Chapter 2
Process Simulators

Process simulator is a computer program that allows modeling different processes depending on the area of study for which it was designed; this way, there are process simulators for industrial, chemical, and biochemical processes. A process simulation software is the best way to perform the simulation of industrial processes; this is due to the large number of equations and numerical methods that are needed to use for proper representation and prediction of behavior in reality.

In addition, the process simulators usually are programmed for using in the operating system of a computer, so it is advisable to verify the compatibility of the software that will be used with the equipment where it is going to work. Currently, there are several process simulators that are distributed commercially and which already have modeling equations for certain equipment and numerical methods programmed for the solution of specific thermodynamic equations. Another important aspect of commercial simulation software is that they have a simple database with components usually used in the chemical and process industry, as well as their physicochemical and thermodynamic properties.

Process simulators have been widely used for analyzing chemical processes (Morgan et al. 2017; Gómez-Ríos et al. 2017; Pauls et al. 2016); these offer a tremendous advantage associated with the implemented thermodynamic correlations as well as the powerful numerical methods for solving the mass and energy balances together with design and constitutive relationships (Hauck et al. 2017). Process simulators allow analyzing the process flowsheets for zero degrees of freedom. Some optimization approaches have been implemented in process simulators; however, important drawbacks have been identified associated with the number of degrees of freedom, the use of explicit constraints, as well as the number of objective functions. Furthermore, the implemented optimization techniques can be prematurely trapped in suboptimal solutions, or even no feasible solutions can be obtained (Coello-Coello et al. 2002) because usually deterministic optimization techniques have been implemented (Ponce-Ortega et al. 2012).

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Nowadays, several process simulators, such as Aspen Plus® and Aspen HYSYS®, are commercially available for simulating complete chemical processes, where common process units and a property database for numerous chemicals are available (Sharma and Rangaiah 2016). Most of chemical and biochemical process simulators are not equipped with adequate optimization tools. However, in very few simulators (e.g., Aspen Plus®), there are some optimization tools, but the formulation of optimization problems and available solution techniques is not good enough (Woinaroschy 2009). For example, the number of degrees of freedom is limited, only deterministic techniques can be implemented, it is complicated to manipulate explicit constraints for not manipulated variables, and only one objective can be considered.

For the proposed multi-objective optimization framework, the first step consists in implementing the flowsheet in the process simulator. The input variables and the operating conditions for the included equipment must be specified. Also, the thermodynamic method and the mathematical solution technique with the maximum number of iterations are necessary to be declared. All these values are for the first simulation process, and it must be run without any error or warning. It is recommended to validate the response variables for checking the values of the results after implementing the optimization approach.

2.1 Aspen Plus®

Aspen Plus® is the market-leading chemical process simulation software used by the bulk, specialty, and biochemical industries for the design and operation (aspentech.com). The main advantages of this simulator consist of a large database of specific chemical compounds and unit operations.

However, models for less common and/or new process units are not readily available in the simulators, but they may be available in the literature or can be developed from first principles. A mathematical model for a new process unit can be implemented in Aspen Custom Modeler (ACM), and then it can be exported to Aspen Plus® or Aspen HYSYS® for simulating processes, having a new process unit besides common process units such as heat exchangers, compressors, reactors, and columns (Sharma and Rangaiah 2016).

For the correct functioning of these simulations, it is necessary to feed the program with values that are within a suitable range, the previous one in order to avoid errors in the equipment so that indeterminacies arise due to the thermodynamic behavior of the substances used and the interconnections of the equipment must be correctly indicated.

Aspen Plus® is a process simulation program that can also be used for many types of thermodynamic calculations or to retrieve and/or correlate thermodynamic and transport data (Sandler 2015). With the purpose of obtaining a better understanding of the use of this software for process simulation, we will present some fundamental aspects for its use. However, it is worth noting that if the reader

requires further information about the use of this specific software, it is better to consult the user guide that the program developers offer on the official website. As the Aspen Plus® V8.8 Help indicates, one can translate any process into an Aspen Plus® process simulation model by performing the following steps:

1. Specify the chemical components used in the process. You can take these components from the Aspen Plus® databanks, or you can define them.
2. Specify the thermodynamic models to represent the physical properties of the components and mixtures in the process. These models are included in the Aspen Plus® software.
3. Define the process flowsheet, which includes:
   (a) Define the unit operations in the process.
   (b) Define the process streams that flow to and from the unit operations.
   (c) Select models from the Aspen Plus® Model Library to describe each unit operation and place them on the process flowsheet.
   (d) Place labeled streams on the process flowsheet and connect them to the unit operation models.
4. Specify the component flow rates and the thermodynamic conditions (e.g., temperature and pressure) of feed streams.
5. Specify the operating conditions for the unit operation models.

With Aspen Plus®, one can interactively change specifications, such as flowsheet configuration, operating conditions, and feed compositions, to run new cases and analyze process alternatives. In addition to process simulation, Aspen Plus® allows to perform a wide range of other tasks such as estimating and regressing physical properties, generating custom graphical and tabular output results, fitting plant data to simulation models, optimizing processes, and interfacing results to spreadsheets (AspenTech 2015).

The user interface of Aspen Plus® is very intuitive and easy to use, due to the remarkable efforts that the developers of this software have implemented to make the use friendlier. This important aspect can be noticed with the improvements that the new version has with respect to the previous one.

To start, open the Aspen Plus V8.x, which you may have to locate depending on the setup of your computer. (It may be on your desktop or you may have to follow the path All Programs > Aspen Tech > Process Modeling V8.x > Aspen Plus > Aspen Plus V8.x.)

When you open Aspen Plus V8.2 or higher version, you will briefly see the Aspen logo of Fig. 2.1. There is then a slight delay while the program connects to the server, and then the Start Using Aspen Plus window with resent simulations appears.

To proceed, click on New, which brings up the window shown in Fig. 2.2 for all versions of Aspen Plus V8.0 or higher.

Click on Blank Simulation and then Create. This will bring up Fig. 2.3.

On the lower-left-hand corner of this window, there are three choices. The first one, which Aspen Plus opens, is Properties; the drop-down menu under Components > Specifications is used to specify the component or components for

Fig. 2.1 Aspen Plus V8.8 Start-up

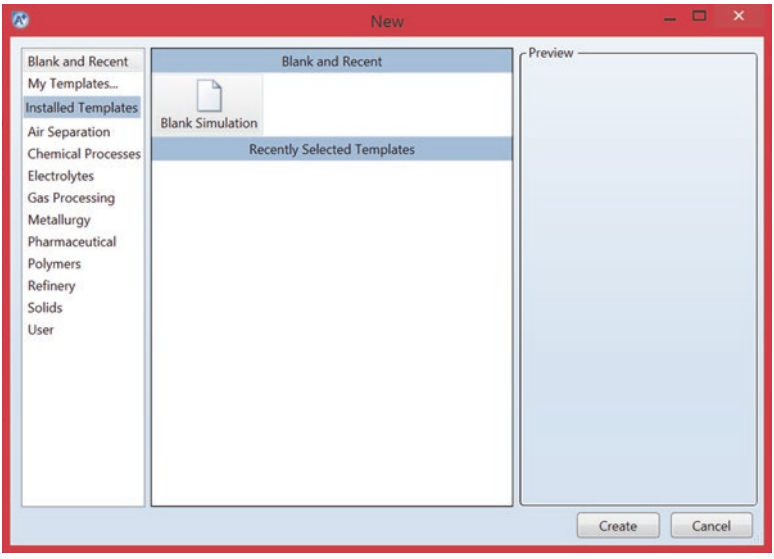


Fig. 2.2 Window to open a New Simulation

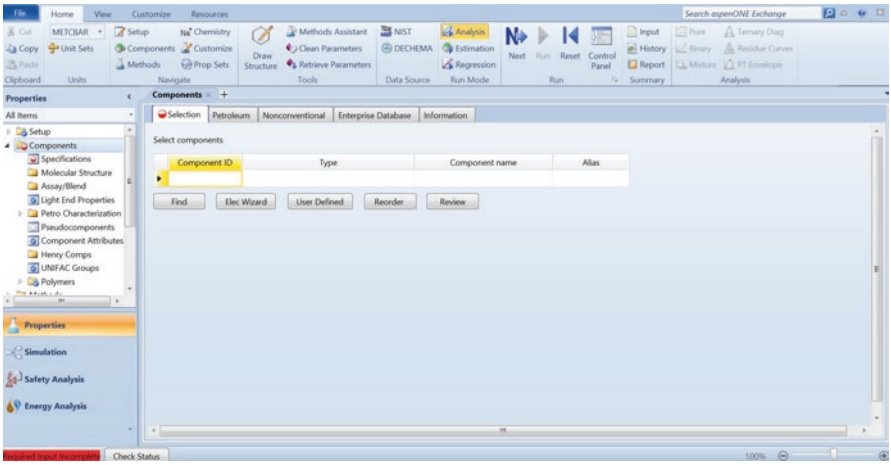


Fig. 2.3 Properties of Aspen Plus

the calculation, and the drop-down menu under Methods is used to specify the thermodynamic models and parameters that will be used in the calculation. The second general area is Simulation that will take you to a flowsheet window, to be discussed later, and the third one is the Energy Analysis that is used to implement energetic analysis and integration. The default is to start with Properties.

For example, we will proceed to entering the component water. There are two ways to enter component names. The simples and most reliable way to ensure that you will get the correct component and its properties from the Aspen Plus® database is to click on the Find box that brings up the Find Compounds window and to enter the component name by typing in water and then clicking on Find Now, which produces the window shown in Fig. 2.4.

A long list of compounds, shown in Fig. 2.4, is generated because the default Contains was used in the Find Compounds window; as a result, every compound in the database that contains water either in its compound name or in its alternate name appears in the list. The compound we are interested will be first on this list, but that will not always be the case. Therefore, a better way to proceed in the Find Compounds window is to click Equals instead of the default Contains and then click Find Now, which produces, instead of a list, only water (Fig. 2.5).

Click on WATER and the Add selected compounds, and for this example, click on Close. You will then see Fig. 2.6.

Another alternative is to type in all or part of the name directly in the Components-Specification window and see whether Aspen Plus® finds the correct name. Notice that water has now been added to the Select components list and that both components and Specifications now have check marks indicating that sufficient information has been provided to proceed to the next step. However, this may not be sufficient information for the problem of interest to the user. If the problem to be solved involves a mixture, one or more additional components may be added following the

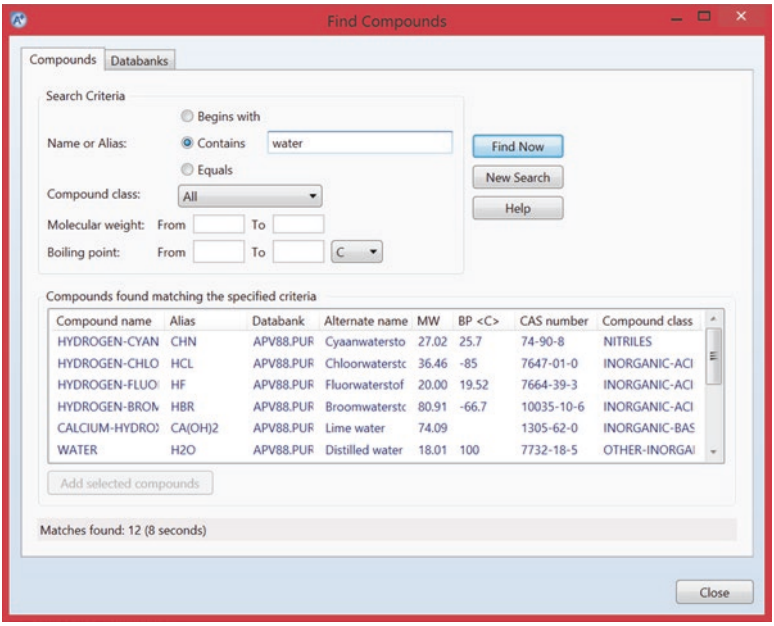


Fig. 2.4 Find Component Window (Contains option)

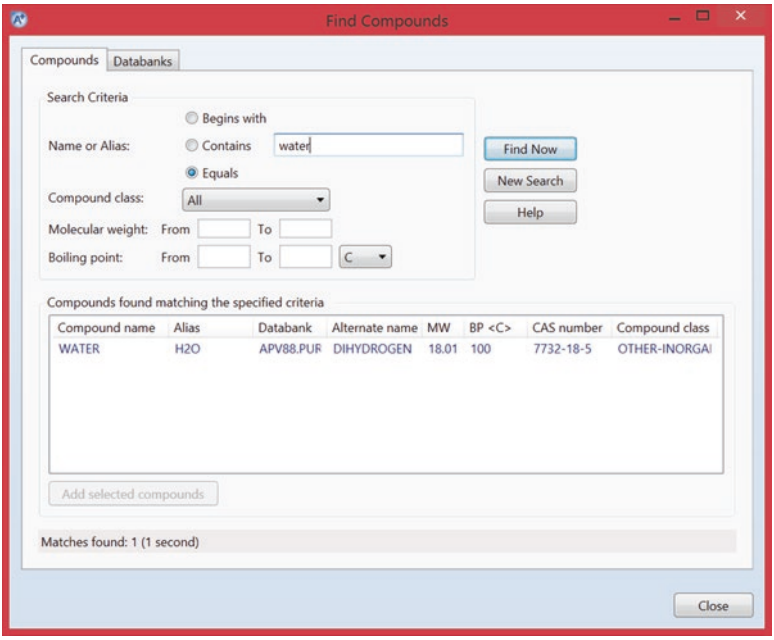


Fig. 2.5 Find Component Window (Equals option)

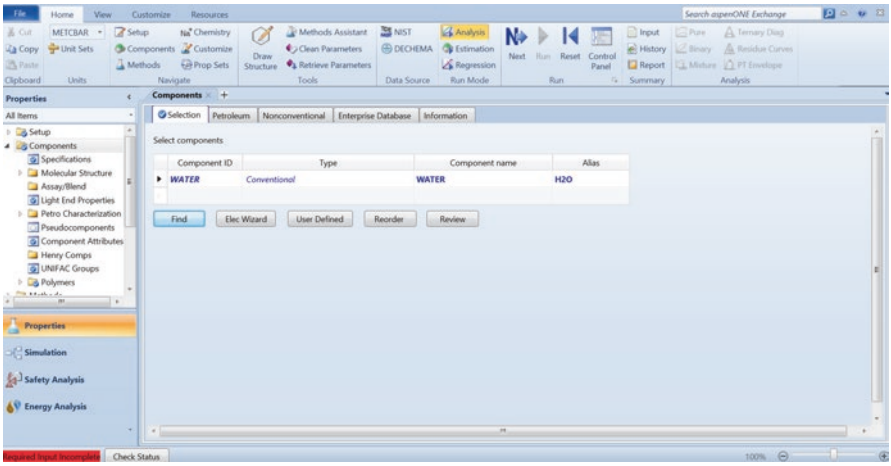


Fig. 2.6 Component window

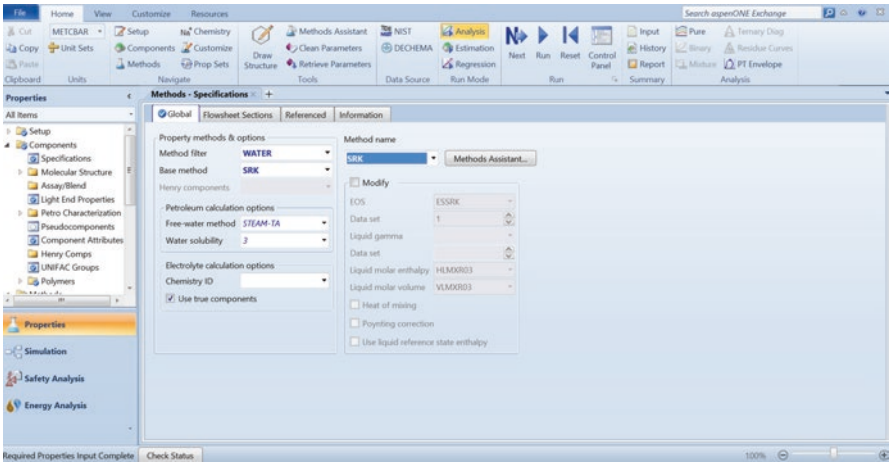


Fig. 2.7 Methods window

procedure described above except that the Close button in the Find Compounds window is used only after all the components have been added.

The next step is to go to Methods by clicking on it. The window shown in Fig. 2.7 appears, and here a number of thermodynamic models can be used through any other equation of state for which parameters are available can be used. Notice that if you need help in choosing a thermodynamic model, you can click on Methods Assistant for help. After accepting the equation by clicking Enter, Methods on the left-hand side of Fig. 2.7 will also have a check.

Checking on Simulation brings up the Main Flowsheet window of Fig. 2.8 together with Model palette at the bottom of the window.

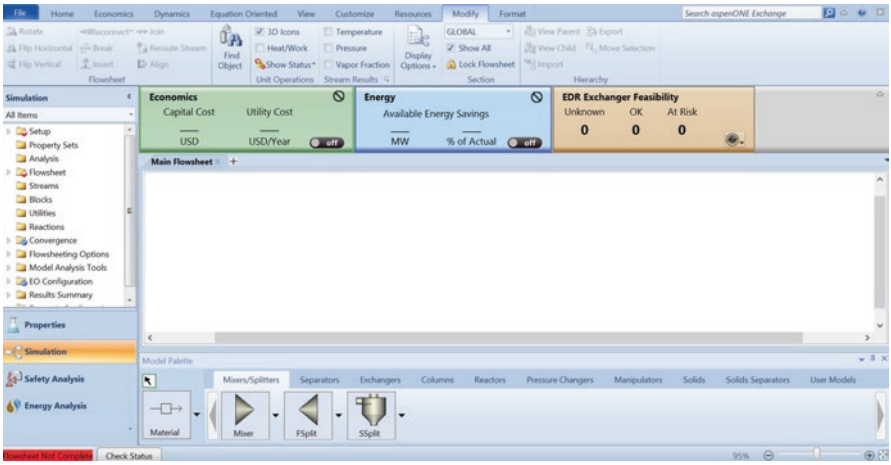


Fig. 2.8 Simulation section of Aspen Plus

The next step is to draw the process flowsheet, or even a single process unit such as a boiler or a turbine, which will be described in the next section.

2.2 Example of the Conventional Rankine Cycle

With the purpose of introducing the reader to the basic principles about how simulations work in the Aspen Plus® process simulator software, this section will present a simple example. As a case study, a conventional Rankine cycle was considered, which consists of a boiler, a turbine, a condenser, and a pump (Fig. 2.9).

The first step to do is to introduce the water component into the Aspen properties part, as shown in the previous section. After that, we proceed to choose the thermodynamic method that will be used to perform the simulation calculations (in this case STEAMNBS with a method filter of WATER). Once this is done, we select the Aspen Simulation part, where we proceed to build the process flowsheet selecting each equipment that conforms the process of the conventional Rankine cycle. To select each equipment, go to the model palette (in case this is not visible, go to the display tab in the show section and select model palette) (Fig. 2.10).

The first unit for the flowsheet process of a conventional Rankine cycle is the boiler. You have to go to the model palette, in the heat exchanger tab, and look for the boiler symbol. To select it, you must click on the corresponding symbol and click again in any part of the work area of the Aspen simulation part (as Fig. 2.11 shows). A small symbol will appear as the one with a default name, which will be "B1"; to change it just click on the symbol and with right click select the "Rename Block" option. Now we can assign a more appropriate name to better identify it; in this case, it can be "BOILER."

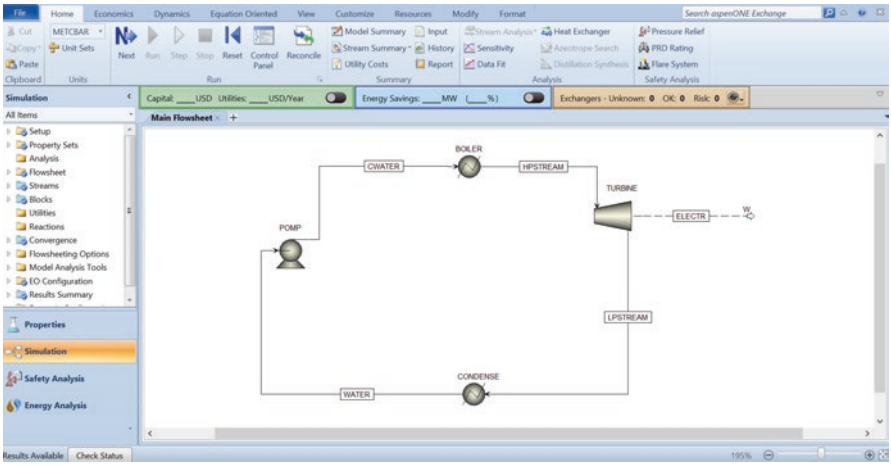


Fig. 2.9 Rankine cycle flowsheet in Aspen Plus®

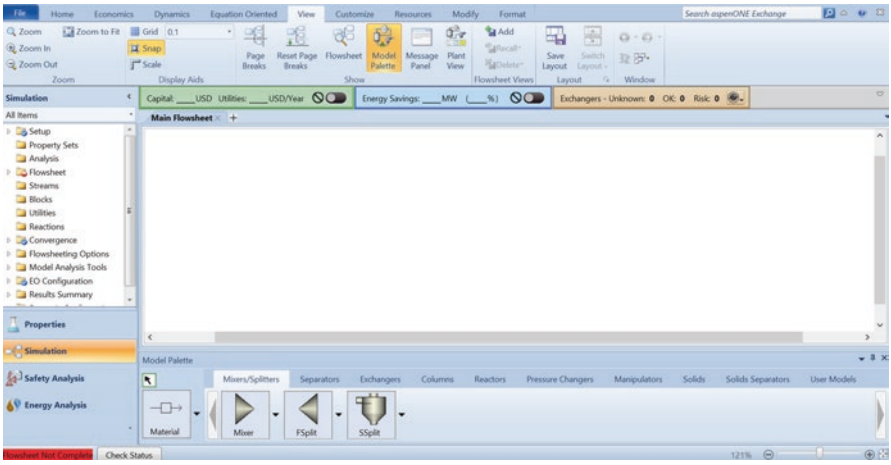


Fig. 2.10 Location of the model palette

In the same way, we proceed to select and rename the rest and the necessary equipment for the flowsheet of the process of a conventional Rankine cycle (Fig. 2.12).

The next step is to complete the processes flowsheet of the conventional Rankine cycle joining the blocks using material streams for that. To do this, select the Material option from the model palette with a click. You will notice that in the blocks of the diagram, there will appear small red and blue arrows; the first common meaning is obligatory to complete the process flowsheet, while the blue ones are optional (Fig. 2.13).

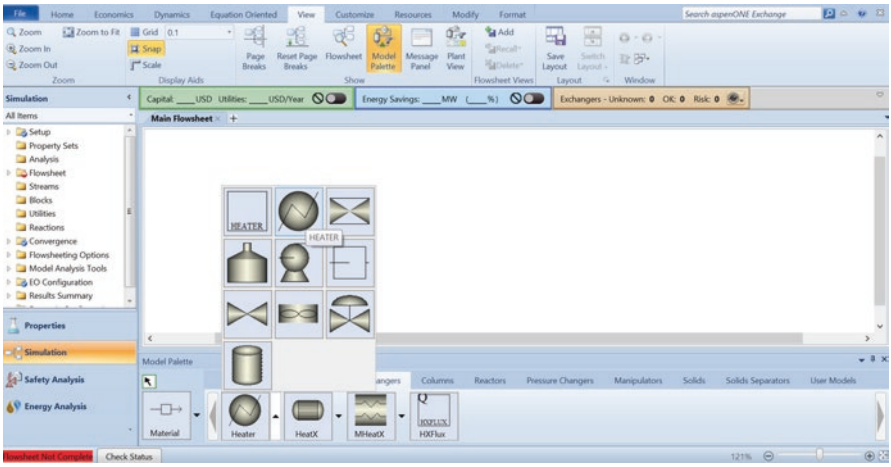


Fig. 2.11 Location of the boiler in the model palette

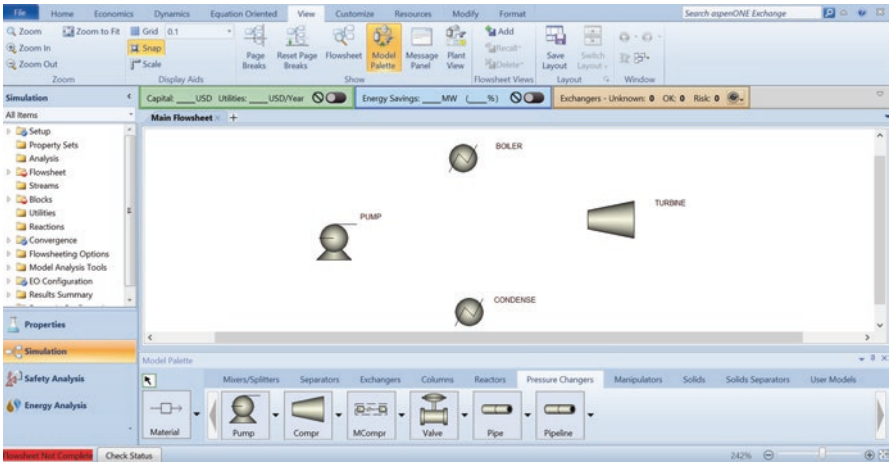


Fig. 2.12 Necessary blocks for the conventional Rankine cycle

Connect the blocks using the material streams. This is done by clicking and holding on an arrow, moving the pointer to the desired location, and releasing it. Rename the streams to obtain the process flowsheet of the conventional Rankine cycle shown in Fig. 2.9.

To proceed, the user must now provide the specifications for the process, which includes the inlet stream component(s) and conditions, pressures and temperatures needed, and the type of each process unit or block (e.g., an isentropic turbine). Click on Streams > WATER and complete with a temperature of 98 °C, a pressure of 1 atm, a total flow rate of 20,000 kg/h, and a molar fraction of 1 in water compound, as shown in Fig. 2.14. This is the only stream that needs to be specified;

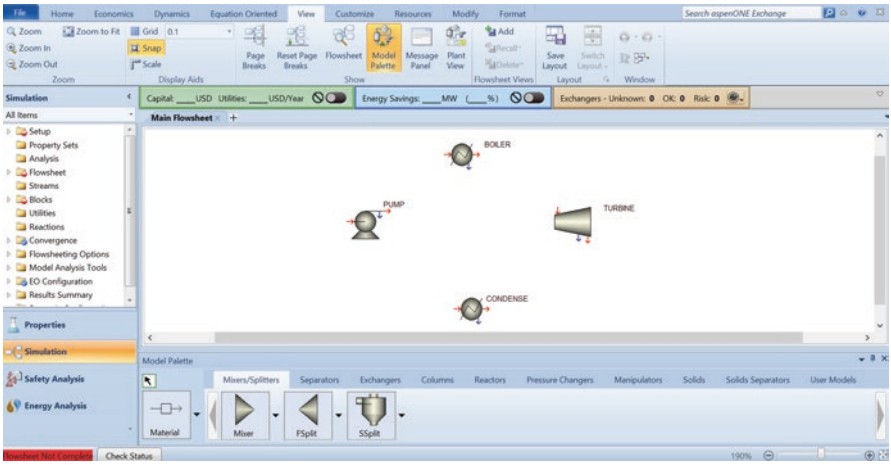


Fig. 2.13 Appearance of the blocks when the stream option is selected

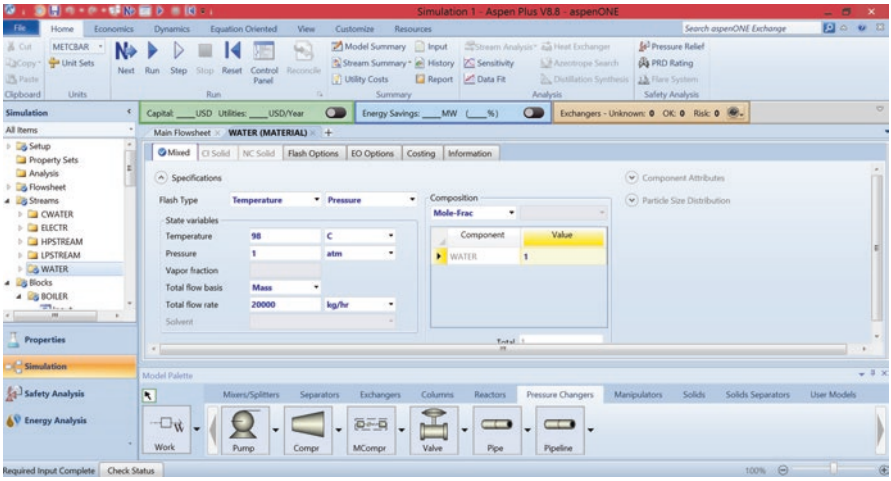


Fig. 2.14 Specification of the WATER stream values

the properties of all the other streams will be computed in the simulation calculation once the actions of the Blocks are chosen.

We then move on to the specifications for the Blocks (process units). First, for the BOILER, we specify a temperature of 460 °C and a pressure of 40 atm (Fig. 2.15).

Next in the block CONDENSE (the condenser), which is a heat exchanger, there are specified the operating conditions, which are a temperature of 98 °C and a pressure of 1 atm (Fig. 2.16).

The pump, PUMP, is operated to discharge a pressure of 40 atm (Fig. 2.17). Other entries are the unchanged defaults.

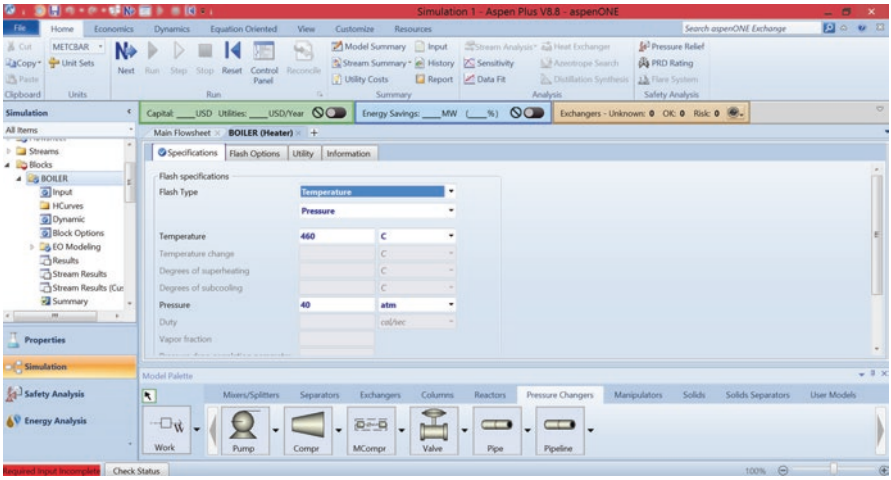


Fig. 2.15 Specification of the BOILER block values

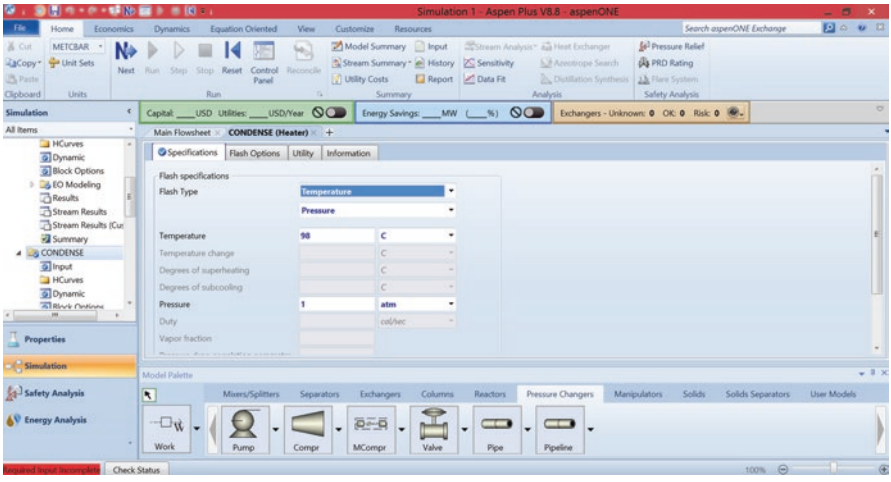


Fig. 2.16 Specification of the CONDENSE block values

Finally, the specifications for the turbine, TURBINE, are that it is operated as an isentropic turbine and it discharges at a pressure of 1 atm (Fig. 2.18).

Now all necessary boxes are checked, and in the lower-right-hand corner of the window, there is the message "Required Input Complete." We are ready to run the simulation. There are five ways to start the simulation. The first way is to press the F5 key (not function F5, just the F5 key). The second and third ways are to press one of the two forward arrow keys on the Main Toolbar and click on the forward arrow above Run (which will gray if not all the information for the simulation has been entered, but turn dark blue when all necessary data have been entered). The final two

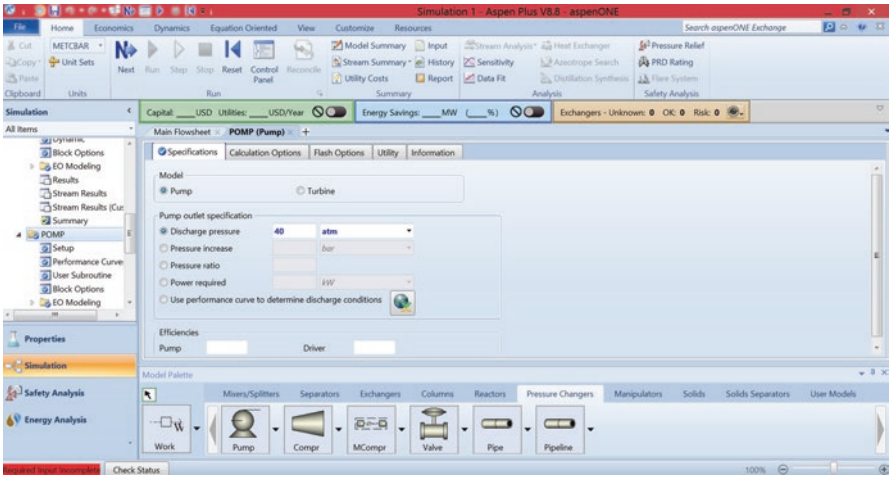


Fig. 2.17 Specification of the PUMP block values

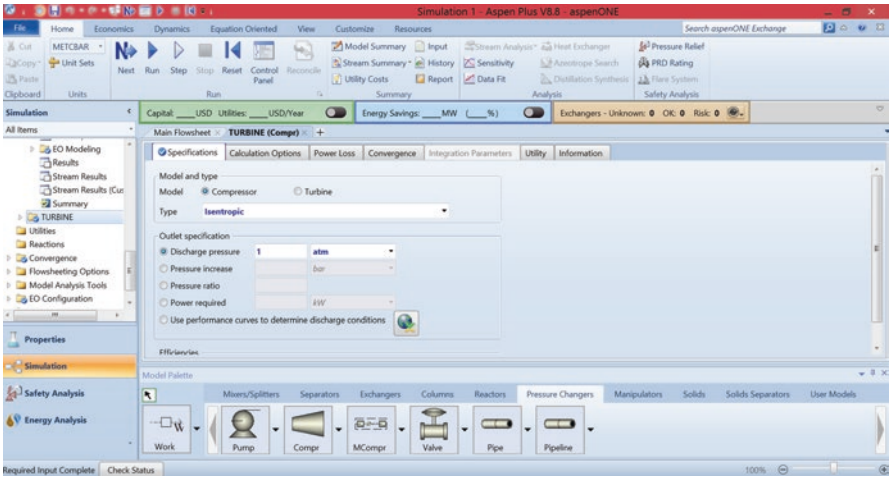


Fig. 2.18 Specification of the TURBINE block values

ways are to click on one of the Aspen Plus Next keys on the Main Toolbar that will bring up the message of Fig. 2.19. Clicking OK will then run the simulation.

After running the simulation, you can check the results clicking on Results Summary (Fig. 2.20).

Then, going to Streams, it brings up a window (Fig. 2.21) containing the table of stream results.

As you can see, Fig. 2.21 shows the Material Streams. If you want to see the work generated in the turbine, you can see it clicking on the Work tab and it brings up a window with the value (Fig. 2.22).

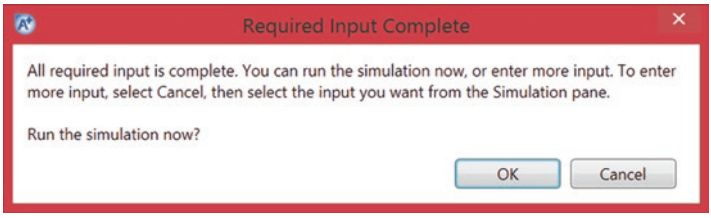


Fig. 2.19 Message before running the simulation

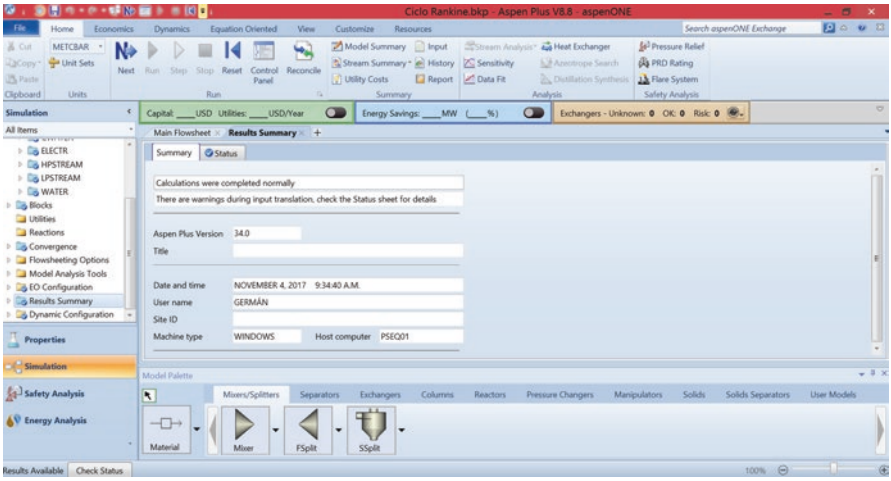


Fig. 2.20 Results Summary after running the simulation

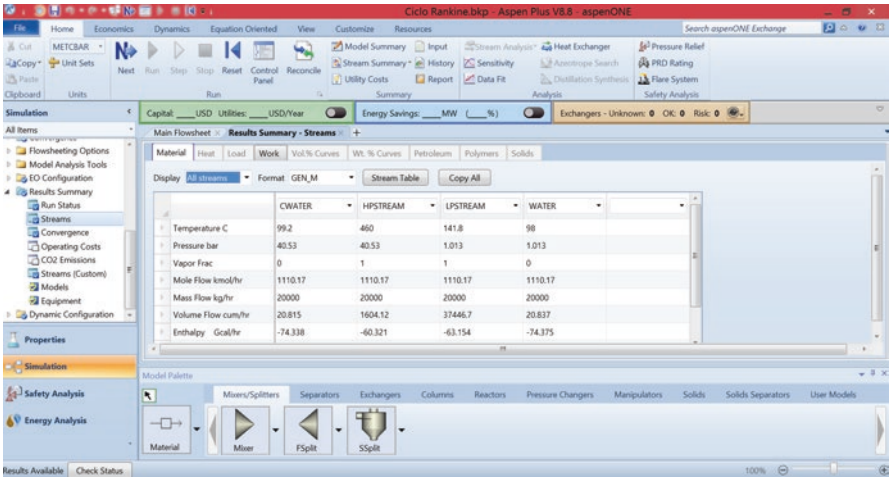


Fig. 2.21 Results Summary Streams Table (Material)

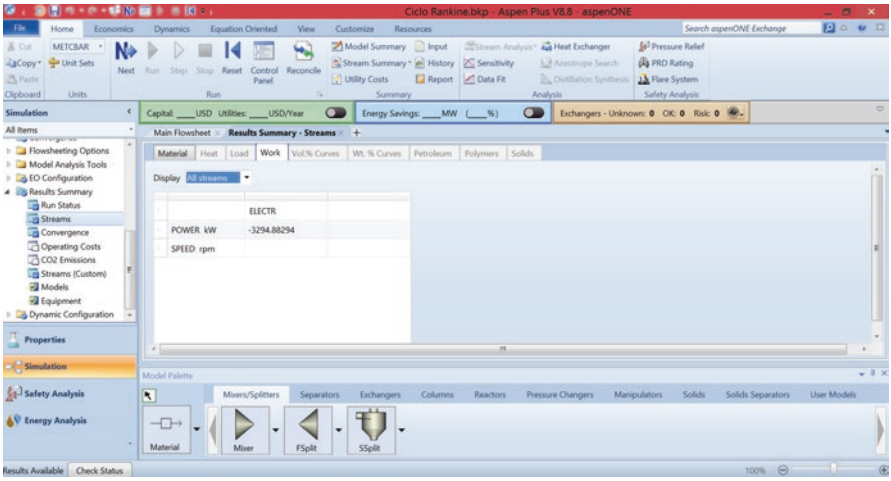


Fig. 2.22 Results Summary Streams Table (Work)

As you can see, Aspen Plus® is a process simulator software with a user interface very easy and intuitive to manipulate. If you need to deep in the use of Aspen Plus, it is recommended to consult a specialized text as mentioned in the bibliography of this book.

2.3 Aspen HYSYS®

Aspen HYSYS® is a process simulation software focused on oil and gas, refining, and engineering processes (aspentech.com). With an extensive array of unit operations, specialized work environments, and a robust solver, modeling in Aspen HYSYS V8 enables the user to:

- Improve equipment design and performance
- Monitor safety and operational issues in the plant
- Analyze processing capacity and operating conditions
- Identify energy savings opportunities and reduce greenhouse gas emissions
- Perform economic evaluation to obtain savings in the process design

Aspen HYSYS V8 builds upon the legacy modeling environment, adding increased value with integrated products and an improved user experience. The ease of use and flexibility of model calculations have been preserved, while new capabilities have also been added.

2.4 SuperPro Designer®

SuperPro Designer® is a software that facilitates modeling, evaluation, and optimization of integrated processes in a wide range of industries (intelligent.com), which includes batch operations and several biochemical processes. The main reason for using this simulator is because it allows the analysis of biochemical processes that other commercial simulators do not include in their modeling options.

SuperPro Designer® is the only commercial process simulator that can handle equally well continuous and batch processes as well as combinations of batch and continuous.

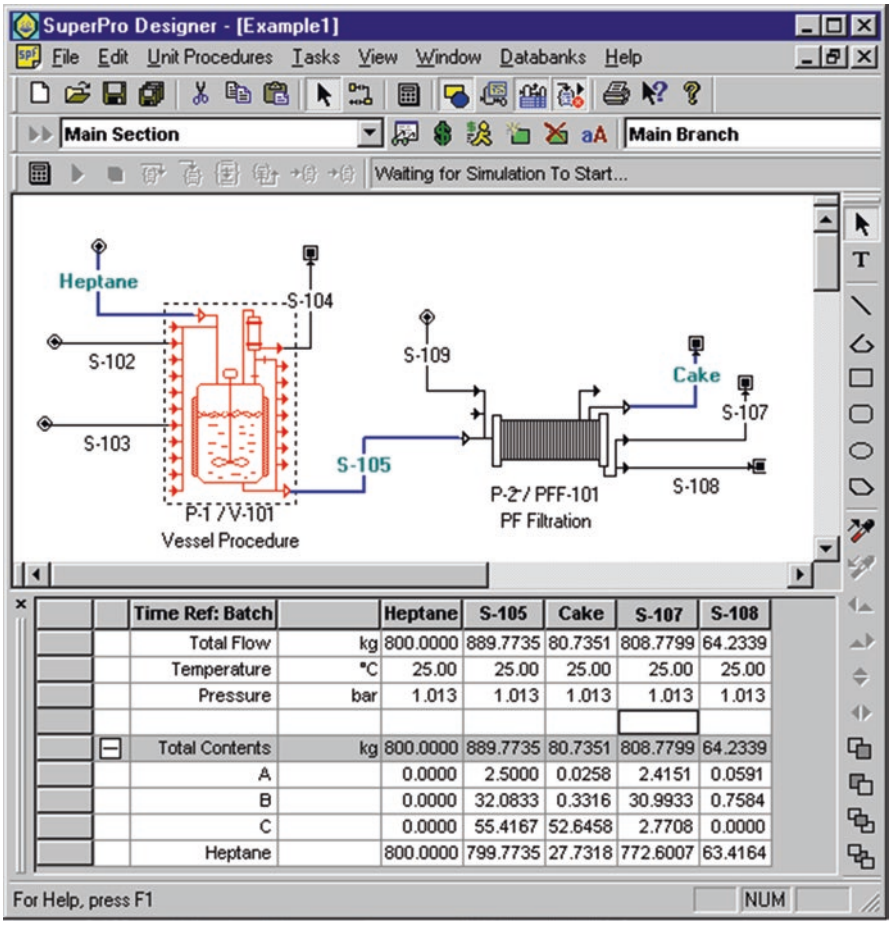
Graphical Interface: This software includes an intuitive and user-friendly interface (see Fig. 2.23). The equipment-looking icons represent unit operations for continuous processes and unit procedures for batch processes.

In this environment, developing a process flowsheet or modifying values is as easy as point and click. The interface is very similar to other MS Windows applications, making its features very intuitive.

Unit Procedures: A unit procedure is a set of operations that take place sequentially in a piece of equipment. For instance, the P-1 vessel unit procedure (see Fig. 2.24) includes the following operations: Charge Solvent, Charge Reactant A, Charge Reactant B, and Transfer to PFF-101. The concept of unit procedures enables the user to model batch processes in great detail. A unit procedure is represented with a single equipment-looking icon on the screen. Multiple procedures can share the same equipment item as long as their cycle times do not overlap.

Operations: For every operation within a unit procedure, the simulator includes a mathematical model that performs material and energy balance calculations. Based on the material balances, it performs equipment-sizing calculations. If multiple operations within a unit procedure dictate different sizes for a certain piece of equipment, the software reconciles the different demands and selects an equipment size that is appropriate for all operations. In other words, the equipment is sized so that it is large enough that it will not be overfilled during any operation, but it is no larger than necessary (in order to minimize capital costs). In addition, the software checks to ensure that the vessel contents will not fall below a user-specified minimum volume (e.g., a minimum stir volume) for applicable operations.

The initialization of operations is done through appropriate windows. For instance, Fig. 2.25 shows the Oper.Cond's tab of a charge operation. Through this, the user specifies either the process time (duration) of the operation or the charge rate (based on mass or volumetric flowrate), and the program uses that information to calculate the duration. A third option is to set the duration of an operation equal to the duration of another operation or equal to the sum of durations of some other operations (through the "Set by Master-Slave Relationship" interface). The Emissions tab is used to specify parameters that affect emissions of volatile organic



		Time Ref: Batch		Heptane	S-105	Cake	S-107	S-108
		Total Flow	kg	800.0000	889.7735	80.7351	808.7799	64.2339
		Temperature	°C	25.00	25.00	25.00	25.00	25.00
		Pressure	bar	1.013	1.013	1.013	1.013	1.013
	⊟	Total Contents	kg	800.0000	889.7735	80.7351	808.7799	64.2339
		A		0.0000	2.5000	0.0258	2.4151	0.0591
		B		0.0000	32.0833	0.3316	30.9933	0.7584
		C		0.0000	55.4167	52.6458	2.7708	0.0000
		Heptane		800.0000	799.7735	27.7318	772.6007	63.4164

Fig. 2.23 User interface of SuperPro Designer®

compounds (VOCs). The Labor tab is used to specify the labor requirement for this operation. The Description tab displays a description of the process generated by the model (e.g., Charge 1000 L of Water at a rate of 150 L/min using stream Water-A). The user has the flexibility to edit the description and enter his/her own comments for documentation purposes. The Scheduling tab is used for specifying the Start Time of this operation relative to other events (e.g., the beginning of the batch, the beginning or end of some other operation in the same or a different procedure, etc.). SuperPro Designer® includes more than 120 operation models.

Component and Mixture Databases: The registration of pure components and mixtures is something that typically precedes the initialization of operations. SuperPro Designer® is equipped with two component databases, its own of 600 compounds and a version of DIPPR that includes 1700 compounds (the DIPPR

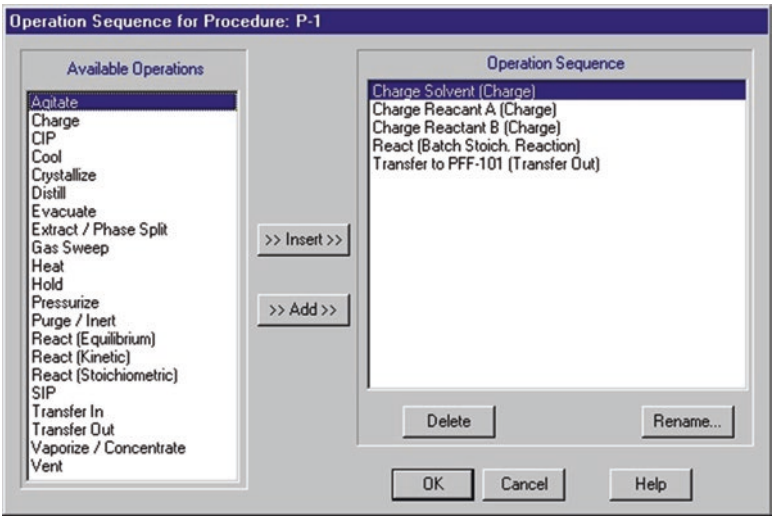


Fig. 2.24 Operation Sequence for Procedure

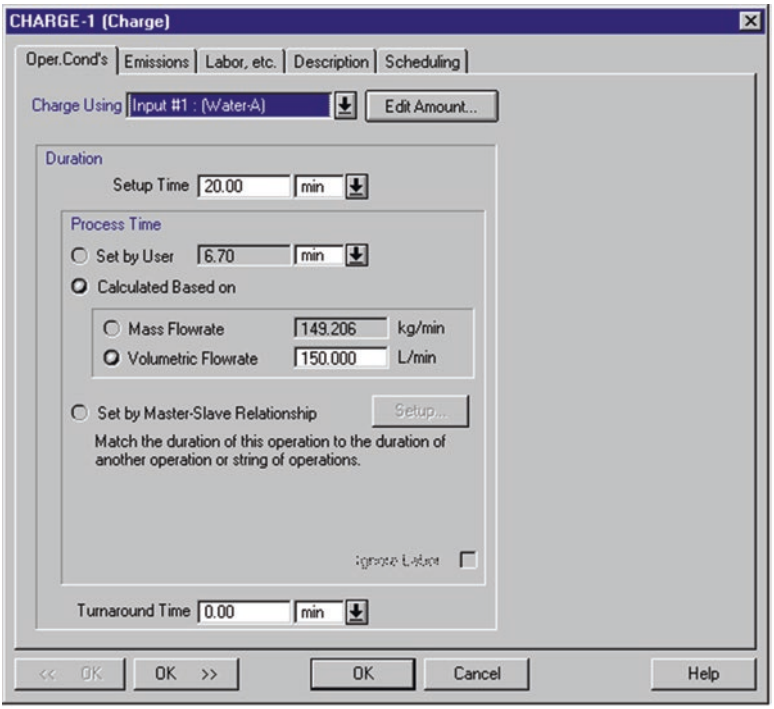


Fig. 2.25 Charge operation of SuperPro Designer

database must be purchased separately from Brigham Young University of Utah). It also comes with a user database where modified and newly created compounds can be saved. All database files are in MS Access format. Furthermore, SuperPro Designer® comes with mixture databases to represent buffers and other solutions that are commonly used in the biotech and other industries. Again, the user has the option to create his/her mixtures and save them in the user database.

For each pure component, the SuperPro Designer® databank includes thermodynamic (e.g., molecular weight, critical pressure and temperature, acentric factor, vapor pressure, density, specific heat, particle size, etc.), environmental (e.g., biodegradation data, octanol to water distribution ratio, Henry's law constant, component contribution to TOC, COD, BOD5, TSS, etc.), cost (e.g., purchasing price, selling price, etc.), and regulatory (e.g., type of pollutant) data.

2.5 PRO/II® Process Engineering

PRO/II® Process Engineering optimizes plant performance by improving process design and operational analysis and performing engineering studies (software.schneider-electric.com). This software was designed to perform rigorous heat and material balance calculations for a wide range of chemical processes. PRO/II® Process Engineering offers a wide variety of thermodynamic models to virtually every industry. PRO/II® Process Engineering is cost-effective, thereby decreasing both capital and operating costs.

PRO/II® is now available via the cloud in addition to the traditional on-premise access method. This cloud access has not only many benefits over on-premise access but also over other products with cloud access due to platform technology developed with simulation users in mind. PRO/II® has the following advantages:

- A secure user access control that allows the administrator to add and delete users or edit privileges as needed
- Simplify IT Overhead with the use of the product on pure on-demand cloud machines via a secure URL with no need for installation
- Seamless maintenance with new versions available as soon as they are released
- Flexible Usage and Pricing with SaaS business model based on minimum usage subscription and flexible, incremental usage credits
- Computer-based introductory training included

2.6 UniSim® Design Suite

Honeywell's UniSim® Design Suite is a process modeling software that provides steady-state and dynamic process simulation in an integrated environment (honeywellprocess.com). It provides powerful tools to help engineers evolve process

optimization designs with lower project risks, prior to committing to capital expenditures. Some applications in process modeling using UniSim® Design Suite include:

- Process flowsheet development
- Utilizing case scenarios tool to optimize designs against business criteria
- Equipment rating across a broad range of operating conditions
- Evaluating the effect of feed changes, upsets and alternate operations on process safety, reliability, and profitability
- Accurately sizing and selecting the appropriate material for blowdown systems
- Monitoring equipment performance against operating objectives

2.7 gPROMS® ProcessBuilder

gPROMS® ProcessBuilder is an advanced process modeling environment for optimizing the design and operation of process plants (psenterprise.com). ProcessBuilder combines industry-leading steady-state and dynamic models with all the power of the gPROMS equation-oriented modeling, analysis, and optimization platform in an easy-to-use process flowsheeting environment (Fig. 2.26).

2.8 Process Simulation Exercises

With the purpose of offering the reader the opportunity to put into practice the knowledge acquired in this chapter, the following exercises are proposed:

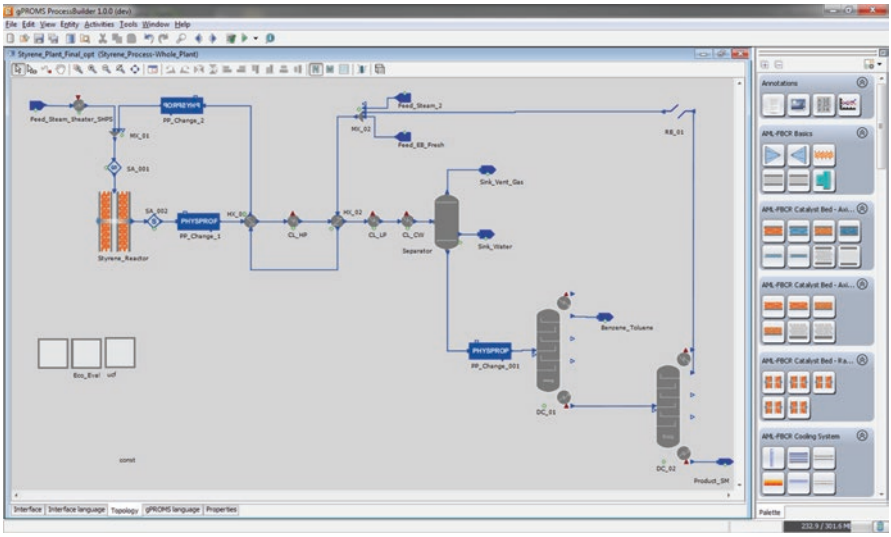


Fig. 2.26 User interface of gPROMS® ProcessBuilder

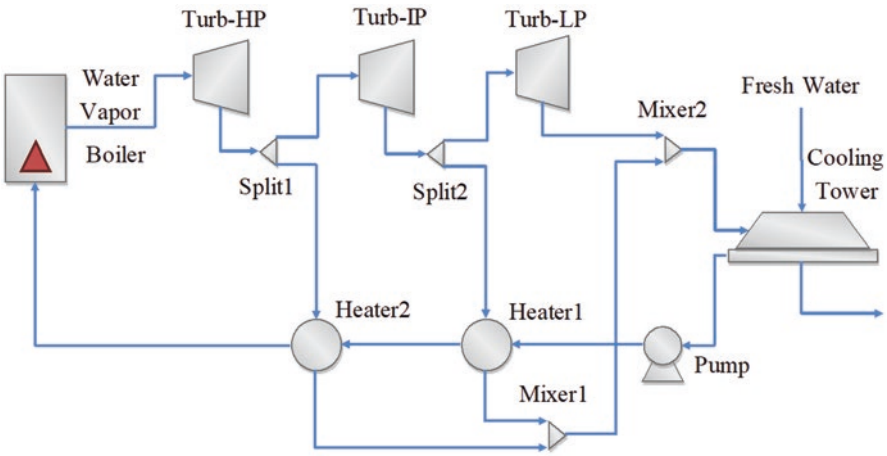


Fig. 2.27 Flowsheet of the regenerative Rankine cycle

1. Implement in Aspen Plus® the process flowsheet of a conventional Rankine cycle just as shown in Sect. 2.2 of this chapter (Fig. 2.12) with the following specifications:

   (a) Change the operating conditions in the boiler with a temperature equal to 500 °C and pressure of 50 atm (the discharge pressure of the pump must be of 50 atm too). What happened with the value of the ELECTR stream? Why?
   (b) Change the total flow rate of the WATER stream, with a value of 30,000 kg/h. What happened with the value of the ELECTR stream? Why?

2. Implement in Aspen Plus® the process flowsheet of a regenerative Rankine cycle, which is shown in Fig. 2.27, using the following operating conditions: a temperature of 580 °C, pressure of 38 atm, and a total flow of 1000 ton/day for the boiler output stream. The hot stream outlet temperature from the condenser is equal to 100 °C, hot stream temperature decrease of 10 °C in the first preheater and 100 °C in the second one, pressure of the pump of 40 atm, temperature of 600 °C, and pressure of 40 atm in the boiler. The split fraction is 0.8 in both splitters, and the pressure decreases are 20, 10, and 5 atm in the HP, LP, and LP turbines, respectively. Explain the results from this simulation.

2.9 Nomenclature

COM	Component Object Module
MS	Microsoft®
OLE	Object Linking and Embedding
VBA	Visual Basic for Application