	Flow Rate (lbmol/hr)			
Species	Reactor Product Stream	Product 1	Product 2	Product 3
H_2	1.5	1.5		
CH_4	19.3	19.2	0.1	
C_6H_6	262.8	1.3	258.1	3.4
C_7H_8	84.7		0.1	84.6
$C_{12}H_{10}$	5.1			5.1

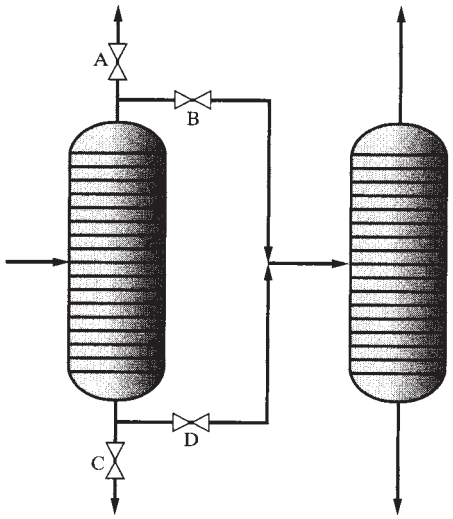

Figure 4.22 Toluene hydrodealkylation process-distillation section.

purge/recycle ratio, which should be adjusted to determine its impact on the recirculation rat equipment sizes, power requirements, and so on; see Exercise 4.4 for this purpose. It is als recommended that the amount of hydrogen added to the process feed stream be adjusted to th amount of hydrogen leaving in the purge stream. This can be accomplished in ASPEN PLU using a design specification. Also, the initial guesses for the recycle streams can be set equ to the values assumed when simulating the reactor section of the process. For the distillatio columns, the RADFRAC subroutine can be used for simulation with the number of stages an the reflux ratio previously calculated by the DSTWU subroutine. See the module *ASPEN – Separators → Distillation → MESH Equations → RADFRAC* on the multimedia CD-RO for an example using the RADFRAC subroutine. In HYSYS.Plant, the **Column** model i used, as described in the module *HYSYS → Separations → Distillation → Column Setup.*

As mentioned in Section 3.5, "Development of the Base-Case Design," the simulatio model prepared for the complete process is often the source of the stream conditions in th PFD (e.g., Figure 3.19). Furthermore, as the design team completes the process integratio step, the model can be improved to represent the more complete PFD.

In this section, several subroutines have been recommended for usage with ASPEN PLU and HYSYS.Plant. These recommendations can be extended readily to permit the simula tions to be carried out with CHEMCAD or PRO/II.

4.4 STEADY-STATE SIMULATION OF THE MONOCHLOROBENZENE SEPARATION PROCESS

Another process, which is considered throughout this text, involves the separation of a mix ture consisting of HCl, benzene, and monochlorobenzene (MCB), the effluent from a reacto to produce MCB by the chlorination of benzene. As discussed in Chapter 7, when separatin a light gaseous species, such as HCl, from two heavier species, it is common to vaporize th

feed partially, followed by separation of the vapor and liquid phases in a *flash separator*. To obtain nearly pure HCl, the benzene and MCB can be absorbed in an absorber. Then, since benzene and MCB have significantly different boiling points, they can be separated by distillation. The process that results from this synthesis strategy is shown in Figure 4.23. Included on the diagram is the design basis (or specifications). Note that a portion of the MCB product is used as the absorbent.

As shown in the flowsheet, the feed is partially vaporized in the preheater, H1, and separated into two phases in the flash vessel, F1. The vapor from F1 is sent to the absorber, A1, where most of the HCl vapor passes through, but the benzene is largely absorbed using recycled MCB as the absorbent. The liquid effluents from F1 and A1 are combined, treated to remove the remaining HCl with insignificant losses of benzene and MCB, and distilled in D1 to separate benzene from MCB. The distillate rate is set equal to the benzene flow rate in the feed to D1, and the reflux ratio is adjusted to obtain the indicated MCB impurity in the distillate. The bottoms are cooled to 120°F in the heat exchanger, H2, after which one-third of the bottoms is removed as MCB product, with the remaining two-thirds recycled to the absorber. Note that this fraction recycled is specified during the *distribution of chemicals* in process synthesis, along with the temperature of the recycle, in an attempt to absorb benzene without sizable amounts of HCl. Furthermore, the temperature of stream S02 is specified to generate an adequate amount of vapor, three equilibrium stages are judged to be sufficient for the absorber (using the approximate Kremser–Brown equations), and the number of stages and the reflux ratio are estimated for the distillation column. Using the process

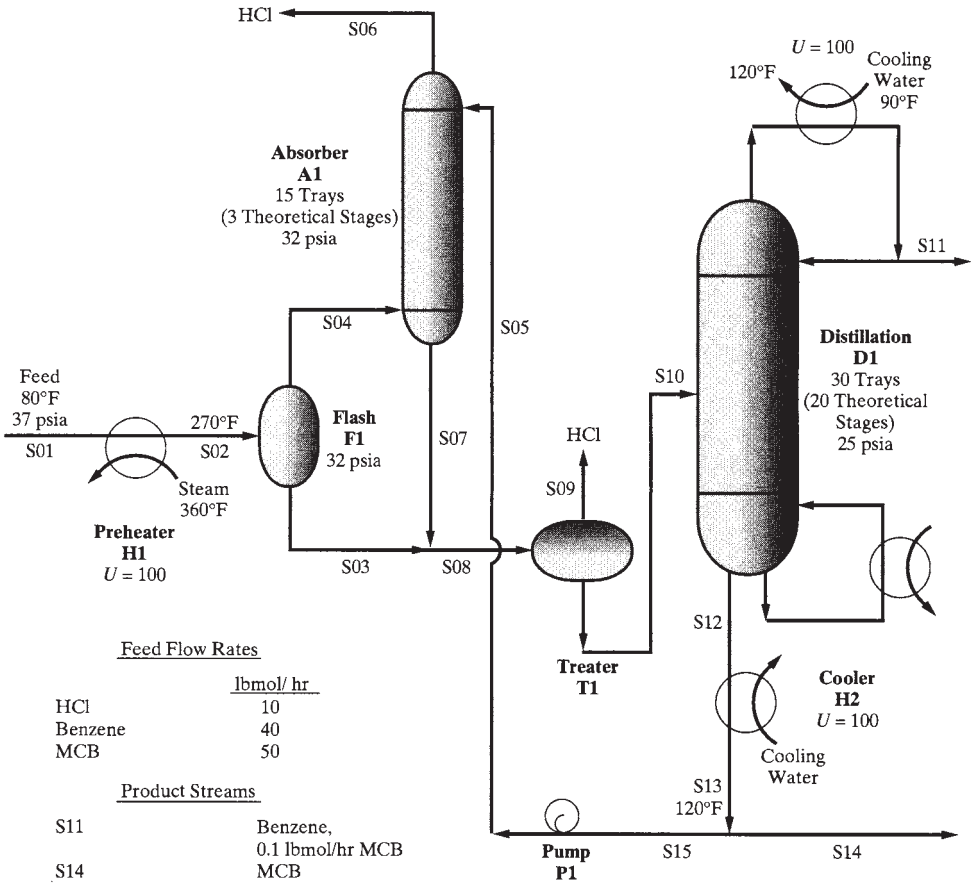

Figure 4.23 Process flowsheet for the MCB separation process.