CHAPTER 16

Solving Material and Energy Balances using Process Simulators (Flowsheeting Codes)

16.1 Main Concepts 768

Your objectives in studying this chapter are to be able to

1. Understand the differences between equation-based and modular-based flowsheeting
2. Understand how material and energy balances are formulated for equation- and modular-based flowsheeting codes

Looking Ahead

In this chapter we survey process simulators (flowsheeting codes) that are used in industrial practice to solve material and energy balances.

16.1 Main Concepts

As explained in Chapter 6, a plant **flowsheet** such as the simple diagram in Figure 16.1 mirrors the stream network and equipment arrangement in a process. Once the process flowsheet is specified, or during its formulation, the solution of the appropriate process material and energy balances is referred to as **process simulation** or **flowsheeting,** and the computer code used in the solution is known as a **process simulator** or **flowsheeting code.** Codes for both steady-state and dynamic processes exist. The essential problem in flowsheeting is to solve (satisfy) a large set of linear and nonlinear equations and constraints to an acceptable degree of precision. Such a program can also, at the same time, determine the size of equipment and piping, evaluate costs, and optimize performance. Figure 16.2 shows the information flow that occurs in a process simulator.

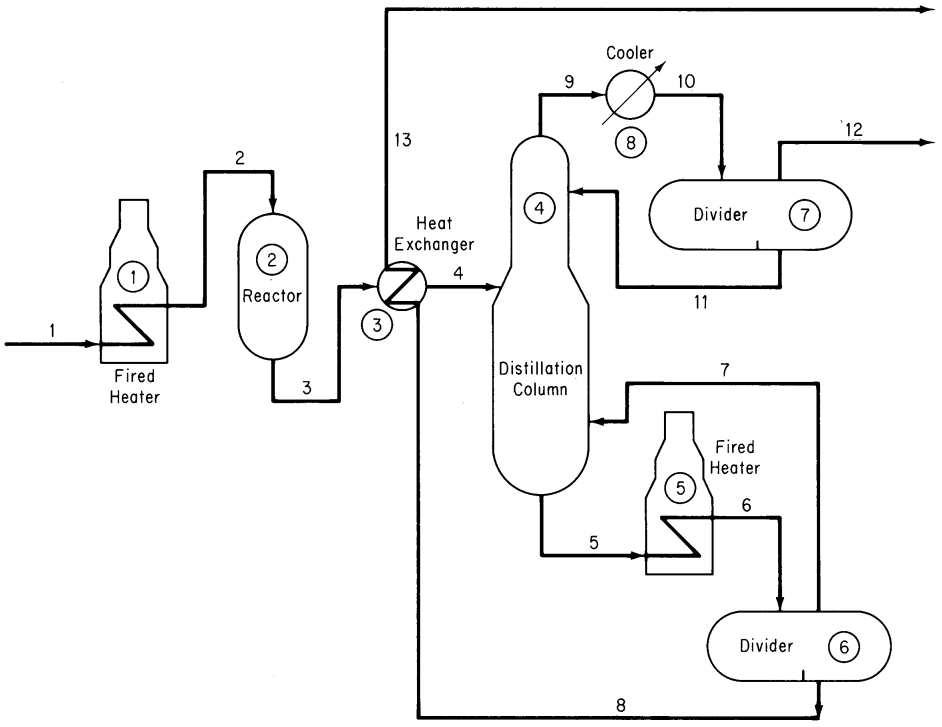


Figure 16.1 Hypothetical process flowsheet showing the materials flow in a process that includes reaction. The encircled numbers denote the unit labels, and the other numbers label the interconnecting streams.

The software must facilitate the transfer of information between equipment and streams, have access to a reliable database, and be flexible enough to accommodate equipment specifications provided by the user to supplement the library of programs that come with the code. Fundamental to all flowsheeting codes is the calculation of mass and energy balances for the entire process. Valid inputs to the material and energy balance phase of the calculations for the flowsheet must be defined in sufficient detail to determine all of the intermediate and product streams and the unit performance variables for all units.

Frequently, process plants contain recycle streams and control loops, and the solution for the stream properties requires iterative calculations. Thus, efficient numerical methods must be used. In addition, appropriate physical properties and thermodynamic data have to be retrieved from a database. Finally, a master program must exist that links all of the building blocks, physical property data, thermodynamic calculations, subroutines,

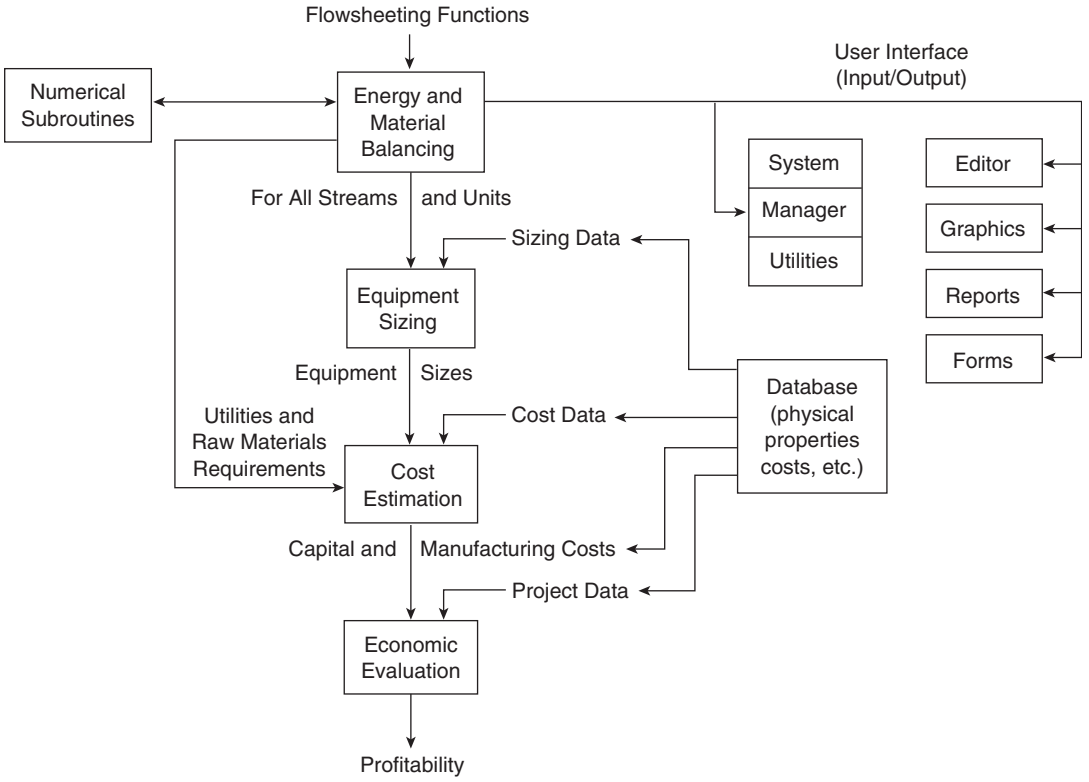


Figure 16.2 Information flow in a typical flowsheeting code

and numerical subroutines, and that also supervises the information flow. You will find that optimization and economic analysis are often the ultimate goals in the use of flowsheeting codes.

Other specific applications include

1. Steady- and unsteady-state simulation to help improve and verify the design of a process and examine complicated or dangerous designs
2. Training of operators
3. Data acquisition and reconciliation
4. Process control, monitoring, diagnostics, and troubleshooting
5. Optimization of process performance
6. Management of information
7. Safety analysis

Typical unit process models found in process simulators for both steady-state and unsteady-state operations include

1. Reactors of various kinds
2. Phase separation equipment

3. Ion exchange and absorption
4. Drying
5. Evaporation
6. Pumps, compressors, blowers
7. Mixers, splitters
8. Heat exchangers
9. Solid-liquid separators
10. Solid-gas separators
11. Storage tanks

Features that you will find in a general process simulator include

1. Unit and equipment models representing operations and procedures
2. Software to solve material and energy balances
3. An extensive database of physical properties
4. Equipment sizing and costing functions
5. Scheduling of batch operations
6. Environmental impact assessment
7. Compatibility with auxiliary graphics, spreadsheets, and word-processing functions
8. Ability to import and export data

Table 16.1 lists some commercial process simulators.

For updated data and information on process simulators refer to www.interduct.tudeltft.nl/Pltools/news/news.html, or to the respective company's Web site.

From the viewpoint of a user of a process simulator code you should realize:

Table 16.1 Vendors of Commercial Process Simulators

Name of Program	Source
ABACUSS II	MIT, Cambridge, MA
Aspen Engineering Suite (AES)	Aspen Technology, Cambridge, MA
CHEMCAD	Chemstations, Houston, TX
DESIGN II	WinSim, Houston, TX
D-SPICE	Fantoft Process Technologies, Houston, TX
HYSIM, HYSYS	Hyprotech, Calgary, Alberta
PRO/II, PROTISS	Simulation Sciences, Fullerton, CA
ProSim	Bryan Research and Engineering, Bryan, TX
SPEEDUP	Aspen Technology Corp., Cambridge, MA
SuperPro Designer	Intelligen, Scotch Plains, NJ

1. Several levels of analysis can be carried out beyond just solving material balances, including solving material plus energy balances, determining equipment sizing, profitability analysis, and much more. Crude, approximate flowsheets are usually studied before fully detailed flowsheets.
2. The results obtained by simulation rest heavily on the type and validity of the choices you make in the selection of the physical property package to be used.
3. You have to realize that the basic function of the process simulator is to solve equations. In spite of the progress made in equation solvers in the last 50 years, the information structure you introduce into the code may yield erroneous or no results. Check essential results by hand. Limits introduced on the range of variables must be valid.
4. A learning curve exists in using a process simulator so that initially a simple problem may take hours to solve, whereas as your familiarity with the simulator increases, it may take only minutes to solve the same problem.
5. GIGO (Garbage In Garbage Out). You have to take care to put appropriate data and connections between units into the data files for the code. Some diagnostics are provided, but they cannot troubleshoot all of your blunders.

Two extremes exist in process simulator software. At one extreme, the entire set of equations (and inequalities) representing the process is written down, including the material and energy balances, the stream connections, and the relations representing the equipment functions. This representation is known as the **equation-oriented method** of flowsheeting. The equations can be solved in a sequential fashion analogous to the modular representation described below, or simultaneously by Newton's method (or the equivalent), or by employing sparse matrix techniques to reduce the extent of matrix manipulations; you can find specific details in the references at the end of this chapter.

At the other extreme, the process can be represented by a collection of modules (**the modular method of flowsheeting**) in which the equations (and other information) representing each subsystem or piece of equipment are collected together and coded so that the module may be used in isolation from the rest of the flowsheet and hence is portable from one flowsheet to another, or can be used repeatedly in a given flowsheet. A module is a model of an individual element in a flowsheet (such as a reactor) that can be coded, analyzed, debugged, and interpreted by itself. In its usual formulation it is an input-output model; that is, given the input values, the module calculates the output values, but the reverse calculation is not feasible. Units represented solely by equations sometimes can yield inputs given the outputs. Some modular-based software codes such as Aspen Plus integrate equations with modules to speed up the calculations.

Another classification of flowsheeting codes focuses on how the equations or modules are solved. One treatment is to solve the equations or

modules sequentially, and the other is to solve them simultaneously. Either the program and/or the user must select the decision variables for recycle and provide estimates of certain stream values to make sure that convergence of the calculations occurs, especially in a process with many recycle streams.

A third classification of flowsheeting codes is whether they solve steady-state or dynamic problems. We consider only the former here.

We will review equation-based process simulators first, although historically modular-based codes were developed first, because they are much closer to the techniques described up to this point in this book, and then turn to consideration of modular-based flowsheeting.

16.1.1 Equation-Based Process Simulation

Sets of linear and/or nonlinear equations can be solved simultaneously using an appropriate computer code. Equation-based flowsheeting codes have some advantages in that the physical property data needed to obtain values for the coefficients in the equations are transparently transmitted from a database at the proper time in the sequence of calculations. Figure 16.3 shows the information flow corresponding to the flowsheet in Figure 16.1.

Figure 16.4 is a set of equations that represents the basic operation of a flash drum.

The interconnections between the unit modules may represent information flow as well as material and energy flow. In the mathematical representation of

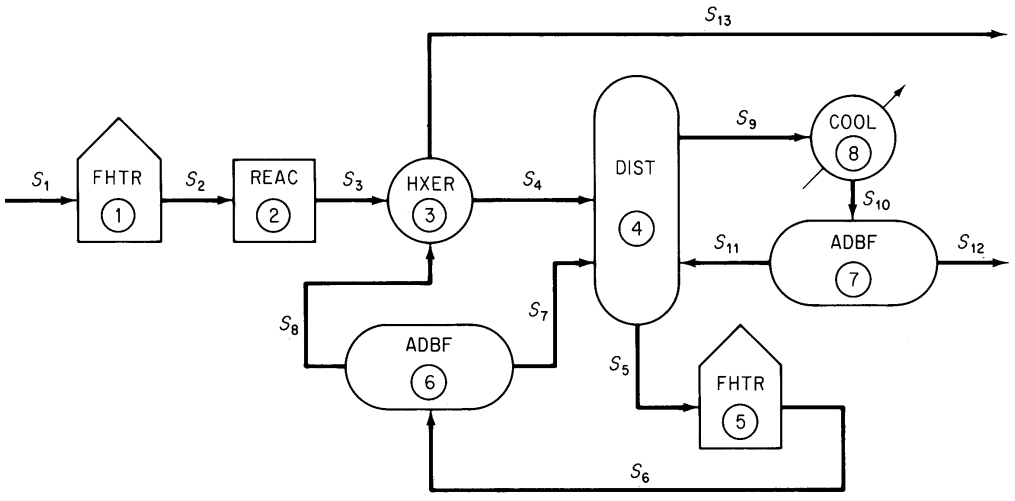
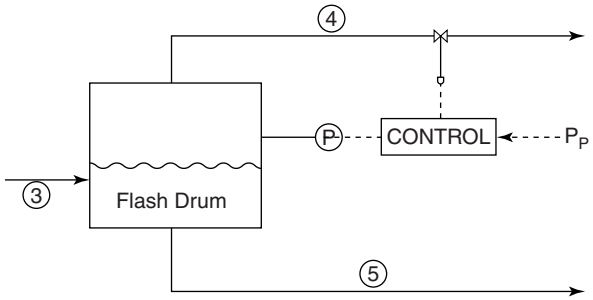


Figure 16.3 Information flowsheet for the hypothetical process in Figure 16.1 (*S* stands for stream; the module or computer code number is encircled.)



Material balances:

$$x_{A3}F_3 - y_{A4}F_4 - x_{A5}F_5 = 0$$
$$x_{P3}F_3 - y_{P4}F_4 - x_{P5}F_5 = 0$$
$$x_{G3}F_3 - y_{G4}F_4 - x_{G5}F_5 = 0$$
$$y_{A4} + y_{P4} + y_{G4} = 1$$
$$x_{A5} + x_{P5} + x_{G5} = 1$$

Equilibrium relations:

$$T_4 = T_5$$
$$y_{A4} = K_A x_{A5}$$
$$y_{P4} = K_P x_{P5}$$
$$y_{G4} = K_G x_{G5}$$

where $\kappa_i = p_i^*(T_4)/p_F \qquad (i = A,P,G)$

Energy balance:

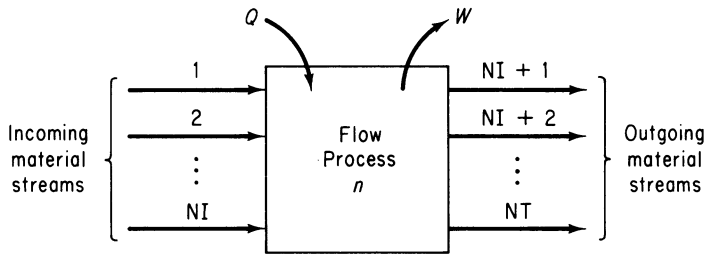
$$F_5(x_{A3}C_A + x_{P3}C_P + x_{G3}C_G)T_3 = F_5(x_{A5}C_A + x_{P5}C_P + x_{G5}C_G)\,T_5 + F_4[(y_{A4}C_A + y_{P4}C_P + y_{G4}c_G)T_4 + y_{A4}\lambda_A + y_{P4}\lambda_P + y_{G4}\lambda_G]$$

Figure 16.4 A set of a linear and two nonlinear equations representing a system of three components, *A*, *P*, and *E*, passing through a flash drum

the plant, the interconnection equations are the material and energy balance flows between model subsystems. Equations for models such as mixing, reaction, heat exchange, and so on must also be listed so that they can be entered into the computer code used to solve the equation. Figure 16.5 (and Table 16.2) lists the common types of equations that might be used for a single subsystem.

In general, similar process units repeatedly occur in a plant and can be represented by the same set of equations that differ only in the names of variables, the number of terms in the summations, and the values of any coefficients in the equations.

System diagram



Total mass balance (or mole balance) without reaction)

$$\sum_{i=1}^{\mathrm{NI}} F_i = \sum_{i=\mathrm{NI}+1}^{\mathrm{NT}} F_i$$

Energy balance

$$\sum_{i=1}^{\mathrm{NI}} F_i H_i + Q_n - W_{s,n} = \sum_{i=\mathrm{N}+1}^{\mathrm{NI}} F_i H_i$$

Vapor-liquid equilibrium distribution

$$y_j = K_j x_j \quad \text{for} \quad j = 1, 2, \ldots, \mathrm{NC}$$

Equilibrium vaporization coefficients

$$K_j = K(T_i, P_i, \overline{W}_i) \quad j = 1, 2, \text{for} \ldots, , \mathrm{NC}$$

Component mass or mole balances

$$\sum_{i=1}^{\mathrm{NI}} F_i w_{i,j} = \sum_{i=\mathrm{NT}+1}^{\mathrm{NT}} F_i w_{i,j}$$

$$\text{for } j = 1, 2, \ldots, \mathrm{NC}$$

Summation of mole or mass fractions

$$\sum_{j=1}^{\mathrm{NC}} w_{i,j} = 1.0 \text{ for } i = 1, 2, \ldots, \mathrm{NI}$$

Physical property functions

$$H_i = H_{\mathrm{VL}}(T_i, P_i, \overline{W}_i)$$
$$S_i = S_{\mathrm{VL}}(T_i, P_i, \overline{W}_i) \quad i = 1, 2, \ldots, \mathrm{NI}$$

Total mole balance (with reaction)

$$\sum_{i=1}^{\mathrm{NI}} F_i + \sum_{l=1}^{\mathrm{NI}} R_l \left[\sum_{j=1}^{\mathrm{NC}} V_{j,l} \right] = \sum_{i=\mathrm{NI}+1}^{\mathrm{NI}} F_i$$

Component mole balances (with reaction)

$$\sum_{i=1}^{\mathrm{NI}} F_i w_{i,j} + \sum_{l=1}^{\mathrm{NR}} V_{j,l} R_l = \sum_{i=\mathrm{NI}+1}^{\mathrm{NT}} F_i w_{i,j} \quad \text{for } j = 1, 2, \ldots, \mathrm{NC}$$

Molar atom balances

$$\sum_{i=1}^{\mathrm{NI}} F_i \left[\sum_{j=1}^{\mathrm{NC}} w_{i,j} a_{j,k} \right] = \sum_{i=\mathrm{NI}+1}^{\mathrm{NT}} F_i \left[\sum_{j=1}^{\mathrm{NC}} w_{i,j} a_{j,k} \right] \quad \text{for } k = 1, 2, \ldots, \mathrm{NE}$$

Mechanical energy balance

$$\sum_{i=1}^{\mathrm{NI}} (K_i + P_i) + \sum_{i=1}^{\mathrm{NI}} \int_{P_{1,i}}^{P_{2,i}} V_i \, dp_i = \sum_{i=\mathrm{NI}+1}^{\mathrm{N}} (K_i + P_i) + \sum_{i=\mathrm{NI}+1}^{\mathrm{NT}} \int_{P_{1,i}}^{P_{2,i}} V_i \, dP_i + W_{s,n} + E_{v,n}$$

Figure 16.5 Generic equations for a steady-state, open system

Table 16.2 Notation for Figure 16.5

$a_{j,k}$	Number of atoms of the kth chemical element in the jth component
F_i	Total flow rate of the ith stream
H_i	Relative enthalpy of the ith stream
K_j	Vaporation coefficient of the jth component
NC	Number of chemical components (compounds)
NE	Number of chemical elements
NI	Number of incoming material streams
NR	Number of chemical reactions
NT	Total number of material streams
p_i	Pressure of the ith stream
Q_n	Heat transfer for the nth process unit
R_l	Reaction expression for the lth chemical reaction
T_i	Temperature of the ith stream
$V_{j,l}$	Stoichiometric coefficient of the jth component in the lth chemical reaction
$w_{i,j}$	Fractional composition (mass of mole) of the jth component in the ith stream
$\bar{W}_i$	Average composition in the ith stream
$W_{s,n}$	Work for the nth process unit
x_j	Mole fraction of component j in the liquid
y_j	Mole fraction of component j in the vapor

Equation-based codes can be formulated to include inequality constraints along with the equations. Such constraints might be of the form $a_1x_1 + a_2x_2 + \ldots \leq b$ and might arise from such factors as

1. Conditions imposed in linearizing any nonlinear equations
2. Process limits for temperature, pressure, concentration
3. Requirements that variables be in a certain order
4. Requirements that variables be positive or integer

As you can see from Figures 16.4 and 16.5, if all of the equations for the material and energy balances plus the phase and chemical equilibrium relationships plus the thermodynamic and kinetic relations are combined, they form a huge, sparse (few variables in any equation) array. The set of equations can be partitioned into subsets of equations that cannot further be decomposed and have to be solved simultaneously. Two important aspects of solving the sets of nonlinear equations in flowsheeting codes, both equation-based and modular, are (1) the procedure for establishing the precedence order in solving the equations, and (2) the treatment of recycle (feedback) of information, material, and/or energy. Details of how to accommodate these important issues efficiently can be found in the references at the end of this chapter.

Whatever the process simulator used to solve material and energy balance problems, you must provide certain input information to the code in an acceptable format. All flowsheeting codes require that you convert the information in the flowsheet (see Figure 16.1) and the information flowsheet as illustrated in Figure 16.3, or something equivalent. In the information flowsheet, you use the name of the mathematical model (or the subroutine in modular-based flowsheeting) that will be used for the calculations instead of the name of the process unit.

Once the information flowsheet is set up, the determination of the process topology is easy; that is, you can immediately write down the stream interconnections between the modules (or subroutines) that have to be included in the input data set. For Figure 16.3 the matrix of stream connections (the **process matrix**) is (a negative sign designates an exit stream):

Unit	Associated Streams				
1	1	−2			
2	2	−3			
3	3	8	−4	−13	
4	4	7	11	−9	−5
5	5	−6			
6	6	−8	−7		
7	10	−11	−12		
8	9	−10			

16.1.2 Modular-Based Process Simulators

Because plants are composed of various unit operations (such as distillation, heat transfer, and so on) and unit processes (such as alkylation, hydrogenation, and so on), chemical engineers historically developed representations of each of these units or processes as self-contained modules. Each module (refer to Figure 16.6) might be composed of equations, equipment sizes, material and energy balance relations, component flow rates, and the temperatures, pressures, and phase conditions of each stream that enters and leaves the physical equipment represented by the module.

Figure 16.7 shows a flash module and the computer code that yields an output for a given input.

Values of certain parameters and variables determine the capital and operating costs for the units. Of course, the interconnections set up for the modules must be such that information can be transferred from module to module concerning the streams, compositions, flow rates, coefficients, and so on. In other words, the modules constitute a set of building blocks that can be arranged in general ways to represent any process.

The sequential modular method of flowsheeting is the one most commonly encountered in commercial computer software. A module exists for each process unit in the information flowsheet. Given the values of each

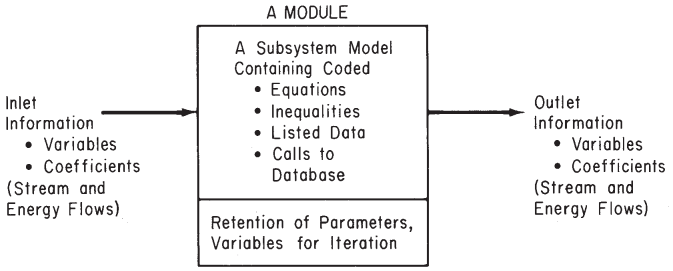


Figure 16.6 A typical process module showing the necessary interconnections of information

input stream composition, flow rate, temperature, pressure, enthalpy, and the equipment parameters, the output of a module can become the input stream to another module for which the calculations can then proceed, and so on, until the material and energy balances are resolved for the entire process. Modules are portable. By portable we mean that a subroutine corresponding to a module can be assembled as an element of a large group of subroutines and successfully represent a certain type of equipment in any process. Figure 16.8 shows icons for typical standardized unit operation modules.

Other modules take care of equipment sizing and cost estimation, perform numerical calculations, handle recycle calculations (described in more detail below), optimize, and serve as controllers (executives for the whole set of modules so that they function in the proper sequence). Internally, a very simple module might just be a table lookup program. However, most modules consist of Fortran or C subroutines that execute a sequence of calculations. Subroutines may consist of hundreds to thousands of lines of code.

Information flows between modules via the material streams. Associated with each stream is an ordered list of numbers that characterize the stream. Table 16.3 lists a typical set of parameters associated with a stream. The presentation of the results of simulations also follows the same format as shown in Table 16.3.

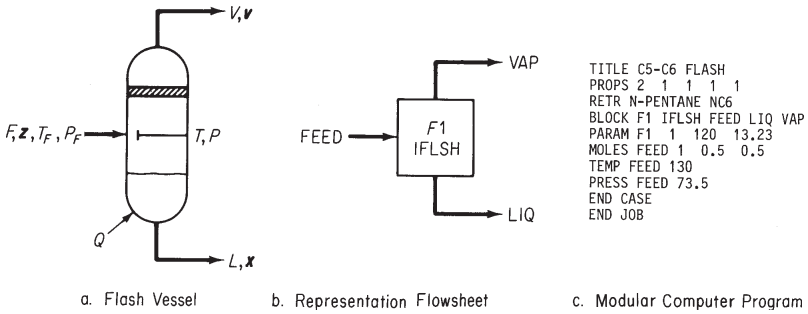


Figure 16.7 A module that represents a flash unit [From J. D. Seader, W. D. Seider, and A. C. Pauls, *Flowtran Simulation: An Introduction*, CACHE, Austin, TX (1987)]

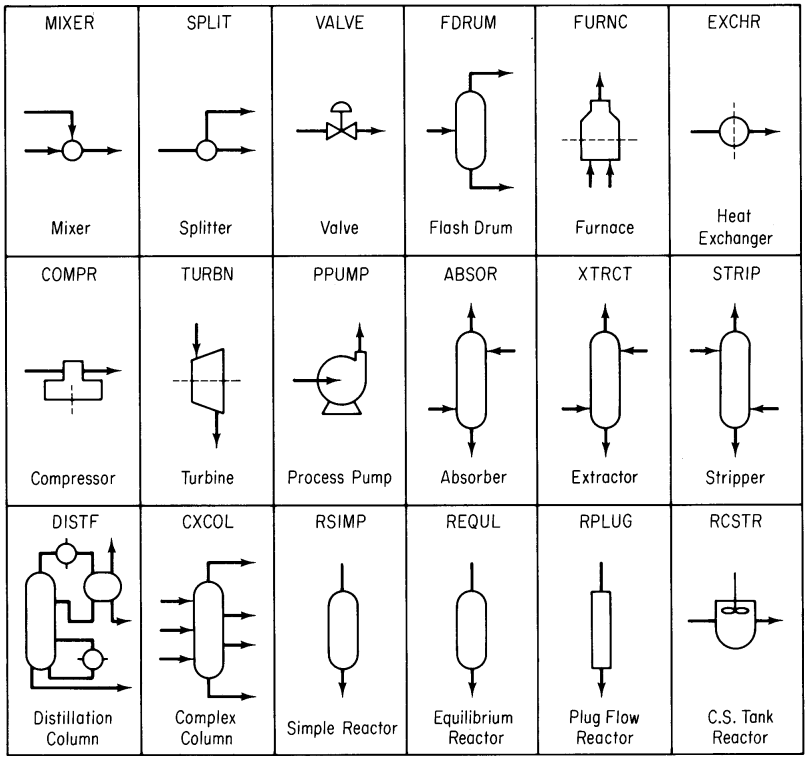


Figure 16.8 Typical process modules used in sequential modular-based flowsheeting codes with their subroutine names

As a user of a modular-based code, you have to provide

1. The process topology
2. Input stream information, including physical properties and connections

Table 16.3 Stream Parameters

1. Stream number*
2. Stream flag (designates type of stream)
3. Total flow, lb mol/hr
4. Temperature, °F
5. Pressure, psia
6. Flow of component 1, lb mol/hr
7. Flow of component 2, lb mol/hr
8. Flow of component 3, lb mol/hr
9. Molecular weight
10. Vapor fraction
11. Enthalpy
12. Sensitivity

*Corresponds to an arbitrary numbering scheme used on the information flowsheet.

3. Design parameters needed in the modules and equipment specifications
4. Convergence criteria

In addition, you sometimes may have to insert a preferred calculation order for the modules. When economic evaluation and optimization are being carried out, you must also provide cost data and optimization criteria.

Modular-based flowsheeting exhibits several advantages in design. The flowsheet architecture is easily understood because it closely follows the process flowsheet. Individual modules can easily be added and removed from the computer package. Furthermore, new modules may be added to or removed from the flowsheet without affecting other modules. Modules at two different levels of accuracy can be substituted for one another.

Modular-based flowsheeting also has certain drawbacks:

1. The output of one module is input to another. The input and output variables in a computer module are fixed so you cannot arbitrarily introduce an output and generate an input as sometimes can be done in equation-based code.
2. The modules require extra computer time to generate reasonably accurate derivatives or their substitutes, especially if a module contains tables, functions with discrete variables, discontinuities, and so on. Perturbation of the input to a module is the primary way in which a finite-difference substitute for a derivative can be generated.
3. The modules may require a fixed precedence order of solution—that is, the output of one module must become the input of another—hence convergence may be slower than in an equation-solving method, and the computational costs may be high.
4. To specify a parameter in a module as a decision variable in the design of a plant, you have to place a control block around the module and adjust the parameter such that design specifications are met. This arrangement creates a loop. If the values of many design variables are to be determined, you might end up with several nested loops of calculation (which do, however, enhance stability). A similar arrangement must be used if you want to impose constraints.
5. Conditions imposed on a process (or a set of equations for that matter) may cause the unit physical states to move from two-phase to single-phase operation, or the reverse. (This situation is true of equation-based codes as well.) You have to foresee and accommodate such changes in state.

An engineer can usually carry out the partitioning and nesting and determine the computational sequence for a flowsheet by inspection if the flowsheet is not too complicated. In some codes, the user supplies the computational

sequence as input. Other codes determine the sequence automatically. In Aspen, for example, the code is capable of determining the entire computational sequence, but the user can supply as many specifications as desired, up to and including the complete computational sequence. Consult one of the supplementary references at the end of this chapter for detailed information on optimal ways of using simulator techniques beyond our scope in this text.

Once the sequence of calculation codes is specified, everything is in order for the solution of material and energy balances. All that has to be done is to calculate the correct values for the stream flow rates and their properties. To execute the calculations, various numerical algorithms can be selected by the user or determined by the simulator. The results can be displayed as tables, graphs, charts, and so on.

Looking Back

In this chapter we described the two main ways of solving the material and energy balances in process simulators: using equation-based and modular-based computer software.

Discussion Question

A number of articles have been written on the subject of paper versus polystyrene as materials for disposable cups. Set up the flowsheets for the production of each, and include all of the quantitative and qualitative factors, both positive and negative, for the production from basic raw materials to the final product. Indicate what material and energy balances are needed, and, if possible, collect data so that they can be solved. Summarize the material and energy usage in the manufacture of a cup.

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Web Sites

The best site by far is

www.interduct.tudelft.nl/Pltools/news/news.html

Other sites are

http://members.ozemail.com.au/~wadsley/models.html
www.umsl.edu/~chemist/books/softpubs.html
www.virtualmaterials.com

Each vendor listed in Table 16.1 has a Web site that contains considerable information and demos pertaining to its particular software.

Problems

16.1 In petroleum refining, lubricating oil is treated with sulfuric acid to remove unsaturated compounds, and after settling, the oil and acid layers are separated. The acid layer is added to water and heated to separate the sulfuric acid from the sludge contained in it. The dilute sulfuric acid, now 20% H_2SO_4 at 82°C, is fed to a Simonson-Mantius evaporator, which is supplied with

saturated steam at 400 kPa gauge to lead coils submerged in the acid, and the condensate leaves at the saturation temperature. A vacuum is maintained at 4.0 kPa by means of a barometric leg. The acid is concentrated to 80% H_2SO_4; the boiling point at 4.0 kPa is 121°C. How many kilograms of acid can be concentrated per 1000 kg of steam condensed?

16.2 You are asked to perform a feasibility study on a continuous stirred tank reactor shown in Figure P16.2 (which is presently idle) to determine if it can be used for the second-order reaction

$$2A \rightarrow B + C$$

Since the reaction is exothermic, a cooling jacket will be used to control the reactor temperature. The total amount of heat transfer may be calculated from an overall heat transfer coefficient (U) by the equation

$$\dot{Q} = UA\,\Delta T$$

where $\dot{Q}$ = total rate of heat transfer from the reactants to the water jacket in the steady state
U = empirical coefficient
A = area of transfer
ΔT = temperature difference (here $T_4 - T_2$)

Some of the energy released by the reaction will appear as sensible heat in stream F_2, and some concern exists as to whether the fixed flow rates will be sufficient to keep the fluids from boiling while still obtaining good conversion. Feed data are as follows:

Component	Feed Rate (lb mol/hr)	C_p [Btu/(lb mol)(°F)]	MW
A	214.58	41.4	46
B	23.0	68.4	76
C	0.0	4.4	16

The consumption rate of A may be expressed as

$$-2k(C_A)^2V_R$$

where

$$C_A = \frac{(F_{1,A})(\rho)}{\Sigma(F_{1,i})(MW_i)} = \text{concentration of } A, \text{ lb mol/ft}^3$$

$$k = k_0 \exp\left(\frac{-E}{RT}\right)$$

k_0, E, R are constants, and T is the absolute temperature.

Solve for the temperatures of the exit streams and the product composition of the steady-state reactor using the following data:

Fixed parameters

Reactor volume $= V_R = 13.3\ \text{ft}^3$
Heat transfer area $= A = 29.9\ \text{ft}^2$
Heat transfer coefficient $= U = 74.5\ \text{Btu/(hr)(ft}^2\text{)(°F)}$

Variable input

Reactant feed rate $= F_i$ (see table above)
Reactant feed temperature $= T_1 = 80°\text{F}$
Water feed rate $= F_3 = 247.7\ \text{lb mol/hr water}$
Water feed temperature $= T_3 = 75°\text{F}$

Physical and thermodynamic data

Reaction rate constant $= k_0 = 34\ \text{ft}^3/\text{(lb mol)/(hr)}$
Activation energy/gas constant $= E/R = 1000°\text{R}$

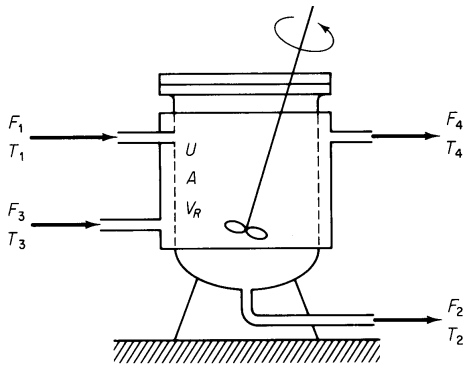


Figure P16.2

Heat of reaction $= \Delta H = -5000\ \text{Btu/lb mol } A$
Heat capacity of water $= C_{pw} = 18\ \text{Btu/(lb mol)(°F)}$
Product component density $= \rho = 55\ \text{lb/ft}^3$

The densities of each of the product components are essentially the same. Assume that the reactor contents are perfectly mixed as well as the water in the jacket, and that the respective exit stream temperatures are the same as the reactor contents or jacket contents.

16.3 The stream flows for a plant are shown in Figure P16.3. Write the material and energy balances for the system and calculate the unknown quantities in the diagram (*A* to *F*). There are two main levels of stream flow: 600 psig and 50 psig. Use the steam tables for the enthalpies.

16.4 Figure P16.4 shows a calciner and the process data. The fuel is natural gas. How can the energy efficiency of this process be improved by process modification? Suggest at least two ways based on the assumption that the supply conditions of the air and fuel remain fixed (but these streams can possibly be passed through heat exchangers). Show all calculations.

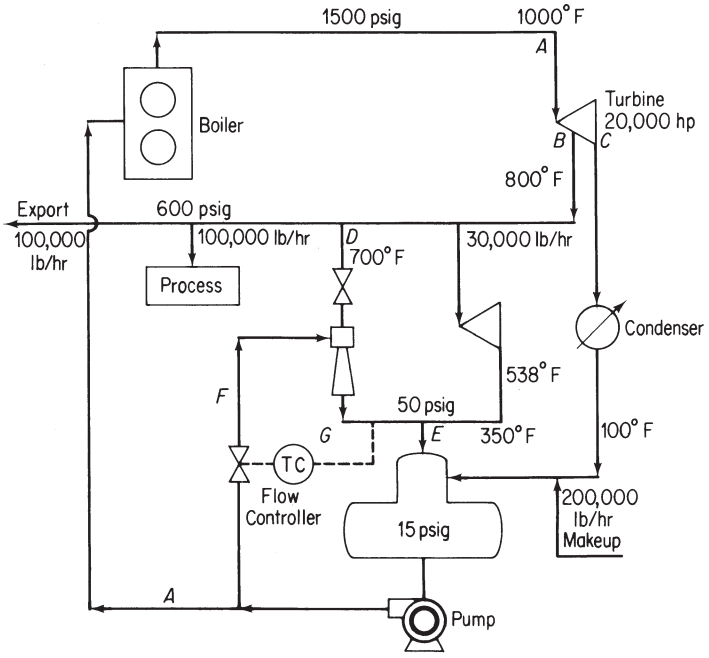


Figure P16.3

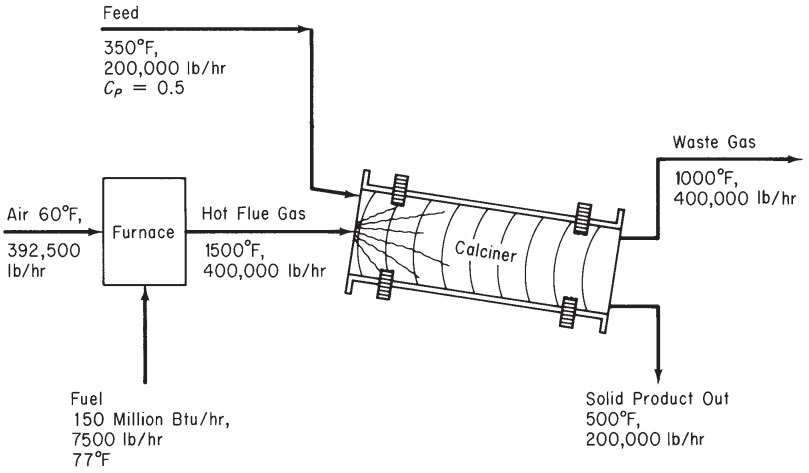


Figure P16.4

16.5 Limestone ($CaCO_3$) is converted into CaO in a continuous vertical kiln (see Figure P16.5). Heat is supplied by combustion of natural gas (CH_4) in direct contact with the limestone using 50% excess air. Determine the kilograms of $CaCO_3$ that can be processed per kilogram of natural gas. Assume that the following average heat capacities apply:

$$C_p \text{ of } CaCO_3 = 234 \text{ J/(g mol)(°C)}$$
$$C_p \text{ of CaO} \quad = 111 \text{ J/(g mol)(°C)}$$

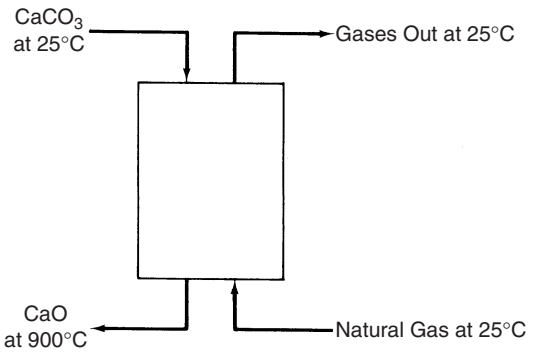


Figure P16.5

16.6 A feed stream of 16,000 lb/hr of 7% by weight NaCl solution is concentrated to a 40% by weight solution in an evaporator. The feed enters the evaporator, where it is heated to 180°F. The water vapor from the solution and the concentrated solution leave at 180°F. Steam at the rate of 15,000 lb/hr enters at 230°F and leaves as condensate at 230°F. See Figure P16.6.

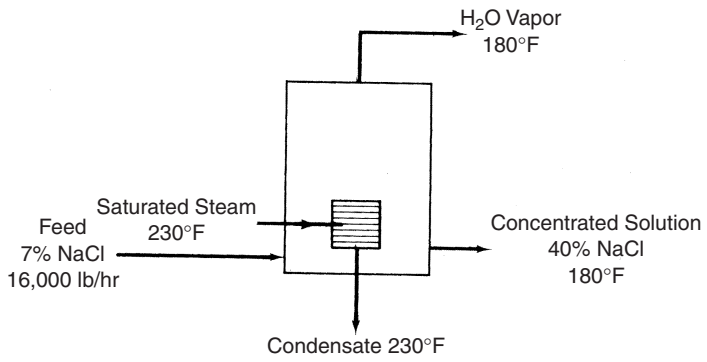


Figure P16.6

a. What is the temperature of the feed as it enters the evaporator?
b. What weight of 40% NaCl is produced per hour?

Assume that the following data apply:

Average C_p 7% NaCl soln: 0.92 Btu/(lb)(°F)
Average C_p 40% NaCl soln: 0.85 Btu/(lb)(°F)
$\Delta \hat{H}_{vap}$ of H_2O at 180°F = 990 Btu/lb
$\Delta \hat{H}_{vap}$ of H_2O at 230°F = 959 Btu/lb

16.7 The Blue Ribbon Sour Mash Company plans to make commercial alcohol by a process shown in Figure P16.7. Grain mash is fed through a heat exchanger where it is heated to 170°F. The alcohol is removed as 60% by weight alcohol from the first fractionating column; the bottoms contain no alcohol. The 60% alcohol is further fractionated to 95% alcohol and essentially pure water in

the second column. Both stills operate at a 3:1 reflux ratio and heat is supplied to the bottom of the columns by steam. Condenser water is obtainable at 80°F. The operating data and physical properties of the streams have been accumulated and are listed for convenience:

Stream	State	Boiling Point (°F)	C_p[Btu/(lb)(°F)] Liquid	Vapor	Heat of Vaporization (Btu/lb)
Feed	Liquid	170	0.96	—	950
60% alcohol	Liquid or vapor	176	0.85	0.56	675
Bottoms I	Liquid	212	1.00	0.50	970
95% alcohol	Liquid or vapor	172	0.72	0.48	650
Bottoms II	Liquid	212	1.0	0.50	970

Prepare the material balances for the process, calculate the precedence order for solution, and

a. Determine the weight of the following streams per hour:
   1. Overhead product, column I
   2. Reflux, column I
   3. Bottoms, column I
   4. Overhead product, column II
   5. Reflux, column II
   6. Bottoms, column II
b. Calculate the temperature of the bottoms leaving Heat Exchanger III.
c. Determine the total heat input to the system in British thermal units per hour.

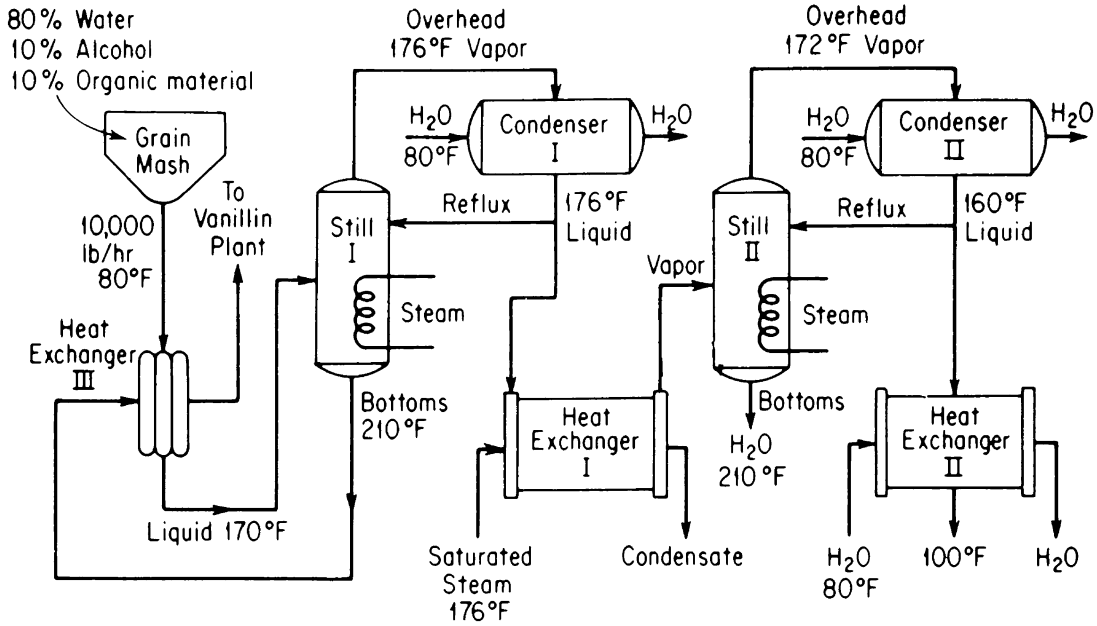


Figure P16.7

d. Calculate the water requirements for each condenser and Heat Exchanger II in gallons per hour if the maximum exit temperature of water from this equipment is 130°F.

16.8 Toluene, manufactured by the conversion of *n*-heptane with a Cr_2O_3-on-Al_2O_3 catalyst

$$CH_3CH_2CH_2CH_2CH_2CH_2CH_3 \rightarrow C_6H_5CH_3 + 4H_2$$

by the method of hydroforming, is recovered by use of a solvent. See Figure P16.8 for the process and conditions.

The yield of toluene is 15 mol % based on the *n*-heptane charged to the reactor. Assume that 10 kg of solvent are used per kilogram of toluene in the extractors.

a. Calculate how much heat has to be added to or removed from the catalytic reactor to make it isothermal at 425°C.
b. Find the temperature of the *n*-heptane and solvent stream leaving the mixersettlers if both streams are at the same temperature.
c. Find the temperature of the solvent stream after it leaves the heat exchanger.
d. Calculate the heat duty of the fractionating column in kilojoules per kilogram of *n*-heptane feed to the process.

	$-\Delta H_f^{\circ *}$ (kJ/g mol)	C_p[J/(g)(°C)] Liquid	C_p[J/(g)(°C)] Vapor	$\Delta H_{vaporization}$ (kJ/kg)	Boiling Point (K)
Toulene†	12.00	2.22	2.30	364	383.8
n-Heptane	−224.4	2.13	1.88	318	371.6
Solvent	—	1.67	2.51	—	434

*As liquids.
†The heat of solution of toluene in the solvent is −23 J/g toluene.

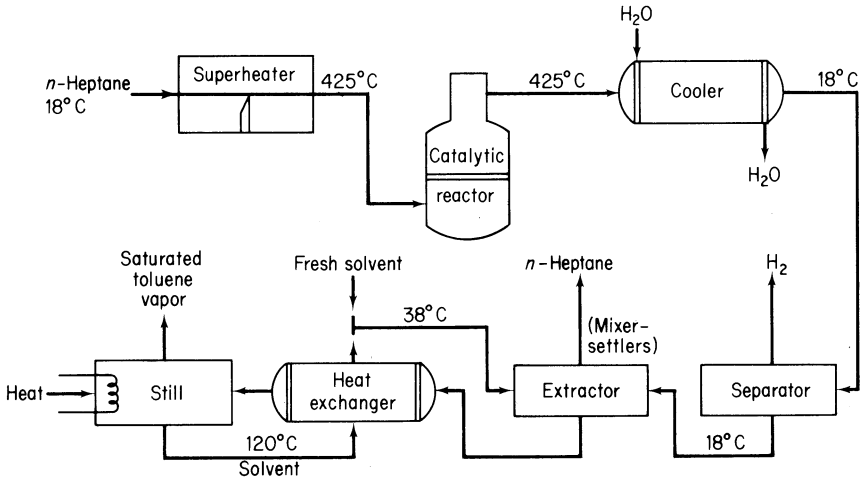


Figure P16.8

16.9 One hundred thousand pounds of a mixture of 50% benzene, 40% toluene, and 10% *o*-xylene is separated every day in a distillation-fractionation plant as shown on the flowsheet for Figure P16.9.

	Boiling Point (°C)	C_p Liquid [cal/(g)(°C)]	Latent Heat of Vap. (cal/g)	C_p Vapor [cal/(g)(°C)]
Benzene	80	0.44	94.2	0.28
Toluene	109	0.48	86.5	0.30
o-Xylene	143	0.48	81.0	0.32
Charge	90	0.46	88.0	0.29
Overhead T_I	80	0.45	93.2	0.285
Residue T_I	120	0.48	83.0	0.31
Residue T_{II}	413	0.48	81.5	0.32

The reflux ratio for Tower I is 6:1; the reflux ratio for Tower II is 4:1; the charge to Tower I is liquid; the chart to Tower II is liquid. Compute:

a. The temperature of the mixture at the outlet of the heat exchanger (marked as T^*)
b. The British thermal units supplied by the steam reboiler in each column
c. The quantity of cooling water required in gallons per day for the whole plant
d. The energy balance around Tower I

16.10 Sulfur dioxide emissions from coal-burning power plants cause serious atmospheric pollution in the eastern and midwestern portions of the United States. Unfortunately, the supply of low-sulfur coal is insufficient to meet the demand. Processes presently under consideration to alleviate the situation include coal gasification followed by desulfurization and stack gas cleaning. One of the more promising stack gas cleaning processes involves reacting SO_2 and O_2 in the stack gas with a solid metal oxide sorbent to give the metal sulfate, and then thermally regenerating the sorbent and absorbing the result SO_3 to produce sulfuric acid. Recent laboratory experiments indicate that sorption and regeneration can be carried out with several metal oxides, but no pilot or full-scale processes have yet been put into operation.

You are asked to provide a preliminary design for a process that will remove 95% of the SO_2 from the stack gas of a 1000 MW power plant. Some data are given below and in the flow diagram of the process (Figure P16.10). The sorbent consists of fine particles of a dispersion of 30% by weight CuO in a matrix of inert porous Al_2O_3. This solid reacts in the fluidized-bed absorber at 315°C. Exit solid is sent to the regenerator, where SO_3 is evolved at 700°C, converting the $CuSO_4$ present back to CuO. The fractional conversion of CuO to $CuSO_4$ that occurs in the sorber is called α and is an important design variable. You are asked to carry out your calculations for $\alpha = 0.2$, 0.5, and 0.8. The SO_3 produced in the regenerator is swept out by recirculating air. The SO_3-laden air is sent to the acid tower, where the SO_3 is absorbed in recirculating sulfuric acid and oleum, part of which is withdrawn as salable by-products. You will notice that the sorber, regenerator, and perhaps the acid tower are adiabatic; their

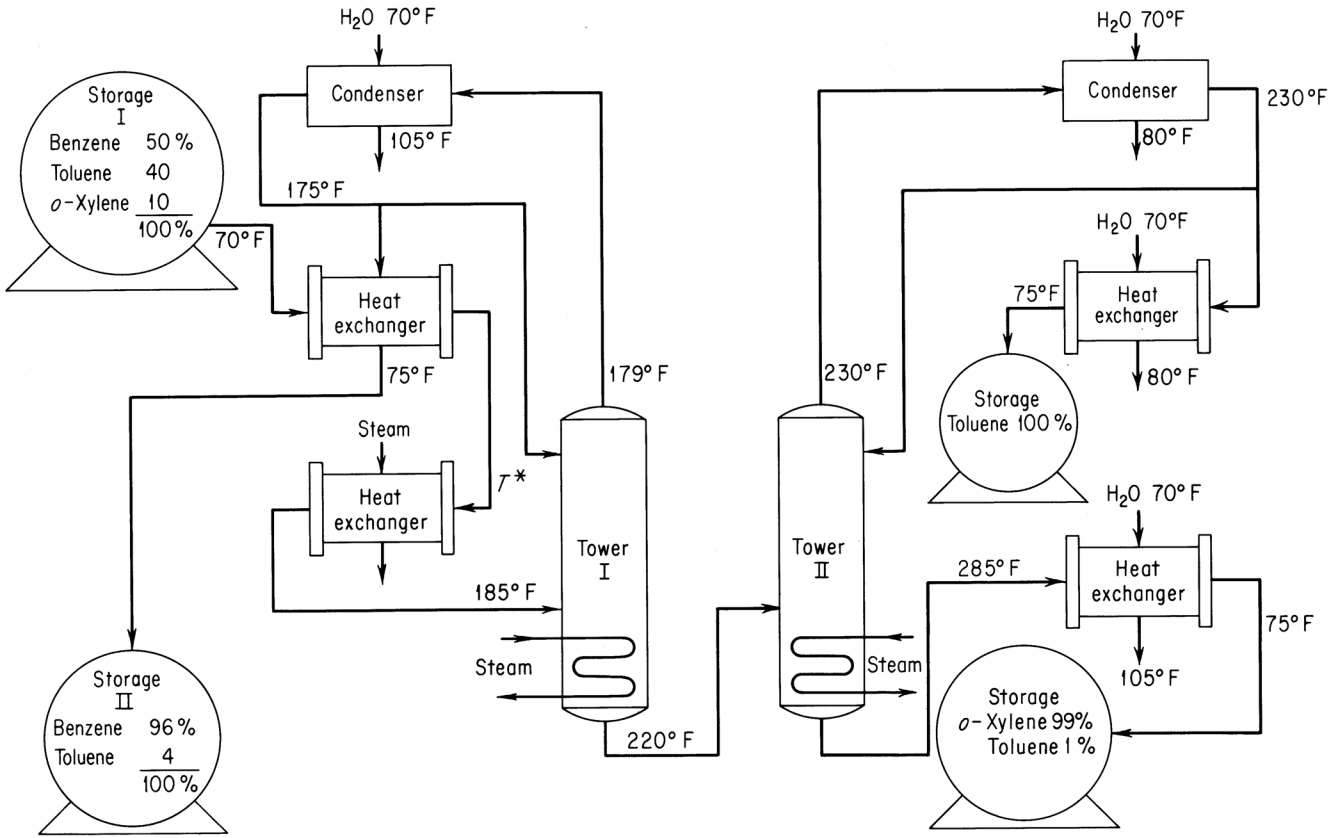

H2O 70° F
Condenser
105° F
175° F
Storage
I
Benzene 50 %
Toluene 40
o-Xylene 10
100 %
70° F
Heat
exchanger
75° F
179° F
Steam
Heat
exchanger
T*
Tower
I
185° F
Steam
220° F
Storage
II
Benzene 96 %
Toluene 4
100 %
H2O 70°F
Condenser
230 °F
80° F
H2O 70°F
75°F
Heat
exchanger
80° F
230° F
Storage
Toluene 100 %
H2O 70° F
Tower
II
285° F
Heat
exchanger
75° F
Steam
105° F
Storage
o-Xylene 99%
Toluene 1 %

Figure P16.9

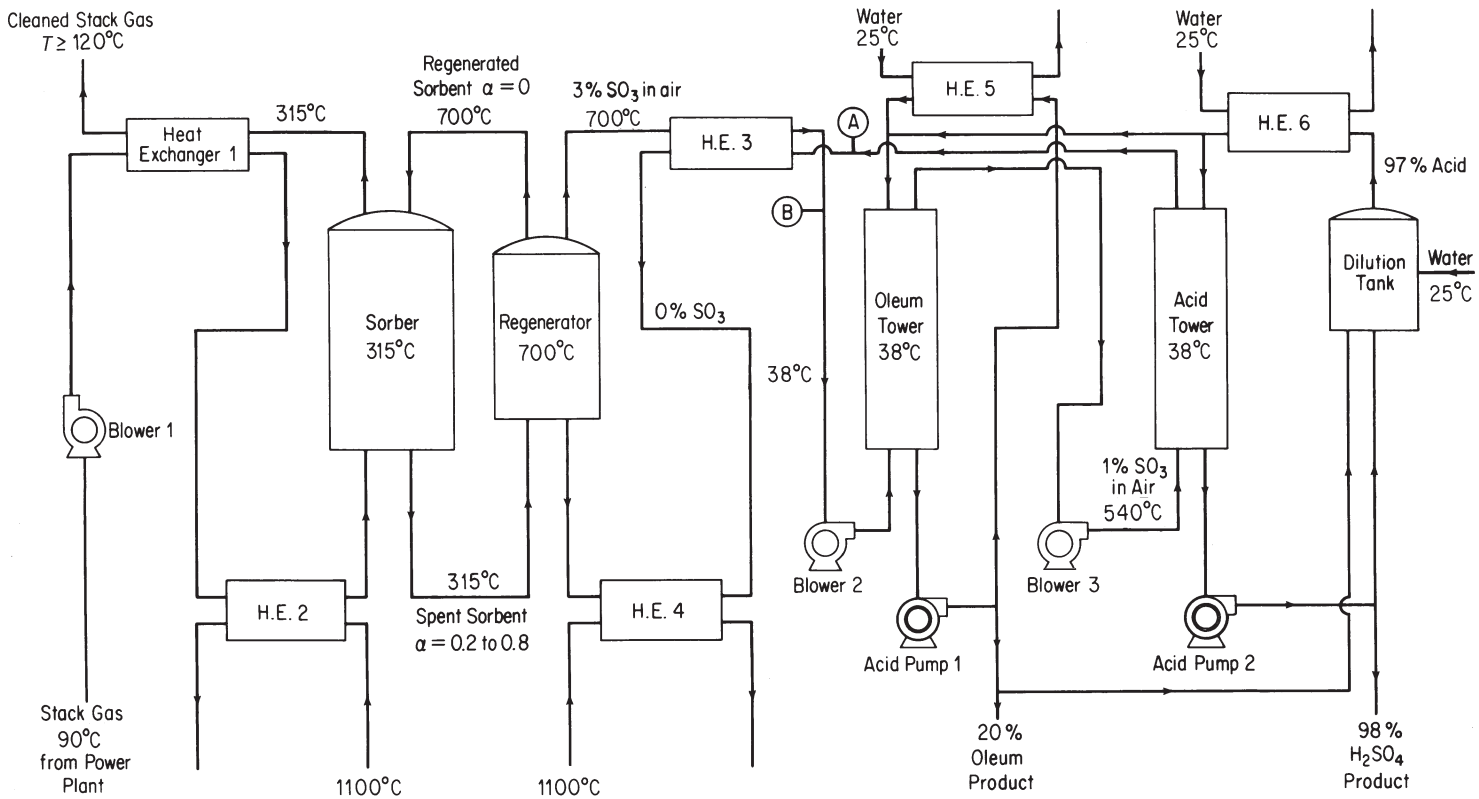


Figure P16.10

temperatures are adjusted by heat exchange with incoming streams. Some of the heat exchangers (nos. 1 and 3) recover heat by countercurrent exchange between the feed and exit streams. Additional heat is provided by withdrawing flue gas from the power plant at any desired high temperature up to 1100°C and then returning it at a lower temperature. Cooling is provided by water at 25°C. As a general rule, the temperature difference across heat-exchanger walls separating the two streams should average about 28°C. The nominal operating pressure of the whole process is 10 kPa. The three blowers provide 6 kPa additional head for the pressure losses in the equipment, and the acid pumps have a discharge pressure of 90 kPa gauge. You are asked to write the material and energy balances and some equipment specifications as follows:

a. Sorber, regenerator, and acid tower. Determine the flow rate, composition, and temperature of all streams entering and leaving.
b. Heat exchangers. Determine the heat load and flow rates, temperatures, and enthalpies of all streams.
c. Blowers. Determine the flow rate and theoretical horsepower.
d. Acid pump. Determine the flow rate and theoretical horsepower.

Use SI units. Also, use a basis of 100 kg of coal burned for all of your calculations; then convert to the operating basis at the end of the calculations.

Power plant operation. The power plant burns 340 metric tons/hr of coal having the analysis given below. The coal is burned with 18% excess air, based on complete combustion to CO_2, H_2O, and SO_2. In the combustion only the ash and nitrogen are left unburned; all the ash has been removed from the stack gas.

Element	Wt %
C	76.6
H	5.2
O	6.2
S	2.3
N	1.6
Ash	8.1

Data on Solids (Units of C_p are J/(g mol)(K); units of H are kJ/g mol)

	Al_2O_3		CuO		$CuSO_4$	
T(K)	C_p	$H_T - H_{298}$	C_p	$H_T - H_{298}$	C_p	$H_T - H_{298}$
298	79.04	0.00	42.13	0.00	98.9	0.00
400	96.19	9.00	47.03	4.56	114.9	10.92
500	106.10	19.16	50.04	9.41	127.2	23.05
600	112.5	30.08	52.30	14.56	136.3	36.23
700	117.0	41.59	54.31	19.87	142.9	50.25
800	120.3	53.47	56.19	25.40	147.7	64.77
900	122.8	65.65	58.03	31.13	151.0	79.71
1000	124.7	77.99	59.87	37.03	153.8	94.98

16.11 When coal is distilled by heating without contact with air, a wide variety of solid, liquid, and gaseous products of commercial importance are produced, as well as some significant air pollutants. The nature and amounts of the products produced depend on the temperature used in the decomposition and the type of coal. At low temperatures (400°C to 750°C) the yield of synthetic gas is small relative to the yield of liquid products, whereas at high temperatures (above 900°C) the reverse is true. For the typical process flowsheet, shown in Figure P16.11:

a. How many tons of the various products are being produced?
b. Make an energy balance around the primary distillation tower and benzol tower.
c. How much (in pounds) of 40% NaOH solution is used per day for the purification of the phenol?
d. How much 50% H_2SO_4 is used per day in the pyridine purification?
e. What weight of Na_2SO_4 is produced per day by the plant?
f. How many cubic feet of gas per day are produced? What percent of the gas (volume) is needed for the ovens?

Products Produced per Ton of Coal Charged	Mean C_p Liquid (cal/g)	Mean C_p Vapor (cal/g)	Mean C_p Solid (cal/g)	Melting Point (°C)	Boiling Point (°C)
Synthetic gas–10,000 ft^3 (555 Btu/ft^3)					
$(NH_4)_2SO_4$, 22 lb					
Benzol, 15 lb	0.50	0.30	—	—	60
Toluol, 5 lb	0.53	0.35	—	—	109.6
Pyridine, 3 lb	0.41	0.28	—	—	114.1
Phenol, 5 lb	0.56	0.45	—	—	182.2
Naphthalene, 7 lb	0.40	0.35	0.281 $+0.00111\,T_{°F}$	80.2	218
Cresols, 20 lb	0.55	0.50	—	—	202
Pitch, 40 lb	0.65	0.60	—	—	400
Coke, 1500 lb	—	—	0.35		—

	ΔH_{vap} (cal/g)	ΔH_{fusion} (cal/g)
Benzol	97.5	—
Toluol	86.53	—
Pyridine	107.36	—
Phenol	90.0	—
Naphthalene	75.5	35.6
Cresols	100.6	—
Pitch	120	—

16.12 A gas consisting of 95 mol % hydrogen and 5 mol % methane at 100°F and 30 psia is to be compressed to 569 psia at a rate of 440 lb mol/hr. A two-stage compressor system has been proposed with intermediate cooling of the gas to 100°F via a heat exchanger. See Figure P16.12. The pressure drop in the heat

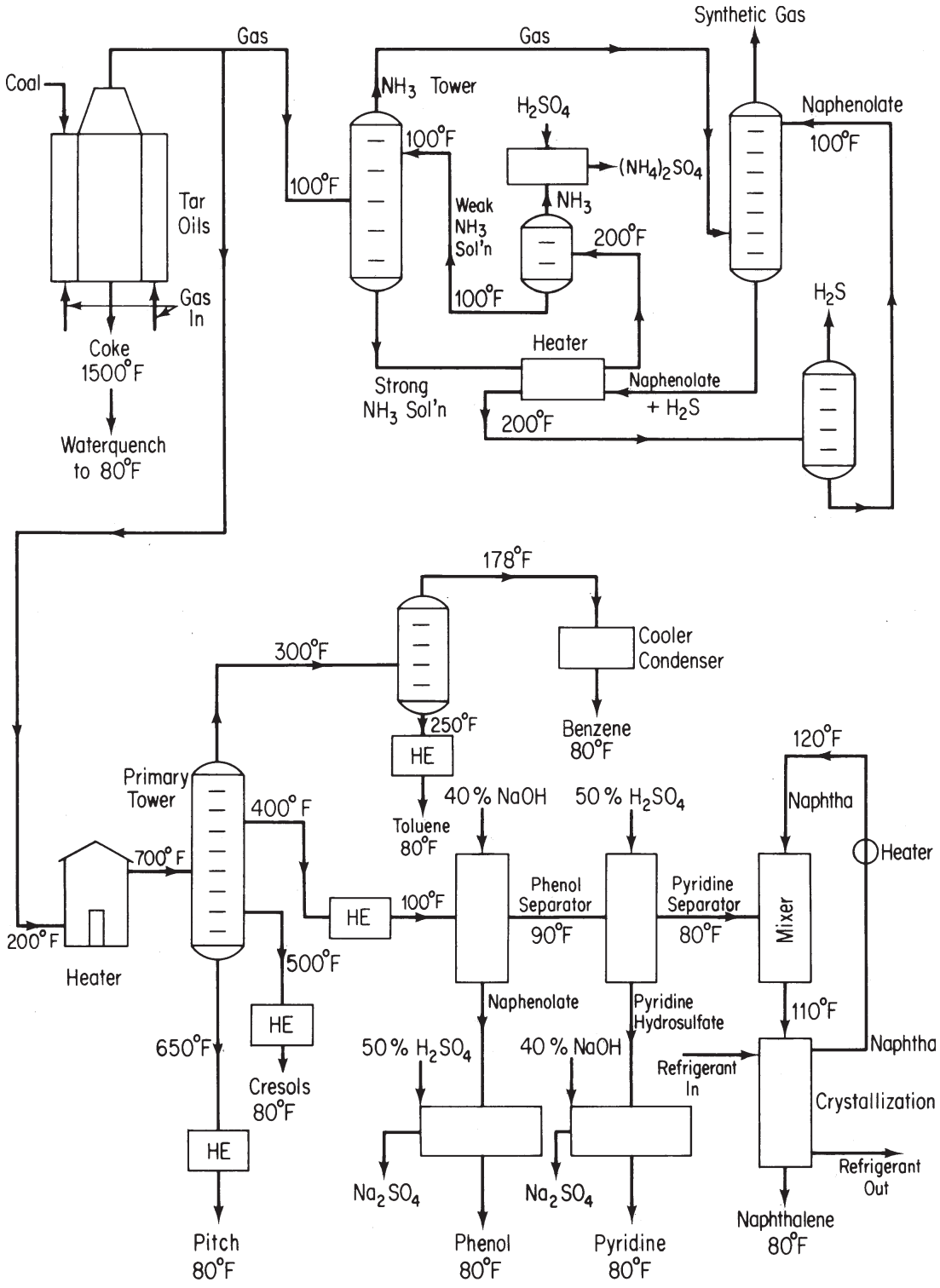


Figure P16.11

exchanger from the inlet stream (*S*1) to the exit stream (*S*2) is 2.0 psia. Using a process simulator program, analyze all of the stream parameters subject to the following constraints: The exit stream from the first stage is 100 psia; both compressors are positive-displacement type and have a mechanical efficiency of 0.8, a polytropic efficiency of 1.2, and a clearance fraction of 0.05.

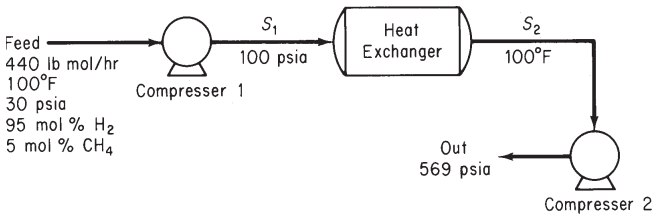


Figure P16.12

16.13 A gas feed mixture at 85°C and 100 psia having the composition shown in Figure P16.13 is flashed to separate the majority of the light from the heavy components. The flash chamber operates at 5°C and 25 psia. To improve the separation process, it has been suggested to introduce a recycle as shown in Figure P16.13. Will a significant improvement be made by adding a 25% recycle of the bottoms? 50%? With the aid of a computer process simulator, determine the molar flow rates of the streams for each of the three cases.

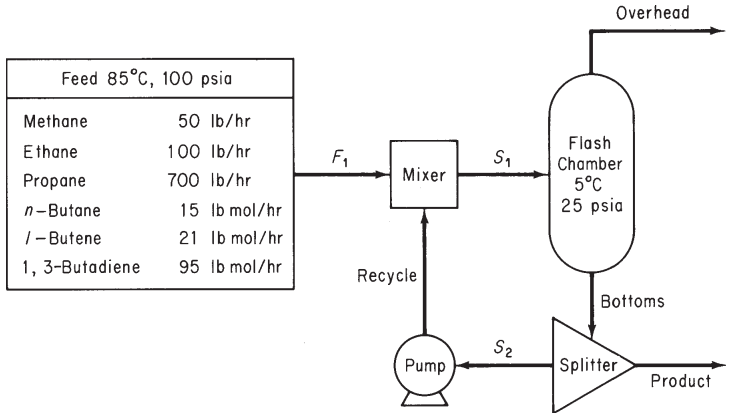


Figure P16.13

16.14 A mixture of three petroleum fractions containing lightweight hydrocarbons is to be purified and recycled back to a process. Each of the fractions is denoted by its normal boiling point: BP135, BP260, and BP500. The gases separated from this feed are to be compressed as shown in Figure P16.14. The inlet feed stream (1) is at 45°C and 450 kPa and has the composition shown. The exit gas (10) is compressed to 6200 kPa by a three-stage compressor process with intercooling of the vapor streams to 60°C by passing through a heat exchanger. The exit pressure for Compressor 1 is 1100 kPa and 2600 kPa for Compressor 2. The efficiencies for Compressors 1, 2, and 3, with reference to an adiabatic compression, are 78%, 75%, and 72%, respectively. Any liquid

fraction drawn off from a separator is recycled to the previous stage. Estimate the heat duty (in kilojoules per hour) of the heat exchangers and the various stream compositions (in kilogram moles per hour) for the system. Note that the separators may be considered as adiabatic flash tanks in which the pressure decrease is zero. This problem has been formulated from *Application Briefs of Process,* the user manual for the computer simulation software package of Simulation Science, Inc.

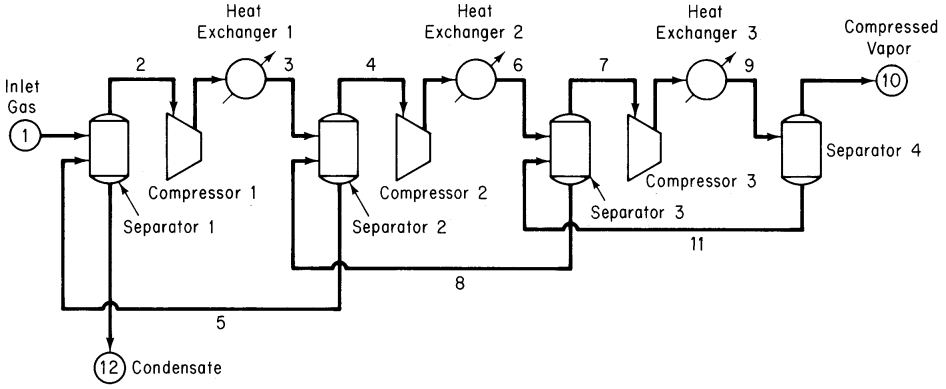


Figure P16.14

Component	kg mol/hr	MW	Sp.Gr.	Normal Boiling Point (°C)
Nitrogen	181			
Carbon dioxide	1920			
Methane	14515			
Ethane	9072			
Propane	7260			
Isobutane	770			
n-Butane	2810			
Isopentane	953			
n-Pentane	1633			
Hexane	1542			
BP135	11975	120	0.757	135
BP260	9072	200	0.836	260
BP500	9072	500	0.950	500

16.15 A demethanizer tower is used in a refinery to separate natural gas from a light hydrocarbon gas mixture stream (1) having the composition listed below. However, initial calculations show that there is considerable energy wastage in the process. A proposed improved system is outlined in Figure P16.15. Calculate the temperature (°F), pressure (psig), and composition (lb mol/hr) of all of the process streams in the proposed system.

Inlet gas at 120°F and 588 psig, stream 1, is cooled in the tube side of a gas-gas heat exchanger by passing the tower overhead, stream 8, through the

shell side. The temperature difference between the exit streams 2 and 10 of the heat exchanger is to be 10°F. Note that the pressure drop through the tube side is 10 psia and 5 psia on the shell side. The feed stream (2) is then passed through a chiller in which the temperature drops to −84°F and a pressure loss of 5 psi results. An adiabatic flash separator is used to separate the partially condensed vapor from the remaining gas. The vapor then passes through an expander turbine and is fed to the first tray of the tower at 125 psig. The liquid stream (5) is passed through a valve, reducing the pressure to that of the third tray on the lower side. The expander transfers 90% of its energy output to the compressor. The efficiency with respect to an adiabatic compression is 80% for the expander and 75% for the compressor. The process requirements are such that the methane-to-ethane ratio in the demethanizer liquids in stream 9 is to be 0.015 by volume; the heat duty on the reboiler is variable to achieve this ratio. A process rate of 23.06×10^6 standard cubic feet per day of feed stream 1 is required.

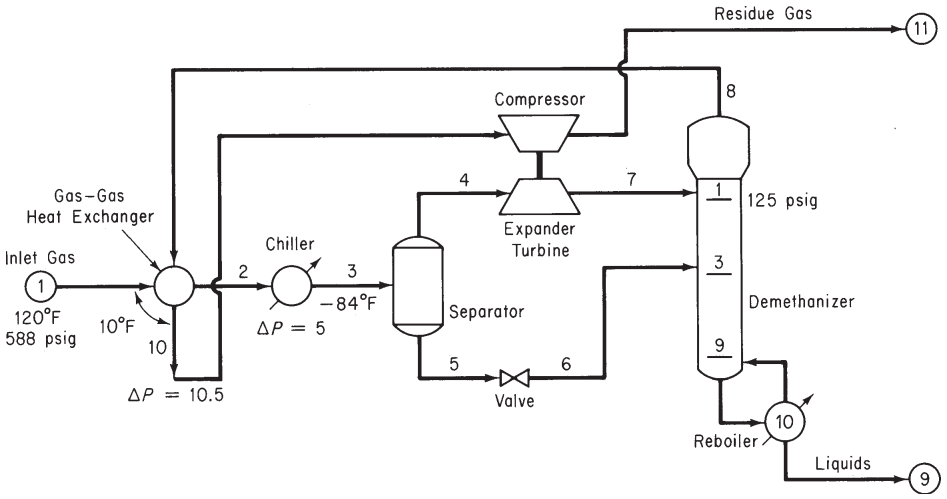


Figure P16.15

Component	Mol %
Nitrogen	7.91
Methane	73.05
Ethane	7.68
Propane	5.69
Isopropane	0.99
n-Butane	2.44
Isopentane	0.69
n-Pentane	0.82
C_6	0.42
C_7	0.31
Total	100.00

The tower has 10 trays, including the reboiler. Note: To reduce the number of trials, the composition of stream 3 may be referenced to stream 1, and if the exit stream of the chiller is given a dummy symbol, the calculation sequence can begin at the separator, thus eliminating the recycle loop.

Carry out the solution of the material and energy balances for the flowsheet in Figure P16.15, determine the component and total mole flows, and determine the enthalpy flows for each stream. Also find the heat duty of each heat exchanger.

This problem has been formulated from *Application Briefs of Process*, the user manual for the computer simulation software package of Simulation Sciences, Inc.

16.16 Determine the values of the unknown quantities in Figure P16.16 by solving the following set of linear material and energy balances that represent the steam balance:

a. $181.60 - x_3 - 132.57 - x_4 - x_5 = -y_1 - y_2 + y_5 + y_4 = 5.1$

b. $1.17x_3 - x_6 = 0$

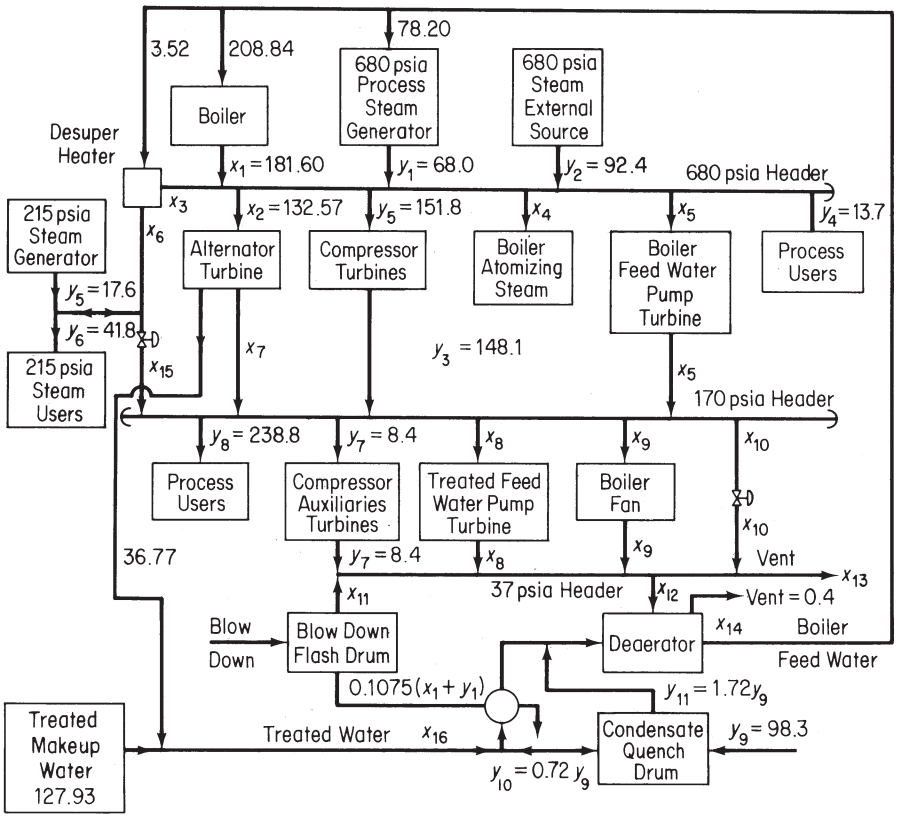


Figure P16.16

c. $132.57 - 0.745x_7 = 61.2$
d. $x_5 + x_7 - x_8 - x_9 - x_{10} + x_5 = y_7 + y_8 = y_3 = 99.1$
e. $x_8 + x_9 + x_{10} + x_{11} - x_{12} - x_{13} = -y_7 = -8.4$
f. $x_6 - x_{15} = y_{12} = y_5 = 24.2$
g. $-1.15(181.60) + x_3 - x_6 + x_{12} + x_{16} = 1.15y_1 - y_9 + 0.4 = -19.7$
h. $181.60 - 4.594x_{12} - 0.11x_{16} = -y_1 + 1.0235y_9 + 2.45 = 35.05$
i. $-0.0423(181.60) + x_{11} = 0.0423y_1 = 2.88$
j. $-0.016(181.60) + x_4 = 0$
k. $x_8 - 0.0147x_{16} = 0$
l. $x_5 - 0.07x_{14} = 0$
m. $-0.0805(181.60) + x_9 = 0$
n. $x_{12} - x_{14} + x_{16} = 0.4 - y_9 = -97.9$

There are four levels of steam: 680, 215, 170, and 37 psia. The 14 x_i, $i = 3, \ldots, 16$, are the unknowns and the y_i are given parameters for the system. Both x_i and y_i have the units of 10^3 lb/hr.