449	Free
T(0)	298.15	Initial
Ta	**298.15**	Fixed
TC(0)	25.0	Free
Tw(0)	298.15	Initial
UserNotes		
Volume	**1.e-005**	Fixed
W_MW	**1.e-006**	
WantToFixTemp	**False**	
Y("C1",0)	2.15161e-004	Free
Y("CO",0)	1.16869e-004	Initial
Y("CO2",0)	0.0046111	Initial
Y("H2",0)	0.99399	Initial
Y("N2",0)	0.00106717	Initial

```
Updating history for cycle and step times...

The batch of 10 cycles has been executed.
and the simulation has been automatically paused.
Press the run button to execute a further 10 cycles.

Run complete at 12:32:52
```

Figure 1.199 Dragging the mole fraction variables from the AllVariables table to the plot.

Step 3: Specify the tank volumes and options

For this problem, if we leave the tank volumes at their very small initial value, and try to calculate compressive terms, we will get occasional unreasonable spikes in temperature due to numerical issues at step changes. To mitigate this, we increase the tank volumes and ignore the compressibility of the gas in the tanks. See Figure 1.208.

Step 4: Determine the Isotherm parameters

Let us suppose that the supplier of your alumina desiccant was "creative" in choosing an isotherm to describe their desiccant's performance. They claim that air is never adsorbed, and provide you with the procedure described in Eq. (1.19) to calculate the equilibrium loading of water:

$$\begin{aligned} P_{\text{sat}} &= \text{IP}_1 e^{\left(\text{IP}_2 - \frac{\text{IP}_3}{T}\right)} \\ P_{\text{rel}} &= Y_{\text{H}_2\text{O}} \frac{P_{\text{Total}}}{P_{\text{sat}}} \\ W_{\text{H}_2\text{O}} &= \text{IP}_4{}^{*} P_{\text{rel}} \end{aligned} \tag{1.19}$$

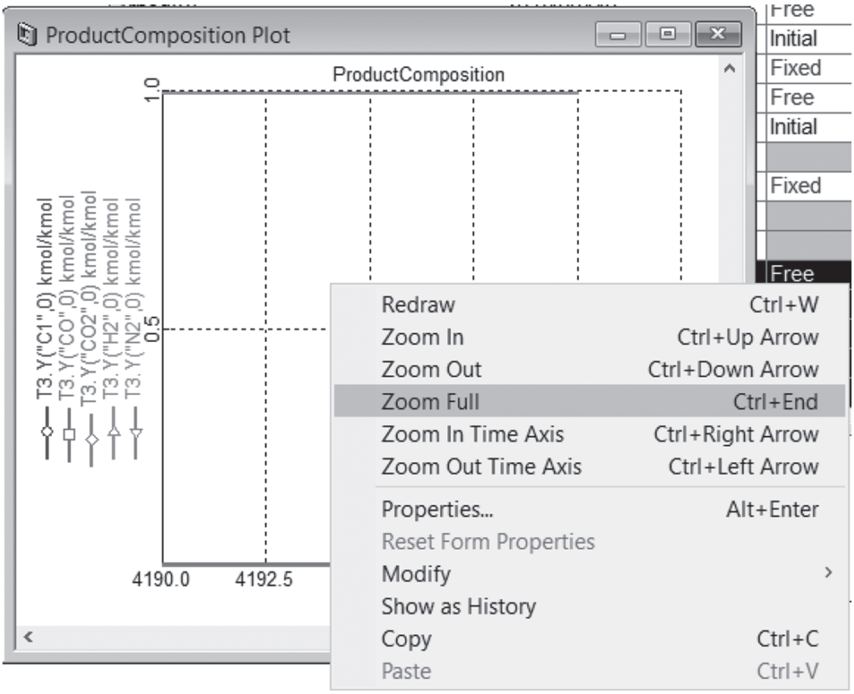


Figure 1.200 Zooming out on the Product Composition plot.

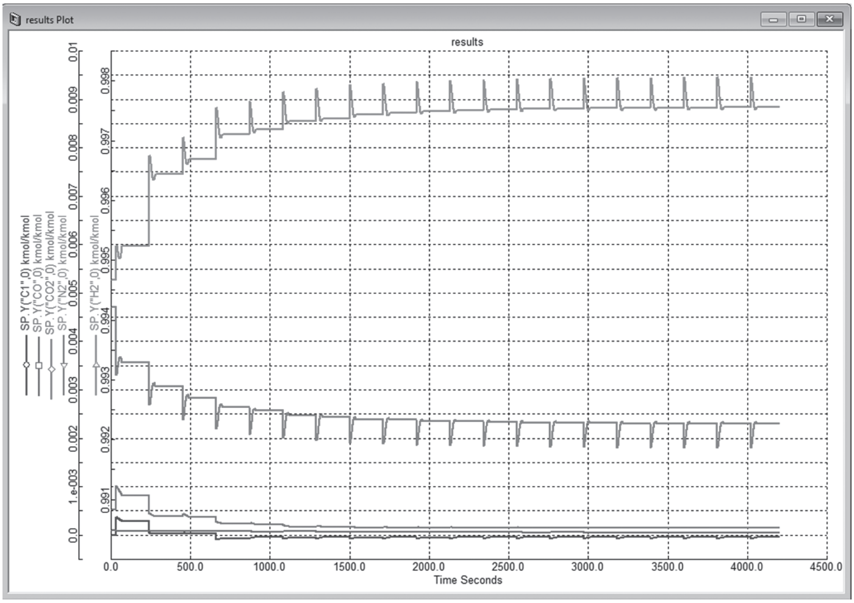


Figure 1.201 The final product composition result.

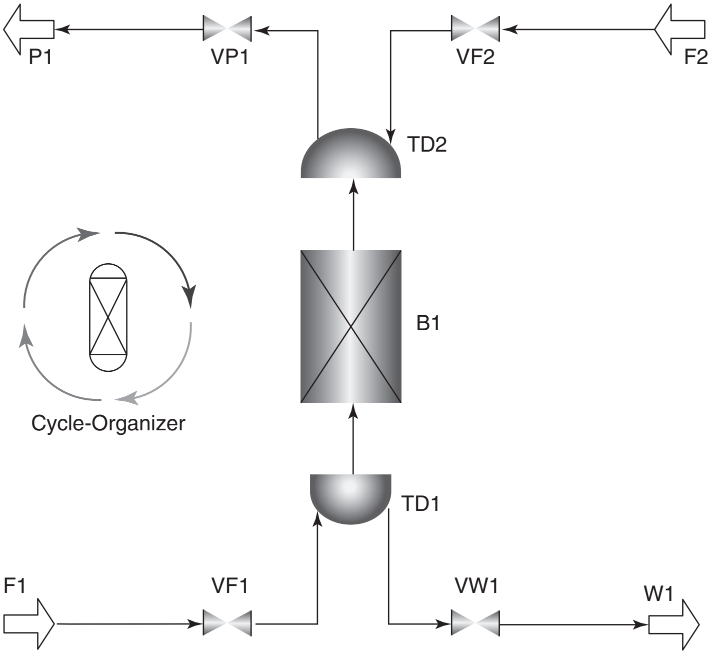


Figure 1.202 The TSA flowsheet. F1 represents the moist air to be dried, while F2 represents a partial recycle of the heated product air that is used to regenerate the adsorbent.

Can we input this multistep procedure into Aspen? What are our options?

- We could use *Flowsheet Constraints* to define the loading in exactly the form provided by the manufacturer.
- We could try to rearrange the equations into something Aspen can handle.

In this case, with some fairly simple observations, we can convert the isotherm into a form Aspen already has implemented. Specifically, let us start by combining all of those steps into one big equation

$$W_{H_2O} = IP_4 \frac{Y_{H_2O} P_{Total}}{IP_1 e^{\left(IP_2 - \frac{IP_3}{T}\right)}} \tag{1.20}$$

Right away, we should notice that $Y_{H_2O} P_{Total}$ is simply partial pressure (p_{H_2O}) and there is no reason to have IP_4/IP_2 as two separate isotherm parameters. We also know that we can simply make the exponent negative to move it into the numerator.

$$W_{H_2O} = IP_5 p_{H_2O} e^{\left(-IP_2 + \frac{IP_3}{T}\right)} \tag{1.21}$$

Now this looks much simpler. However, we still have the $e^{\left(-IP_2 + \frac{IP_3}{T}\right)}$ term, which does not appear in any comparable built-in isotherm. Fortunately, we know that it is possible to write $e^{\left(-IP_2 + \frac{IP_3}{T}\right)}$ as $e^{-IP_2} e^{\left(\frac{IP_3}{T}\right)}$ and that e^{-IP_2} is itself a constant. So it is finally possible to write the equation as

$$W_{H_2O} = IP_6 p_{H_2O} e^{\left(\frac{IP_3}{T}\right)} \tag{1.22}$$

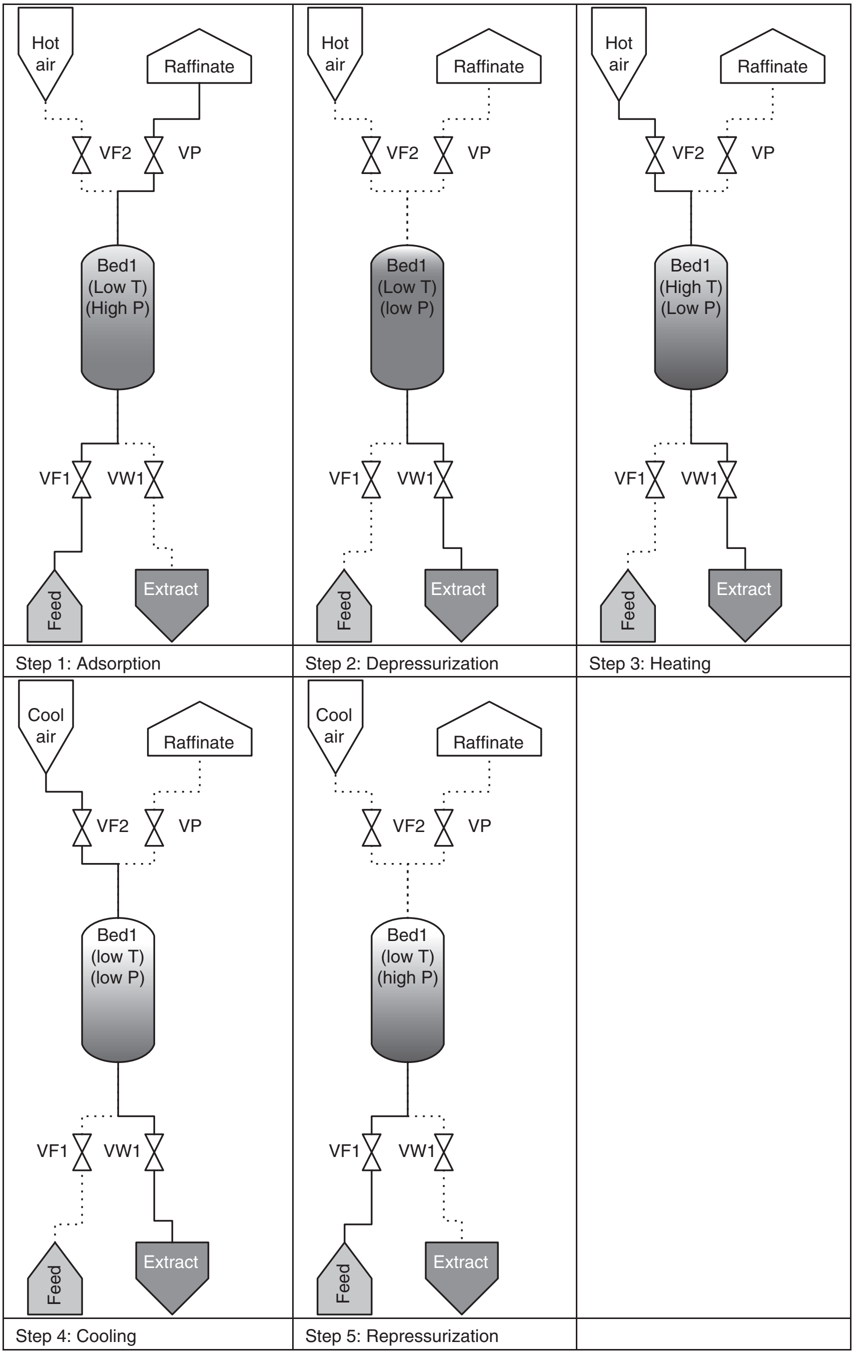
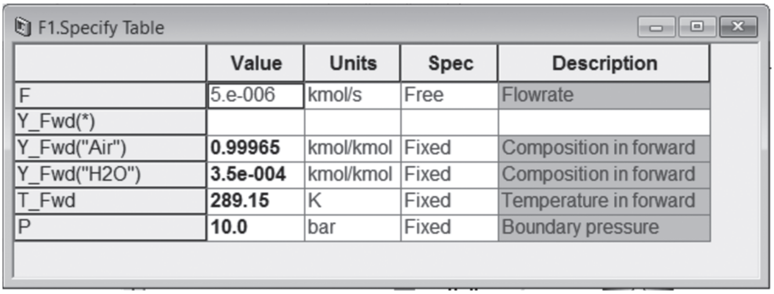
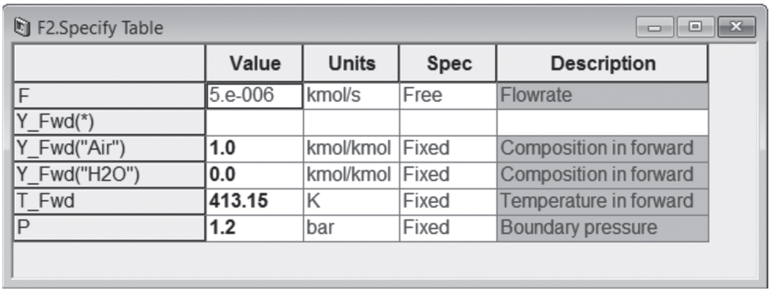


Figure 1.203 The one-bed TSA cycle.



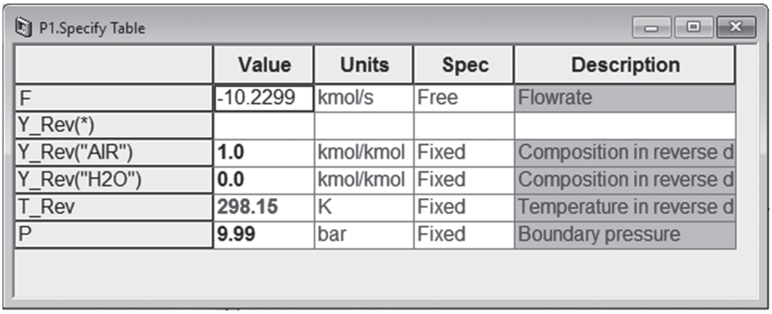
	Value	Units	Spec	Description
F	5.e-006	kmol/s	Free	Flowrate
Y_Fwd(*)				
Y_Fwd("Air")	**0.99965**	kmol/kmol	Fixed	Composition in forward
Y_Fwd("H2O")	**3.5e-004**	kmol/kmol	Fixed	Composition in forward
T_Fwd	**289.15**	K	Fixed	Temperature in forward
P	**10.0**	bar	Fixed	Boundary pressure

Figure 1.204 Moist air feed conditions.



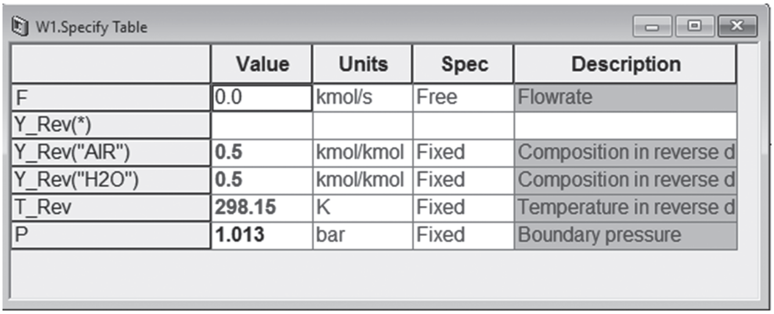
	Value	Units	Spec	Description
F	5.e-006	kmol/s	Free	Flowrate
Y_Fwd(*)				
Y_Fwd("Air")	**1.0**	kmol/kmol	Fixed	Composition in forward
Y_Fwd("H2O")	**0.0**	kmol/kmol	Fixed	Composition in forward
T_Fwd	**413.15**	K	Fixed	Temperature in forward
P	**1.2**	bar	Fixed	Boundary pressure

Figure 1.205 Hot regeneration air conditions.



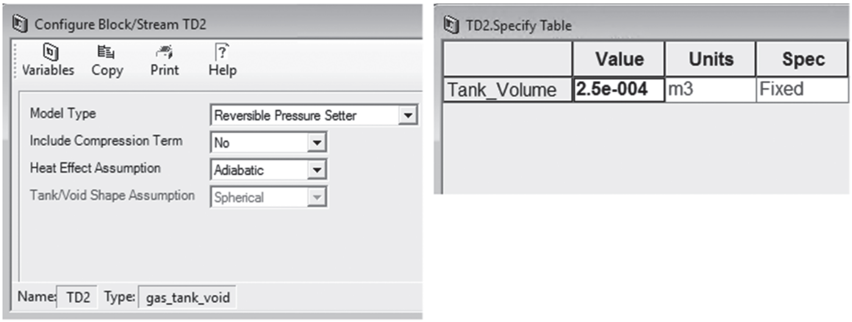
	Value	Units	Spec	Description
F	-10.2299	kmol/s	Free	Flowrate
Y_Rev(*)				
Y_Rev("AIR")	**1.0**	kmol/kmol	Fixed	Composition in reverse d
Y_Rev("H2O")	**0.0**	kmol/kmol	Fixed	Composition in reverse d
T_Rev	**298.15**	K	Fixed	Temperature in reverse d
P	**9.99**	bar	Fixed	Boundary pressure

Figure 1.206 Dry air collection conditions.



	Value	Units	Spec	Description
F	0.0	kmol/s	Free	Flowrate
Y_Rev(*)				
Y_Rev("AIR")	**0.5**	kmol/kmol	Fixed	Composition in reverse d
Y_Rev("H2O")	**0.5**	kmol/kmol	Fixed	Composition in reverse d
T_Rev	**298.15**	K	Fixed	Temperature in reverse d
P	**1.013**	bar	Fixed	Boundary pressure

Figure 1.207 Wet product collection conditions.



Model Type: Reversible Pressure Setter
Include Compression Term: No
Heat Effect Assumption: Adiabatic
Tank/Void Shape Assumption: Spherical
Name: TD2 Type: gas_tank_void

TD2.Specify Table

	Value	Units	Spec
Tank_Volume	2.5e-004	m3	Fixed

Figure 1.208 Specifying the tank options.

which is clearly a simple Henry's Law style of isotherm. In this case, IP_6 can be expressed as a function of the manufacturer's parameters as

$$IP_6 = \frac{IP_4}{IP_1} e^{-IP_2} \tag{1.23}$$

Step 5: Specify thecolumn behavior

Apply the following assumptions to the packed bed according to Table 1.13.

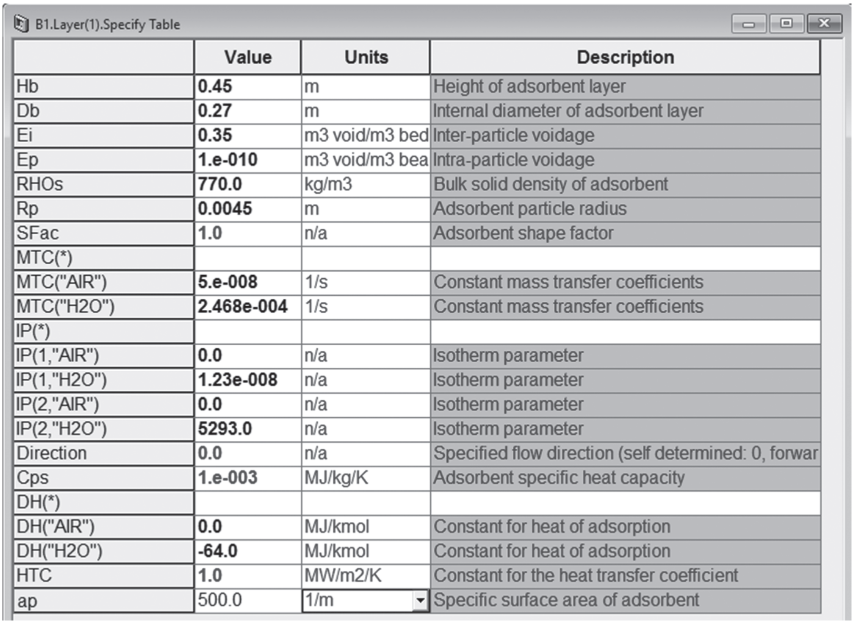
Table 1.13 Specifications of the adsorption column.

Discretization method	QDS (quadratic differencing scheme)	*Nodes*	20
Material balance	Convection only	*Pressure drop assumption*	Ergun
Kinetic film model	Linear lumped resistance	*Based on*	Solid phase concentration
Mass transfer coefficient	Constant		
Isotherm	Henry 2 (based on partial pressure)		
Energy balance	Nonisothermal	*Conduction*	No
Consider solid phase	No	*Heat of adsorption*	Constant
Heat transfer to environment	Adiabatic	*Heat capacity*	Constant

Once these options have been entered, specify the values for the column shown in Figure 1.209.

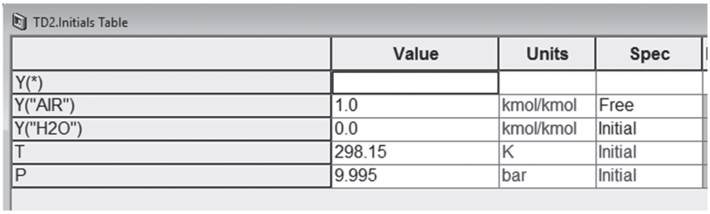
Step 6: Specify the initial conditions

We would like this separation to start with fully dry air in the column and tanks. To do this, we need to modify their initial conditions. On the column configuration sheet, click on the preset/initials button. The tanks and bed should be set to be completely dry at $t = 0$. See Figures 1.210 and 1.211.



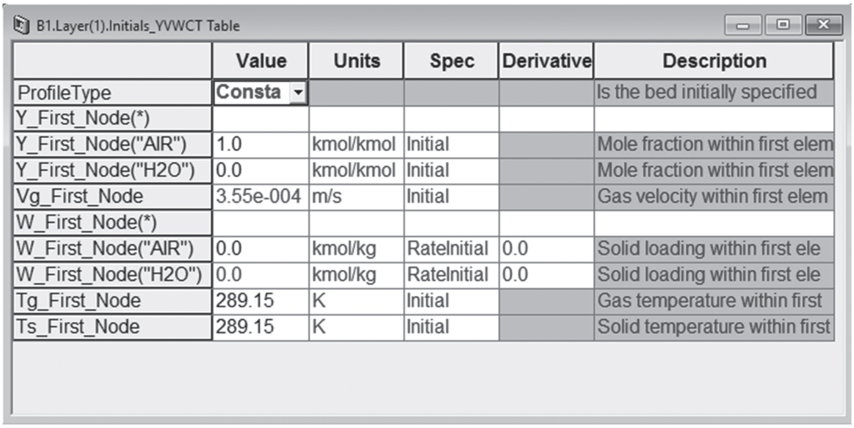
	Value	Units	Description
Hb	**0.45**	m	Height of adsorbent layer
Db	**0.27**	m	Internal diameter of adsorbent layer
Ei	**0.35**	m3 void/m3 bed	Inter-particle voidage
Ep	**1.e-010**	m3 void/m3 bea	Intra-particle voidage
RHOs	**770.0**	kg/m3	Bulk solid density of adsorbent
Rp	**0.0045**	m	Adsorbent particle radius
SFac	**1.0**	n/a	Adsorbent shape factor
MTC(*)			
MTC("AIR")	**5.e-008**	1/s	Constant mass transfer coefficients
MTC("H2O")	**2.468e-004**	1/s	Constant mass transfer coefficients
IP(*)			
IP(1,"AIR")	**0.0**	n/a	Isotherm parameter
IP(1,"H2O")	**1.23e-008**	n/a	Isotherm parameter
IP(2,"AIR")	**0.0**	n/a	Isotherm parameter
IP(2,"H2O")	**5293.0**	n/a	Isotherm parameter
Direction	**0.0**	n/a	Specified flow direction (self determined: 0, forwar
Cps	**1.e-003**	MJ/kg/K	Adsorbent specific heat capacity
DH(*)			
DH("AIR")	**0.0**	MJ/kmol	Constant for heat of adsorption
DH("H2O")	**-64.0**	MJ/kmol	Constant for heat of adsorption
HTC	**1.0**	MW/m2/K	Constant for the heat transfer coefficient
ap	500.0	1/m	Specific surface area of adsorbent

Figure 1.209 Column parameters for air drying.



	Value	Units	Spec
Y(*)			
Y("AIR")	1.0	kmol/kmol	Free
Y("H2O")	0.0	kmol/kmol	Initial
T	298.15	K	Initial
P	9.995	bar	Initial

Figure 1.210 Set the tanks to contain dry air.



	Value	Units	Spec	Derivative	Description
ProfileType	**Consta**				Is the bed initially specified
Y_First_Node(*)					
Y_First_Node("AIR")	1.0	kmol/kmol	Initial		Mole fraction within first elem
Y_First_Node("H2O")	0.0	kmol/kmol	Initial		Mole fraction within first elem
Vg_First_Node	3.55e-004	m/s	Initial		Gas velocity within first elem
W_First_Node(*)					
W_First_Node("AIR")	0.0	kmol/kg	RateInitial	0.0	Solid loading within first ele
W_First_Node("H2O")	0.0	kmol/kg	RateInitial	0.0	Solid loading within first ele
Tg_First_Node	289.15	K	Initial		Gas temperature within first
Ts_First_Node	289.15	K	Initial		Solid temperature within first

Figure 1.211 Set the column to contain dry air.

Step 7: Create the Cycle Organizer steps

Create five steps according to Table 1.14. Figures 1.212–1.216 show the manipulated variables of steps 1–5. The steps will use different manipulated variables, so it is best to not copy the values from one step to the next.

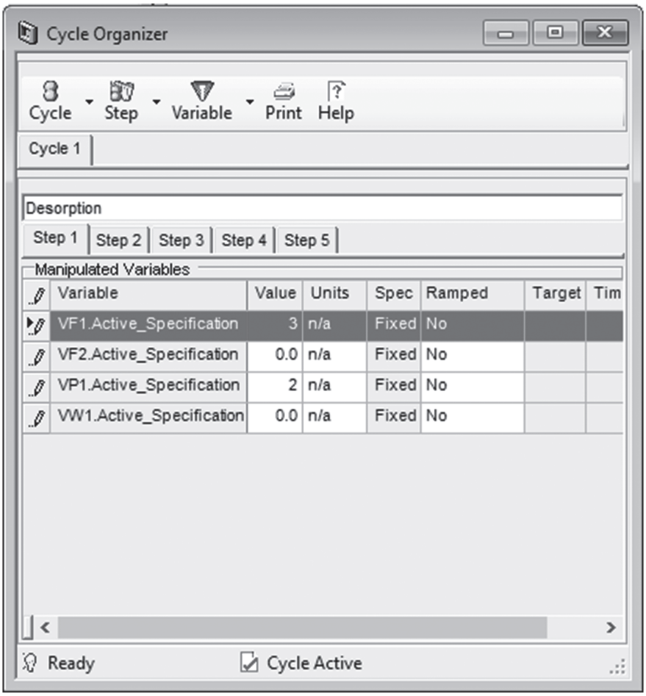
Step 8: Specify the manipulated variables

Refer to Figure 1.7 and Table 1.5 for the four ASs for valves within Aspen Adsorption: (1) AS = 0, valve is fully closed; (2) AS = 1, valve is fully open; and (3) AS = 2, the gas flow rate through the valve is linearly dependent on the pressure drop across the valve according to Eq. (1.12); and (4) AS = 3, the valve has a fixed flow rate.

Step 9: Set the cycle to run twice

Table 1.14 A five-step TSA cycle.

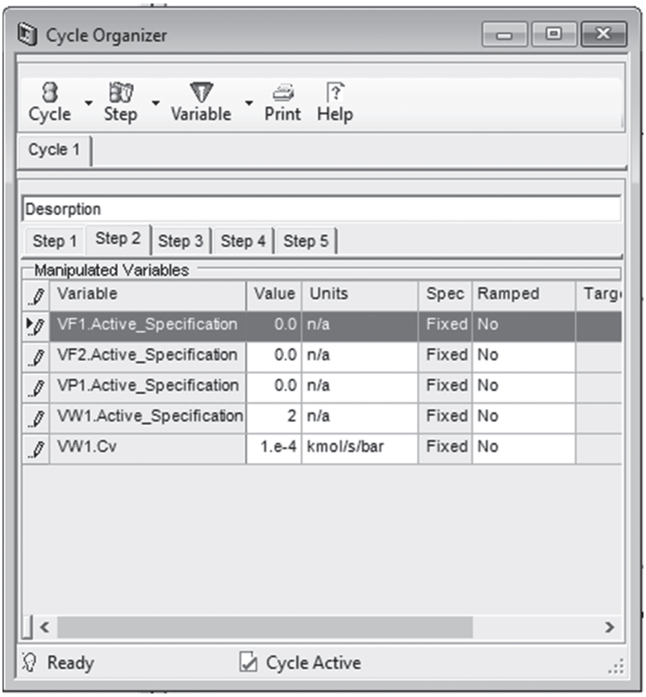
	Description	Duration (min)
Step 1	Adsorption	151
Step 2	Depressurization	1
Step 3	Heating	47
Step 4	Cooling	72
Step 5	Repressurization	Dependent on step 2



Desorption

Variable	Value	Units	Spec	Ramped	Target	Tim
VF1.Active_Specification	3	n/a	Fixed	No		
VF2.Active_Specification	0.0	n/a	Fixed	No		
VP1.Active_Specification	2	n/a	Fixed	No		
VW1.Active_Specification	0.0	n/a	Fixed	No		

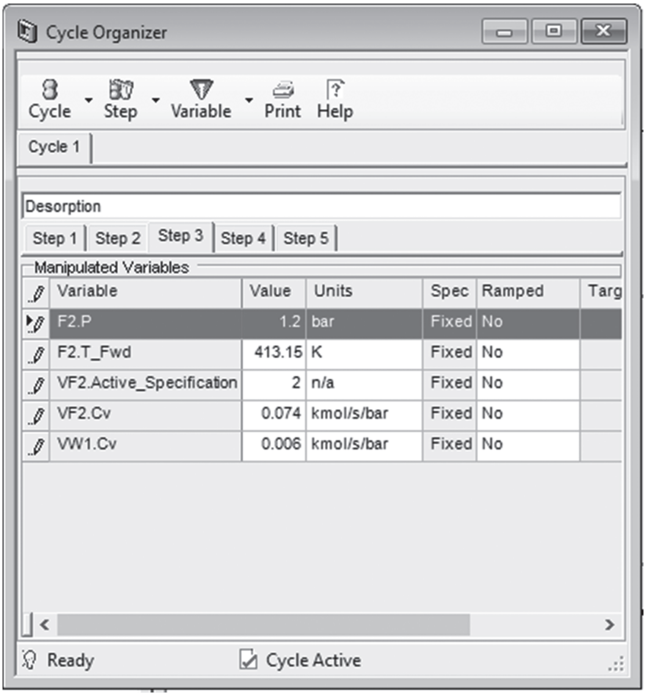
Figure 1.212 Step 1 (adsorption) manipulated variables.



Desorption

Variable	Value	Units	Spec	Ramped	Targ
VF1.Active_Specification	0.0	n/a	Fixed	No	
VF2.Active_Specification	0.0	n/a	Fixed	No	
VP1.Active_Specification	0.0	n/a	Fixed	No	
VW1.Active_Specification	2	n/a	Fixed	No	
VW1.Cv	1.e-4	kmol/s/bar	Fixed	No	

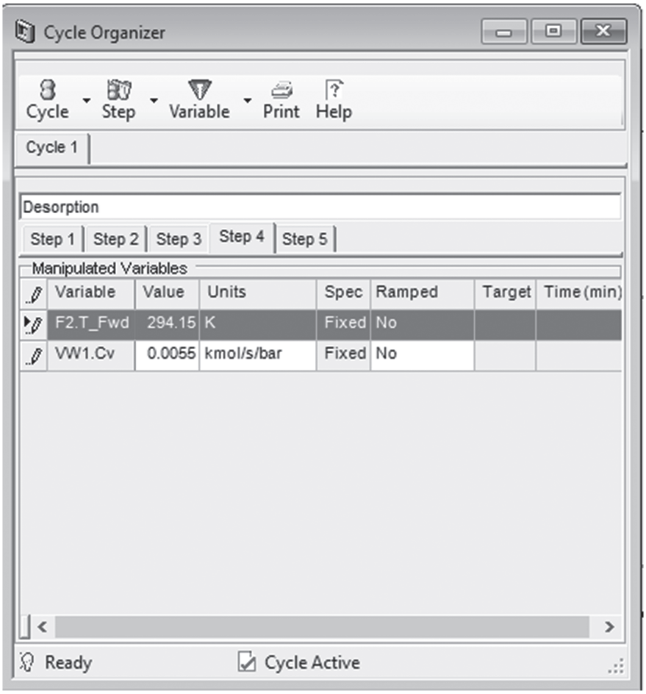
Figure 1.213 Step 2 (depressurizatin) manipulated variables.



Desorption

Variable	Value	Units	Spec	Ramped	Targ
F2.P	1.2	bar	Fixed	No	
F2.T_Fwd	413.15	K	Fixed	No	
VF2.Active_Specification	2	n/a	Fixed	No	
VF2.Cv	0.074	kmol/s/bar	Fixed	No	
VW1.Cv	0.006	kmol/s/bar	Fixed	No	

Figure 1.214 Step 3 (heating) manipulated variables.

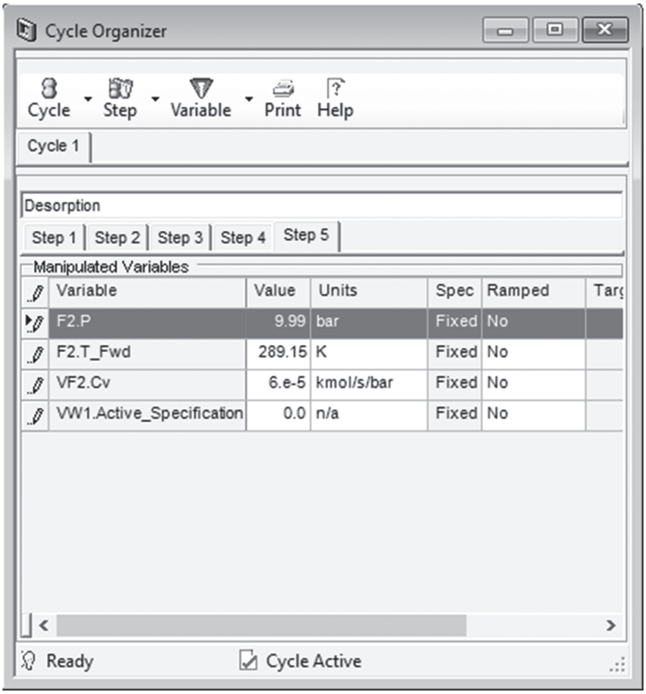


Desorption

Manipulated Variables

Variable	Value	Units	Spec	Ramped	Target	Time (min)
F2.T_Fwd	294.15	K	Fixed	No		
VW1.Cv	0.0055	kmol/s/bar	Fixed	No		

Figure 1.215 Step 4 (cooling) manipulated variables.



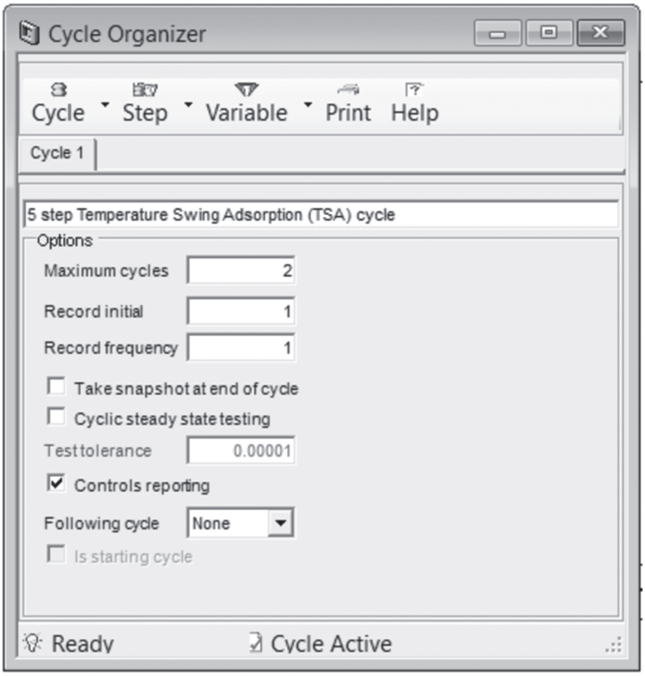
Desorption

Manipulated Variables

Variable	Value	Units	Spec	Ramped	Targ
F2.P	9.99	bar	Fixed	No	
F2.T_Fwd	289.15	K	Fixed	No	
VF2.Cv	6.e-5	kmol/s/bar	Fixed	No	
VW1.Active_Specification	0.0	n/a	Fixed	No	

Figure 1.216 Step 5 (repressurization) manipulated variables.

This process reaches the steady state quite quickly, and therefore, we only need to run very few cycles to see the trends (Figure 1.217).



5 step Temperature Swing Adsorption (TSA) cycle

Options

Maximum cycles 2

Record initial 1

Record frequency 1

☐ Take snapshot at end of cycle

☐ Cyclic steady state testing

Test tolerance 0.00001

☑ Controls reporting

Following cycle None

☐ Is starting cycle

Ready Cycle Active

Figure 1.217 Limiting the cycle to two iterations.

Step 10: Change the integration options

Use the Solver Options button to edit the integration options. Specifically, to improve the speed of the simulation, we want to increase the "Maximum step size" to 10 s (Figure 2.218).

Next, change the run options so that the communication interval is also 10 s (Figure 2.219).

Step 11: Initialize the flowsheet

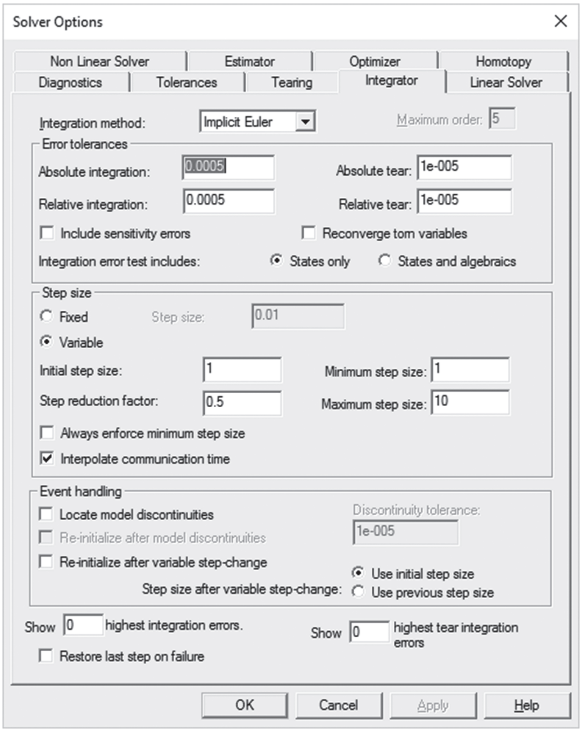
Use the "Check and Initial" entry in the flowsheet menu to initialize the flowsheet (Figure 1.220).

Step 12: Run the simulation and view the results

Create a plot to display the axial temperature profile in the bed (Figure 1.221), and leave this plot open while the simulation executes.

To see how the temperatures at either end of the column change over time, create a plot of the temperatures of the tanks at either end of the column. This will give us some additional insight into the temperature gradients across the column (Figure 1.222).

Finally, we will want to know what the actual product composition is. To do this, create a plot of the mole fraction of water and air in the P1 block. As we can see, we have successfully dried the air from an initial mole fraction of 3.5e−4 to below 1e−5 (Figure 1.223).



Integration method: Implicit Euler
Maximum order: 5

Error tolerances
Absolute integration: 0.0005
Absolute tear: 1e-005
Relative integration: 0.0005
Relative tear: 1e-005
☐ Include sensitivity errors
☐ Reconverge torn variables
Integration error test includes: ● States only ○ States and algebraics

Step size
○ Fixed
Step size: 0.01
● Variable
Initial step size: 1
Minimum step size: 1
Step reduction factor: 0.5
Maximum step size: 10
☐ Always enforce minimum step size
☑ Interpolate communication time

Event handling
☐ Locate model discontinuities
☐ Re-initialize after model discontinuities
Discontinuity tolerance: 1e-005
☐ Re-initialize after variable step-change
Step size after variable step-change: ● Use initial step size ○ Use previous step size

Show 0 highest integration errors.
Show 0 highest tear integration errors
☐ Restore last step on failure

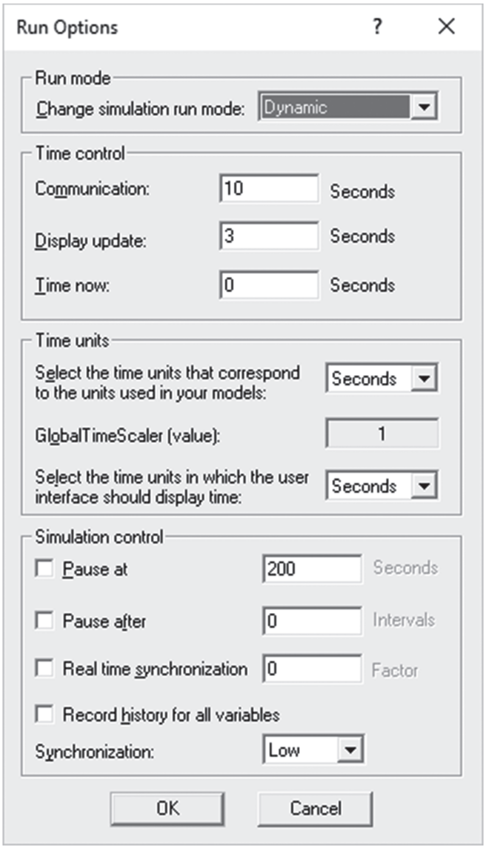
Figure 1.218 Increasing the maximum step size.

1.11 Conclusions

This chapter has covered a number of crucial modeling considerations involved in building simulations of gas adsorption processes. Specifically, the key requirements in each model are as follows:

1) Knowledge of which chemical species will be present in the simulation, as well as their properties. We discuss in Section 1.4 several possible methods for modeling the behavior of both the gas and solid phases and offered guidance on selecting the methods.
2) Knowledge of the solid–gas interaction equilibrium and kinetics. We cover several major equilibrium models in Section 1.3, and kinetic assumptions in Section 1.4. We show how to employ these equations in Aspen Adsorption.
3) Detailed knowledge of the model libraries available in Aspen Adsorption, and how they can combine to approximate real-world unit operations. Each workshop discussed covers a different set of the models and options available. At the conclusion of these three workshops, the reader should have a command of the majority of the important gas process models, and be well positioned to model a wide variety of industrial processes.
4) A detailed schedule of the valve operation required to implement the “swing” in temperature or PSA. Each workshop uses a slightly different switching scheme, and we discuss the methods for implementing both time-based and

Figure 1.219 Changing the Run options.



Run Options

Run mode

Change simulation run mode: Dynamic

Time control

Communication: 10 Seconds

Display update: 3 Seconds

Time now: 0 Seconds

Time units

Select the time units that correspond to the units used in your models: Seconds

GlobalTimeScaler (value): 1

Select the time units in which the user interface should display time: Seconds

Simulation control

☐ Pause at 200 Seconds

☐ Pause after 0 Intervals

☐ Real time synchronization 0 Factor

☐ Record history for all variables

Synchronization: Low

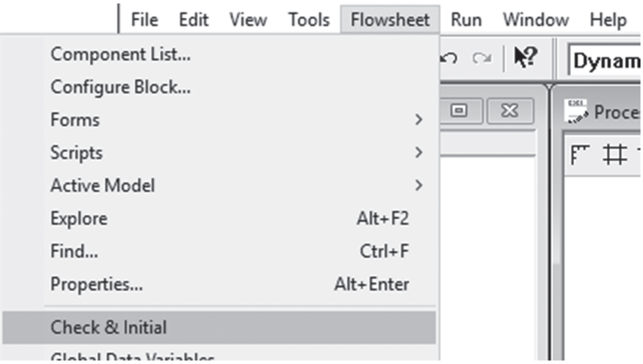


Figure 1.220 Initializing the flowsheet.

event-based scheduling. We also cover how to use a gas_interaction model to speed up computation, and how to schedule around that model.

5) Collecting data from the completed simulation. We discuss strategies for structuring the data collection in the H2 workshop. Specifically, we want to

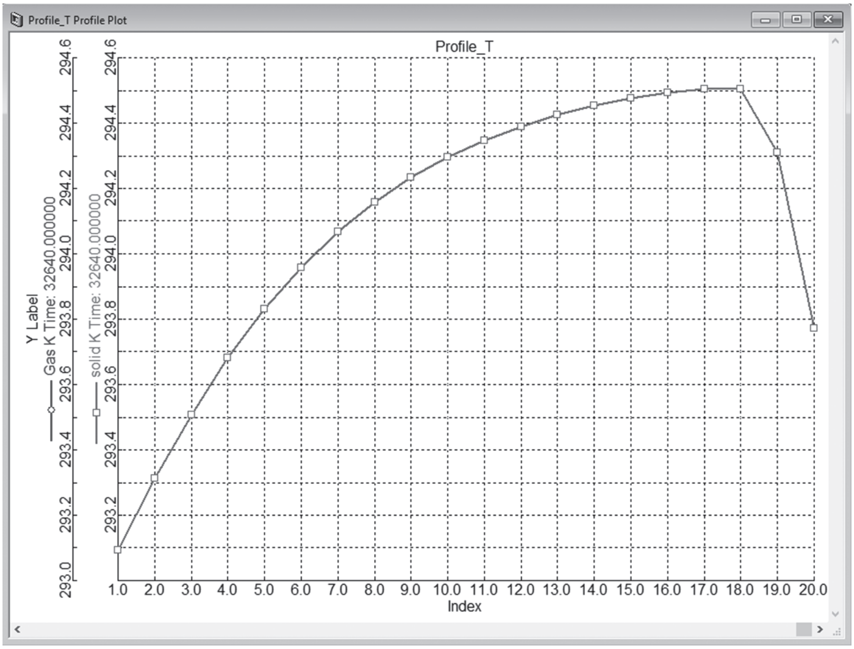


Figure 1.221 The axial temperature profile.

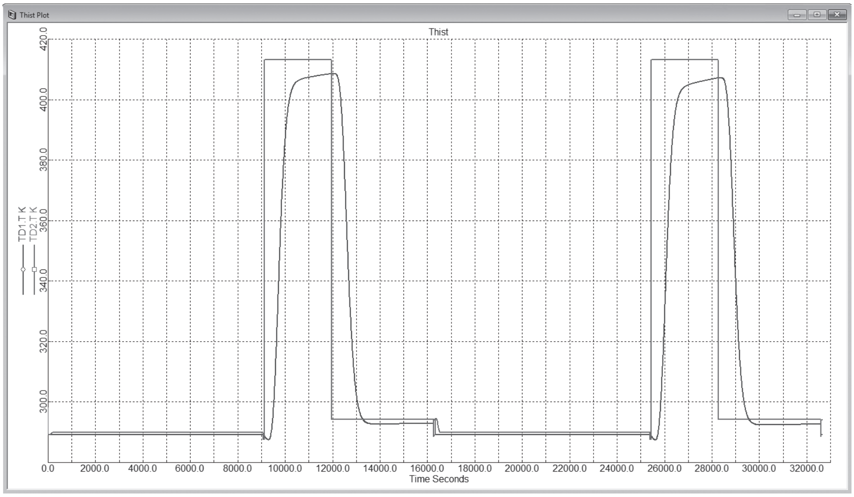


Figure 1.222 Temperature of the top and bottom tanks over time.

avoid errors due to division by trace quantities, and avoid making the results too dependent on the model's time discretization settings.

The techniques described in this chapter will allow the reader to quickly implement detailed, predictive models of gas adsorption processes. The lessons learned

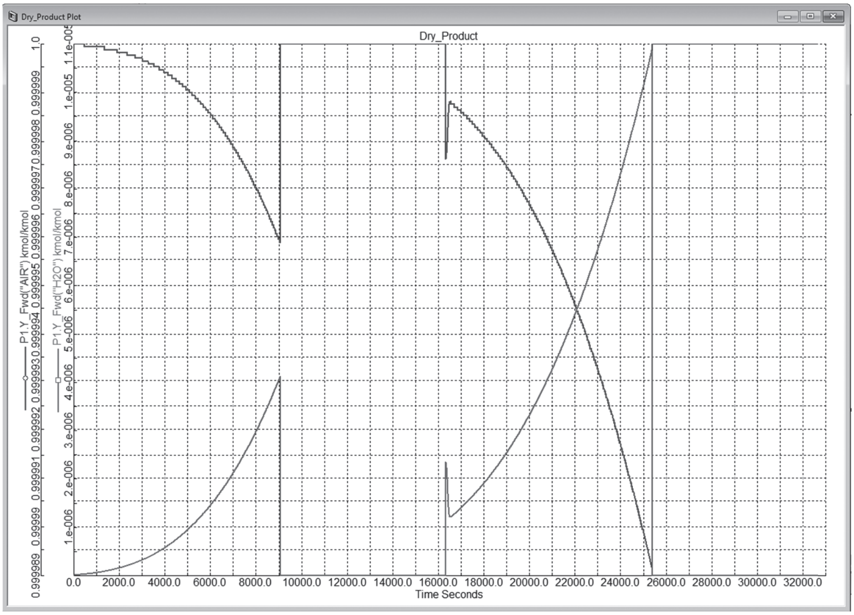


Figure 1.223 Product Composition. Notice that the mole fraction of water stays below 1.1e−5.

here will reappear in Chapter 3, when we employ them to model chromatographic processes.

1.12 Practice Problems

1.12.1 Introducing a gas_interaction Unit into Workshop 1

Using what you learned about the gas_interaction block in workshop 2, re-do workshop 1 using a single bed and gas_interaction unit (Figure 1.224). Consider the differences between the two flowsheets, especially about how the blowdown is implemented.

Here, the buffer tank should actually have a significant volume (e.g. 3m^3). Also, set the valves VP1 to have a Cv value of 0.00162 and the VB1 valve to have a Cv value of 1.5e−5.

Task 1: Re-create this plot of the LP stream using one gas_bed and one gas_interaction block (Figure 1.225). Once you have completed the process, save the file as `AirSepSingleBed.ada`.

Note that in this case, the simulation achieves a greater oxygen purity than the Air Separation workshop (nearly 99% purity in this case vs 95% purity in the workshop.) Why is that? Can you modify the Air Separation workshop to achieve similar purity? (Hint, change the VP1 and VP2 valves to use Cv instead of simply being on/off).

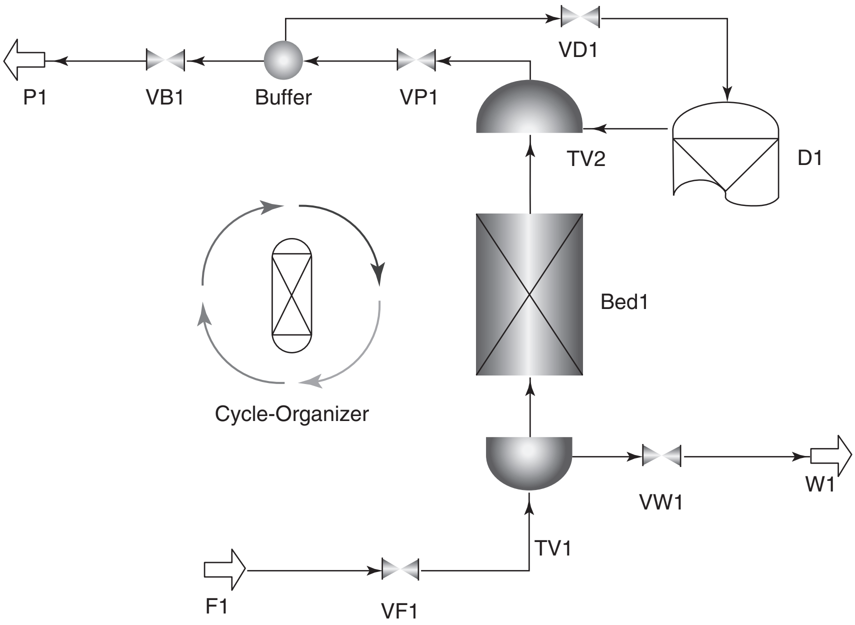


Figure 1.224 One possible flowsheet solution.

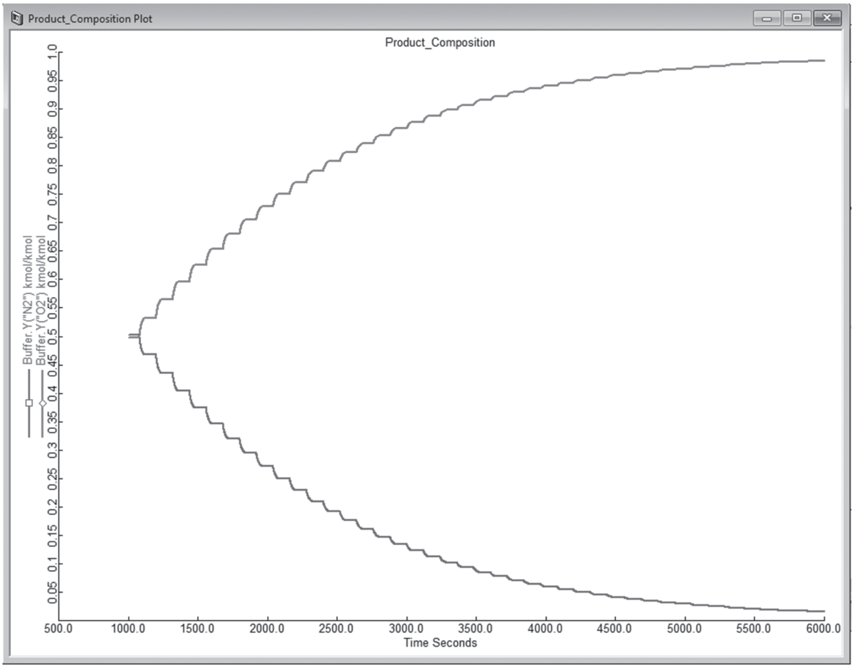


Figure 1.225 The product composition of a single bed air separator.

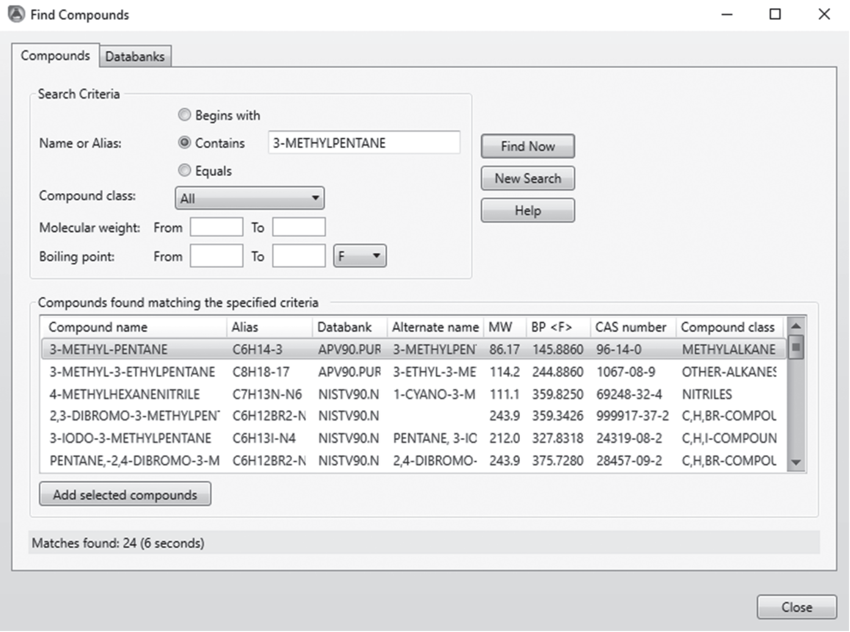
1.12.2 Naphtha Upgrading Using Adsorption

Bárcia et al. [25] discovered a new adsorbent (zeolite beta) that has properties very suitable for upgrading naphtha. Create a very simple flowsheet with only a feed, bed, and product block.

Make the following assumptions:

1) The gas phase is IDEAL, and consists of
    a) *n*-pentane (nP).
    b) *n*-hexane (nH).
    c) Iso-pentane (iP).
    d) Helium.
    e) 3-methylpentane (3MP).
    f) 2,3-dimethylbutane (23dmb).
    g) 2,2-dimethylbutane (22dmb).

    Task 1: Use the "Find" button to search for all of these components in the Aspen property databanks (Figure 1.226).
2) The dual-site Langmuir model is appropriate (partial pressure based), and Table 1.15 gives the isotherm parameters.
3) The bed has the following properties (Table 1.16).The mass transfer coefficients of the components are given in Table 1.17.Inside the bed, the Ergun equation, Eq. (1.11) for pressure drop applies, and mass transfer resistances are handled with the solid-phase linear lumped resistance model Eq. (1.15).



Name or Alias: ● Contains 3-METHYLPENTANE

Compound class: All

Molecular weight: From To

Boiling point: From To F

Compounds found matching the specified criteria

Compound name	Alias	Databank	Alternate name	MW	BP <F>	CAS number	Compound class
3-METHYL-PENTANE	C6H14-3	APV90.PUR	3-METHYLPEN	86.17	145.8860	96-14-0	METHYLALKANE
3-METHYL-3-ETHYLPENTANE	C8H18-17	APV90.PUR	3-ETHYL-3-ME	114.2	244.8860	1067-08-9	OTHER-ALKANE
4-METHYLHEXANENITRILE	C7H13N-N6	NISTV90.N	1-CYANO-3-M	111.1	359.8250	69248-32-4	NITRILES
2,3-DIBROMO-3-METHYLPEN	C6H12BR2-N	NISTV90.N		243.9	359.3426	999917-37-2	C,H,BR-COMPOL
3-IODO-3-METHYLPENTANE	C6H13I-N4	NISTV90.N	PENTANE, 3-IC	212.0	327.8318	24319-08-2	C,H,I-COMPOUN
PENTANE,-2,4-DIBROMO-3-M	C6H12BR2-N	NISTV90.N	2,4-DIBROMO-	243.9	375.7280	28457-09-2	C,H,BR-COMPOL

Matches found: 24 (6 seconds)

Figure 1.226 The Aspen tool for compound searches.

Table 1.15 Isotherm parameters.

	IP1	IP2	IP3	IP4	IP5	IP6	IP7	IP8
3MP	0.37	−1.50	0.80	−1.50	1.80	−5.25	3.62	−5.25
22DMB	0.42	−14.57	0.83	−14.57	0.23	−8.21	3.78	−8.21
23DMB	0.45	−12.17	0.82	−12.17	0.76	−7.63	3.76	−7.63
HE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
IPEN	0.58	−11.04	0.82	−11.04	0.26	−4.99	3.60	−4.99
NHEX	0.31	20.44	0.75	20.44	4.09	−1.46	3.43	−1.46
NPEN	0.63	−8.42	0.82	−8.42	0.73	−6.70	3.71	−6.70

Table 1.16 Bed properties.

Diameter (cm)	0.46
Length (cm)	10
Bulk porosity (ε_b)	0.49
Adsorbent particle diameter (cm)	0.159
Bulk density (kg m^{-3})	1130

Table 1.17 Mass transfer coefficients.

3M	0.5549
22DMB	1.8355
23DMB	0.8165
He	5.0
IP	1.5698
NH	0.2668
NP	0.959

Initially, assume that the bed is isothermal. Also, ensure that the initial concentrations in the bed are *slightly* greater than zero.

4) The feed stream has the following properties (Table 1.18).

Table 1.18 Stream properties.

Pressure (kPa)	8
T (K)	523

There is an equimolar mixture of the components in the feed.

The product stream is collected at a pressure of 5 kPa.

Task 2: Ensure that your flowsheet is correctly constructed (Figure 1.227).

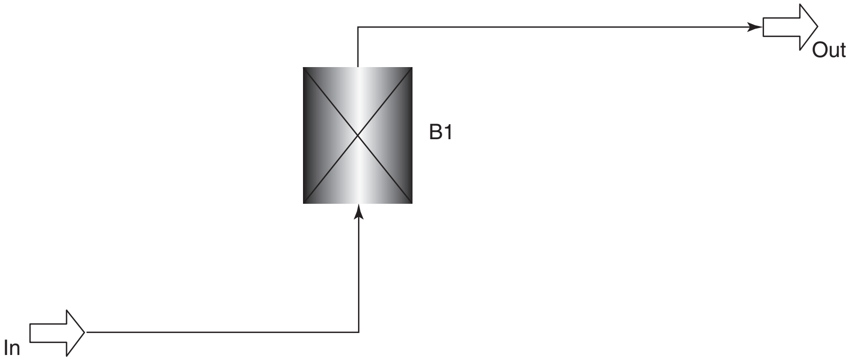


Figure 1.227 The correct flowsheet layout.

Task 3: Enter the following flowsheet constraints:

```
Fip as RealVariable;
Fnp as RealVariable;
F22 as RealVariable;
F23 as RealVariable;
F3mp as RealVariable;
FnHex as RealVariable;

Fip = (B3.F * B3.Y_Fwd("IP")) / (B2.F*B2.Y_Fwd("IP"));
Fnp = (B3.F * B3.Y_Fwd("NP")) / (B2.F*B2.Y_Fwd("NP"));
F22 = (B3.F * B3.Y_Fwd("22DMB")) / (B2.F*B2.Y_Fwd("22DMB"));
F23 = (B3.F * B3.Y_Fwd("23DMB")) / (B2.F*B2.Y_Fwd("23DMB"));
F3mp = (B3.F * B3.Y_Fwd("3M")) / (B2.F*B2.Y_Fwd("3M"));
FnHex = (B3.F * B3.Y_Fwd("NH")) / (B2.F*B2.Y_Fwd("NH"));
```

Ensure that these constrains are compiled.

Task 4: Run the simulation, and create a plot of the ratios defined in the flowsheet constraints.

Confirm that your enriched product stream achieves the correct concentrations of components (Figures 1.228 and 1.229).

Some notes on the discrepancy between the simulation and literature data:

- Our simulation is isothermal, while the actual adsorption unit is closer to adiabatic with a heat of adsorption.
- The literature uses a tri-site Langmuir model, while we restrict ourselves to a dual-site model. The isotherm parameters for this problem were generated by regressing a dual-site model against data generated by the tri-site model.
- Given these discrepancies, the qualitative agreement we have here is remarkably good.

Once you have completed this workshop, save the file as **NapthaIsothermal.ada**.

As an additional challenge, can you build that bed into a PSA unit?

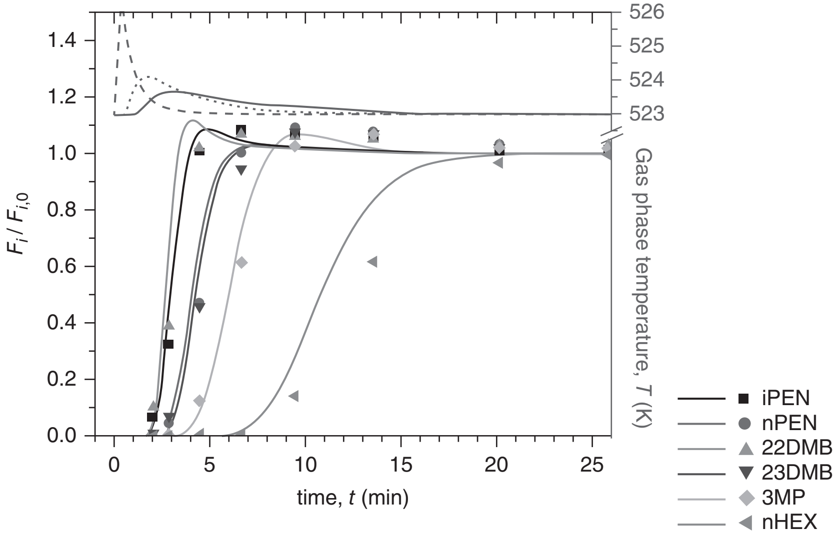


Figure 1.228 The product concentrations from literature. Kneabel and Hill 1985 [26]. Reproduced with permission of Elsevier.

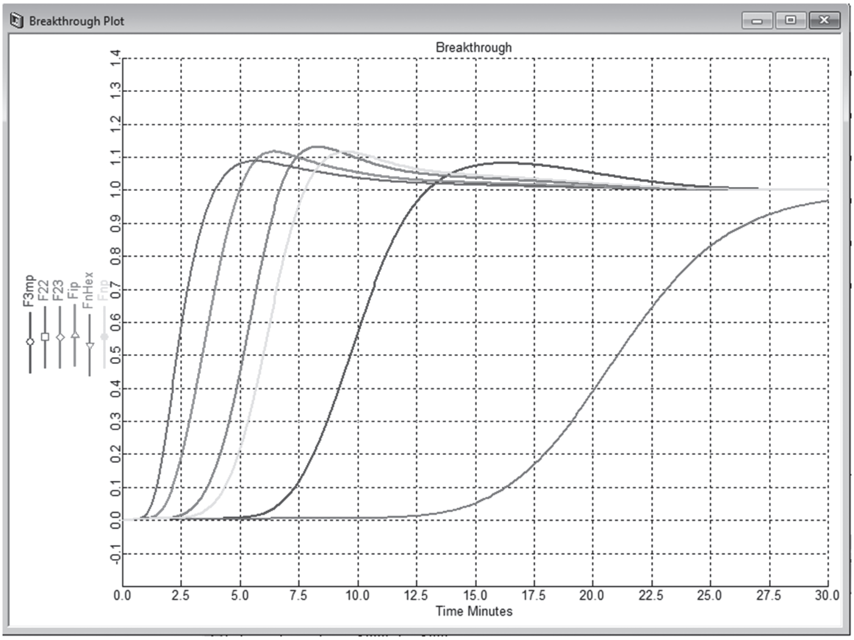


Figure 1.229 The actual simulation results.

1.13 Nomenclature

Variables	Units	Description
$a_{i,1}$	[—]	bi-Langmuir isotherm parameter a_1 for component i
$a_{i,2}$	[—]	bi-Langmuir isotherm parameter a_2 for component i
$b_{i,1}$	$[\mathrm{l\,g^{-1}}]$	bi-Langmuir isotherm parameter b_1 for component i
$b_{i,2}$	$[\mathrm{l\,g^{-1}}]$	bi-Langmuir isotherm parameter b_2 for component i
D_L	$[\mathrm{cm^2\,min^{-1}}]$	axial dispersion coefficient
Dia	[cm]	column diameter
F	N/A	Feed stream
IP1	[—]	isotherm parameter 1 in Aspen
IP2	[—]	isotherm parameter 2 in Aspen
k_i	$[\mathrm{1\,s^{-1}}]$	mass transfer coefficient for component i
K_i	[—]	equilibrium constant for component i
L	[m]	column length
P	[bar]	bed pressure drop
P_i	[bar]	partial pressure drop for component i
Pe	[—]	particle Peclet number
q_i	$[\mathrm{g\,g^{-1}}]$	solid loading for component i
q_i^*	$[\mathrm{g\,g^{-1}}]$	equilibrium solid loading for component i
r_p	[μm]	particle radius
S	$[\mathrm{cm^2}]$	cross-sectional area of the bed
U	$[\mathrm{m\,s^{-1}}]$	the superficial velocity of the gas flow
V_bed	$[\mathrm{cm^3}]$	bed volume per column
V_j^D	$[\mathrm{cm^3}]$	dead volume through the column
XFac	[—]	volume correction factor
Z	[m]	axial distance through the column
ΔP_j	[bar]	pressure drop in zone j
ΔP_max	[bar]	maximum pressure drop through the column
ϕ	$\left[\dfrac{\mathrm{m^3\,void}}{\mathrm{m^3}}\right]$	overall bed voidage
ε_i	$\left[\dfrac{\mathrm{m^3\,void}}{\mathrm{m^3}}\right]$	interparticle voidage
ε_p	$\left[\dfrac{\mathrm{m^3\,void}}{\mathrm{m^3}}\right]$	intraparticle voidage
μ	[cp]	liquid viscosity
ψ	[—]	particle shape factor
φ	$\left[\dfrac{\mathrm{bar^*min}}{\mathrm{cm^2}}\right]$	pressure drop coefficient

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