King Fahd University of Petroleum & Minerals

Department of Chemical Engineering

CHE 425

Engineering Economics and Design Principles

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CHAPTER 11

Synthesis of a Process Using a Simulator and Simulator Troubleshooting

Introduction

Past

- Material and energy balances done with hand
- Design achieved through:
  - Simplified analyses
  - Shortcut method
  - Years of experience

Present

- Design done with process simulators
- Example of simulators:
  - CHEMCAD
  - ASPEN PLUS
  - ASPEN HYSYS
  - PRO/II

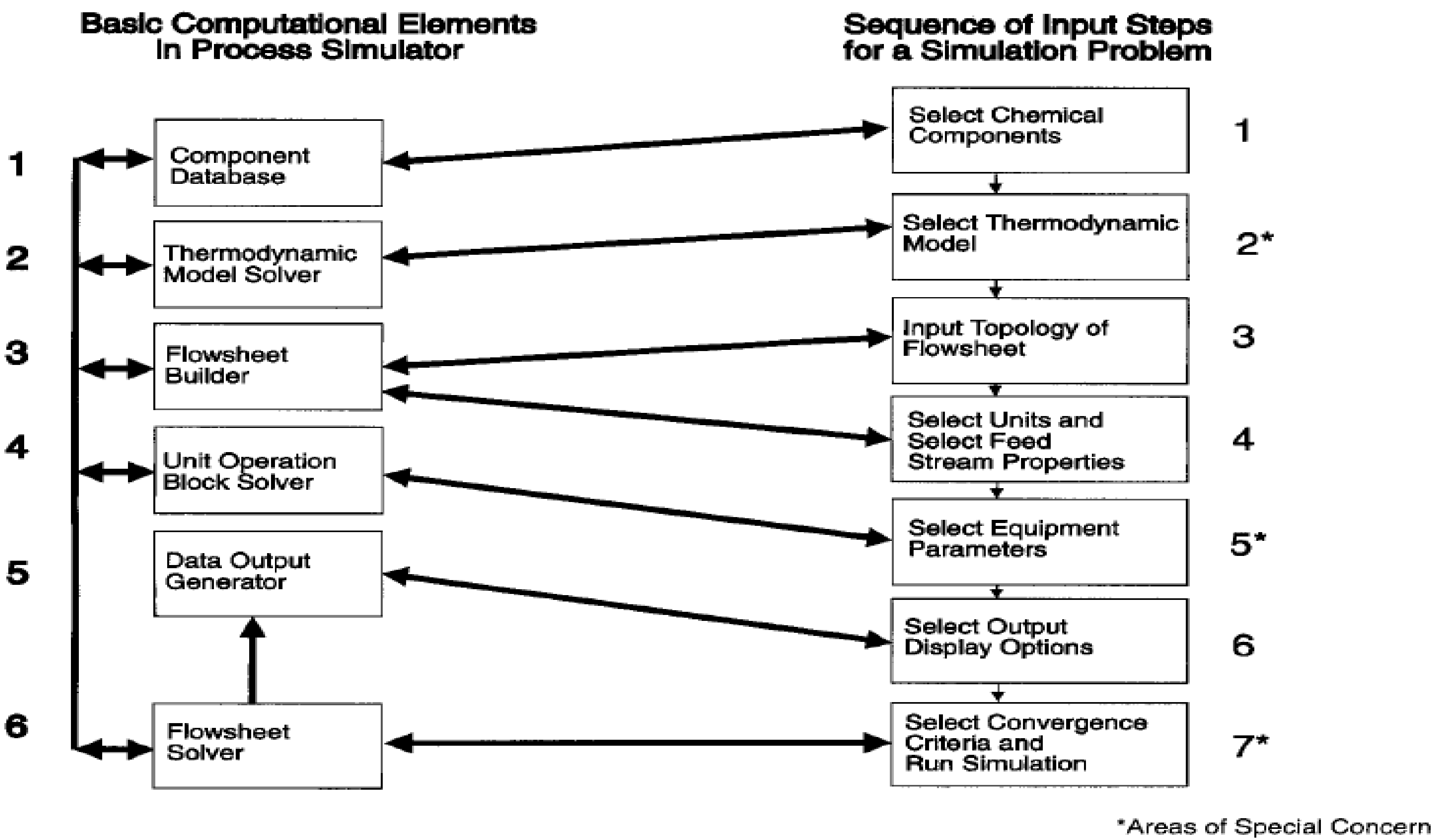
Process Simulator

- Simulation software is a great asset to the experienced engineer.
- However, it can be potentially dangerous in the hands of a neophyte engineer.
- <u>NOTE:</u> The engineer is responsible for analyzing the results from the simulator.

Purpose of the Chapter

- Emphasize the general approach of setting up processes.
- Highlight common problems encountered by users of process simulators.
- Offer solutions to the problems.

The Structure of Process Simulator



Types of Solution Algorithms

- Sequential Modular
- Equation Solving (Simultaneous nonmodular)
- Simultaneous Modular

The Sequential Modular Algorithm is the Most Widely Used.

Sequential Modular Simulator

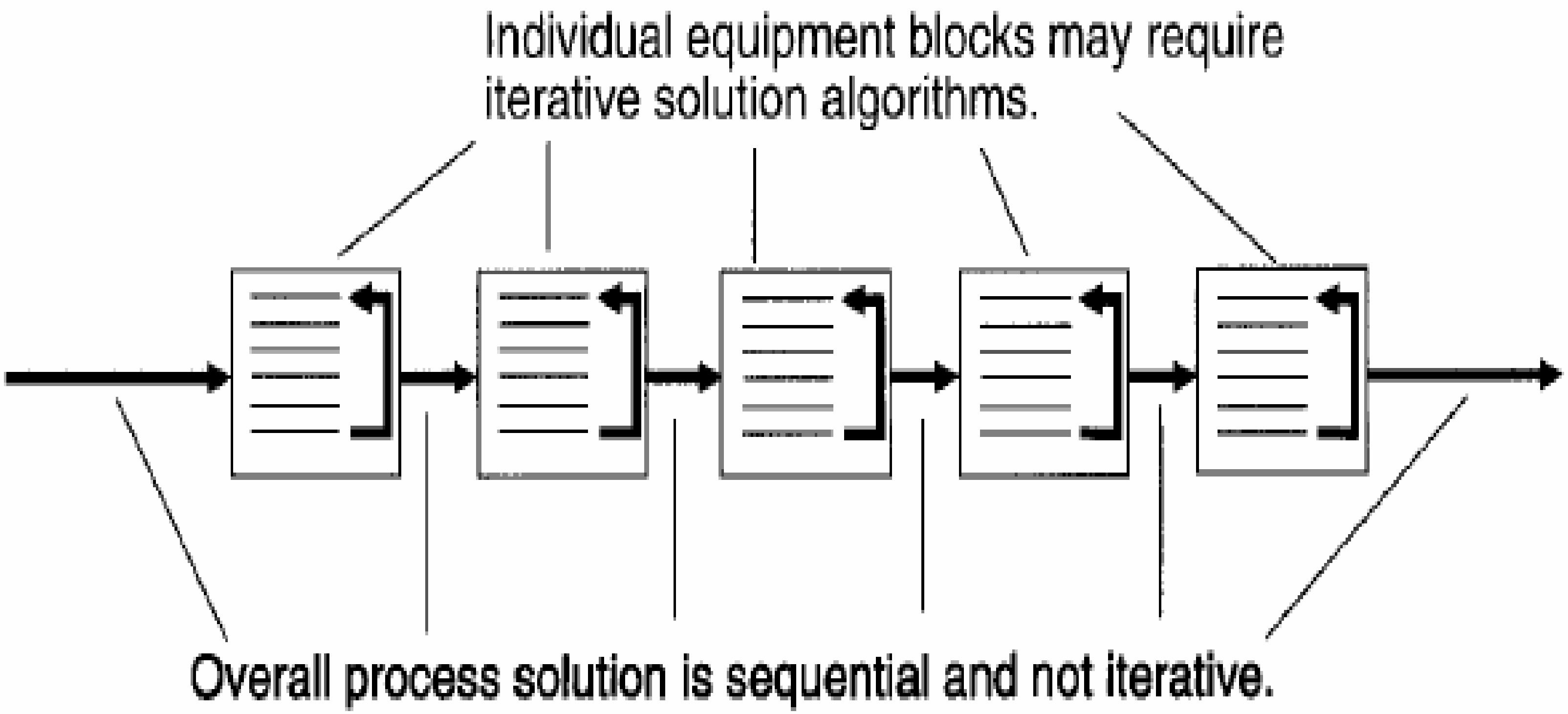


Figure 11.2 Solution Sequence Using Sequential Modular Simulator for a Process Containing No Recycles

Use of Tear Streams

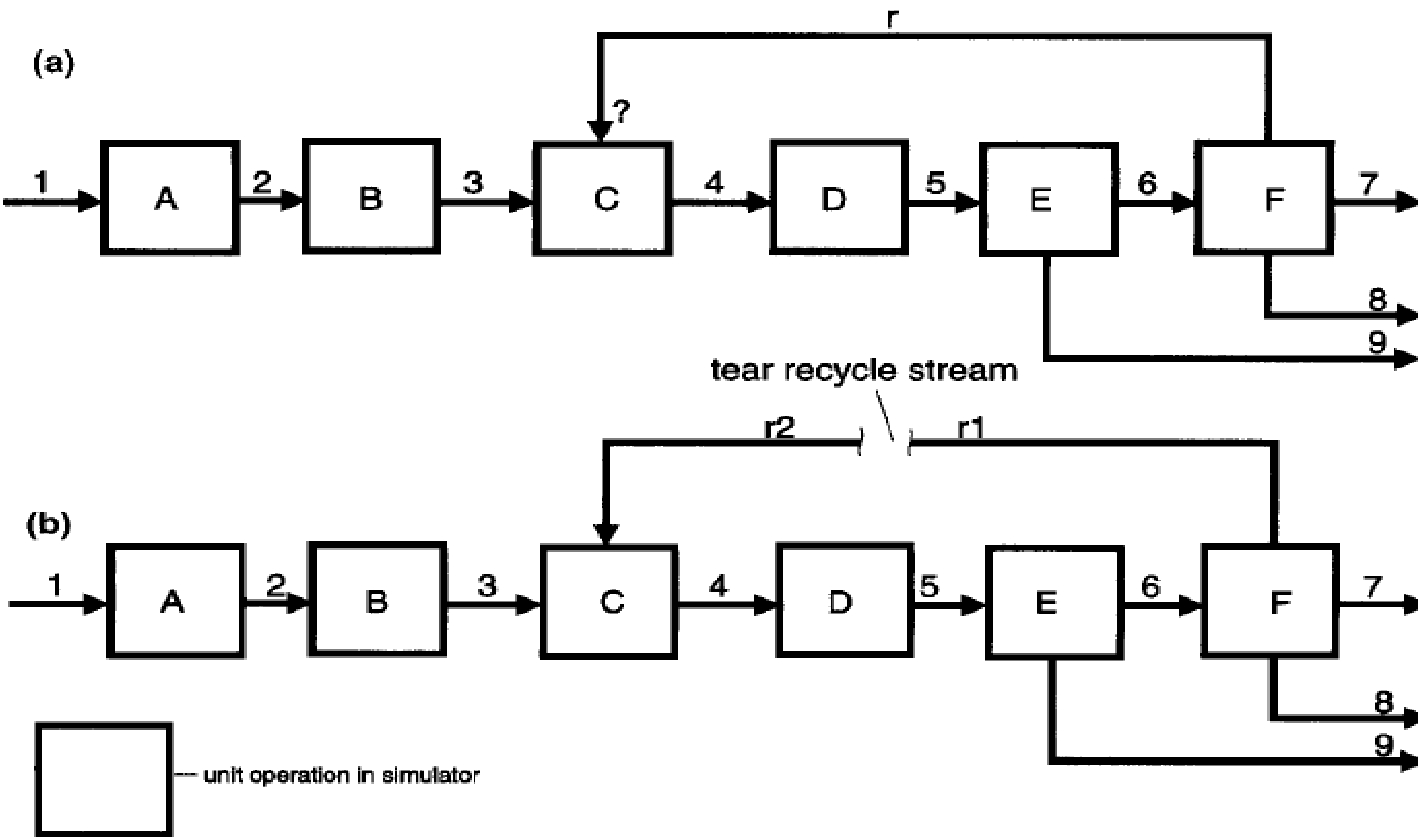


Figure 11.3 The Use of Tear Streams to Solve Problems with Recycles Using the Sequential Modular Algorithm

INFORMATION REQUIRED TO COMPLETE A PROCESS SIMULATION – INPUT DATA

- Selection of Chemical Components
- Selection of Physical Property Model(s)
- Input Topology of the Flowsheet
- Select Feed Stream Properties
- Select Equipment Parameters
- Selection of Output Display Options
- Selection of Convergence Criteria and Running the Simulation

Selection of Chemical Components

- **Identify all components**
  - **Inerts, Reactants, Products, By-Products, Utilities and Waste Products.**
- **Simulators contain databank of many components**
- **"User added components" - For components not available in the simulator databank.**

Selection of Physical Property Model(s)

- Selecting the best physical property model is an extremely important part of any simulation.
- Wrong property package ➡ Wrong results
- Physical Properties (Pure & Mixtures)
  - Transport Properties (Viscosity, Thermal Conductivity, Diffusivity)
  - Thermodynamic Properties (Enthalpy, Fugacity, K-Factors, Critical Constants)
  - Other Properties (Density, Mol Wt., Surface Tension)
- All simulators have built-in procedures to estimate pure component properties from group-contribution and other techniques.

Example 11.1

Example 11.1

Consider the HCl absorber (T-602) in the separation section of the allyl chloride process, Figure C.3 (Appendix C, on the CD). This equipment is shown in Figure E11.1. The function of the absorber is to contact countercurrently Stream 10a, containing mainly propylene and hydrogen chloride, with water, Stream 11. The HCl is highly soluble in water and is almost completely absorbed to form 32 wt% hydrochloric acid, Stream 12. The gas leaving the top of the absorber, Stream 13, is almost pure propylene which is cleaned and then recycled.

Example 11.1 (cont.)

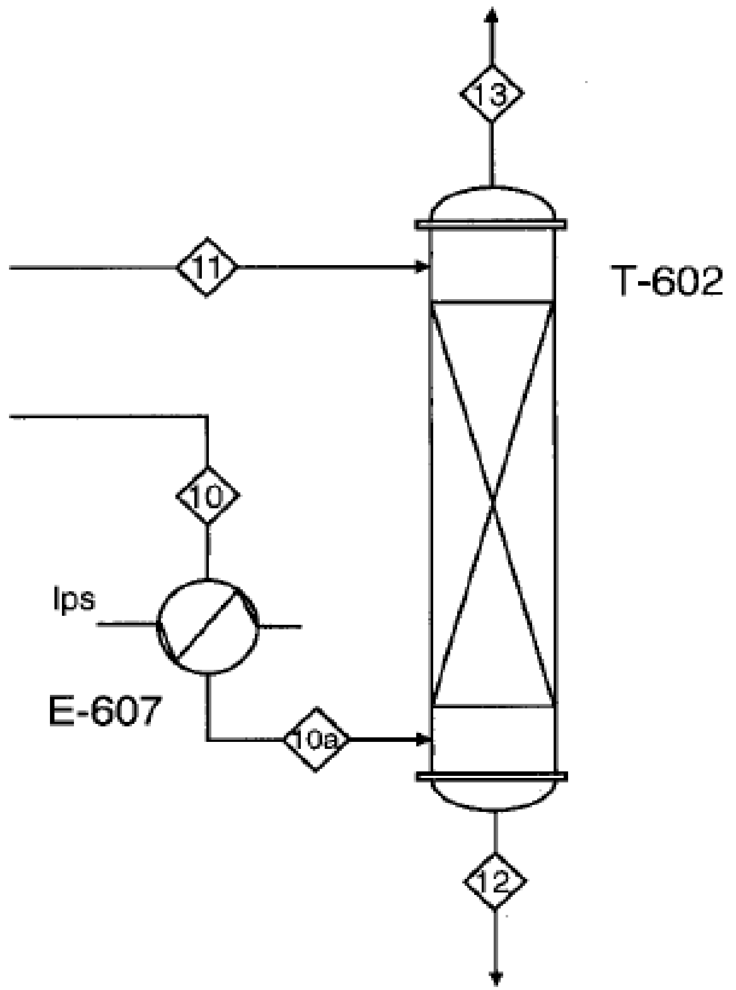


Figure E11.1 HCl Absorber in Allyl Chloride Separation Section (Unit 600)

Example 11.1 (cont.)

Table E11.1 Results of Simulation of HCl Absorption Using Two Different Physical Property Models

Phase Component Flows (kmol/h)	Using SRK Model		Using PPAQ* Model	
	Stream 12 Liquid	Stream 13 Vapor	Stream 12 Liquid	Stream 13 Vapor
Propylene	0.05	57.48	—	57.53
Allyl chloride	0.01	—	0.01	—
Hydrogen chloride	0.91	18.78	19.11	0.58
Water	81.37	0.63	81.88	0.12
Total	82.34	76.89	101.00	58.23

*This is a model used in the CHEMCAD™ simulator especially for HCl-water and similar systems.

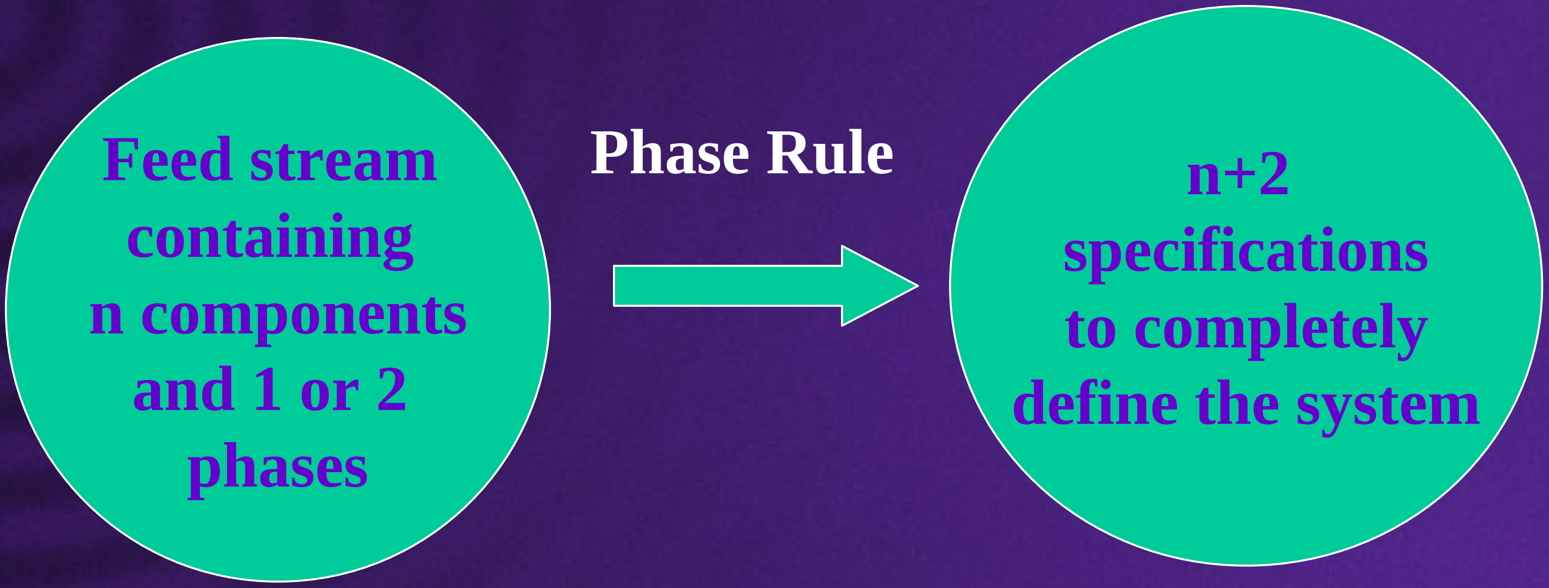
"You absolutely must have confidence in the thermodynamics that you have chosen to represent your chemicals and unit operations. This is your responsibility, not that of the software simulation package. If you relinquish your responsibility to the simulation package, be prepared for dire consequences."

Input the Topology of the Flowsheet

- **Make a sketch on paper and have it in front of you when you construct the flowsheet in the simulator.**
- **Every time streams combine ADD a “mixer”.**
- **Every time streams split ADD a “splitter”.**

Select Feed Stream Properties

- **Sequential modular approach requires that:**
  - **All feed streams must be specified.**
  - **Estimates of recycle streams should be made.**



Select Feed Stream Properties (cont.)

System	No of components In the Feed	No of Phases	Specification to completely define the system
I	1	2	Flowrate+vf+T Flowrate+vf+P
II	n	1	n components flowrates+T+P
III	n	2	n components flowrates+T+P n components flowrates+vf+P n components flowrates+vf+T **Note:** Avoid specifying vf for multi components system

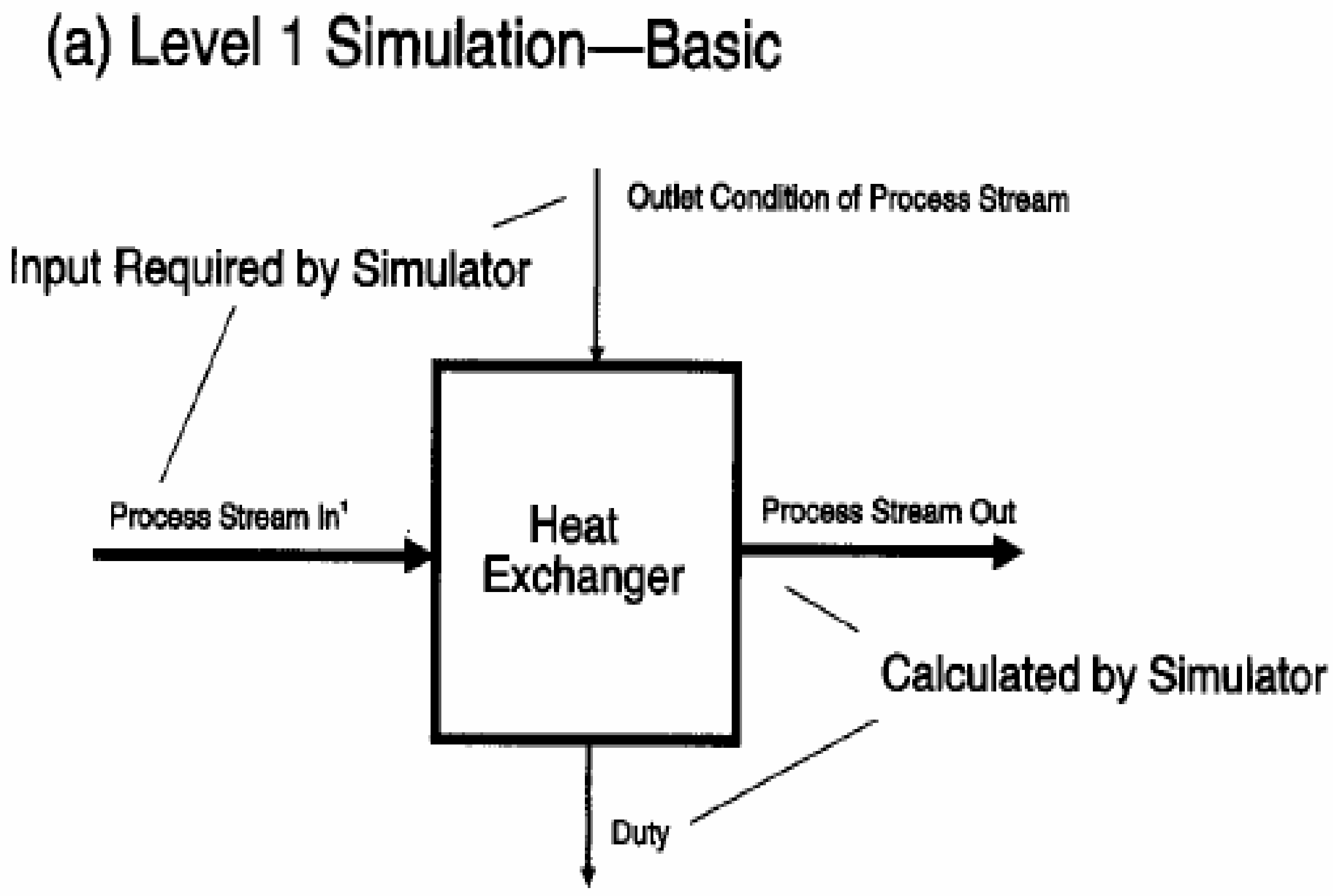
Select Feed Stream Properties (cont.)

Use the vapor fraction (*vf*) to define feed streams only for saturated vapor (*vf* = 1), saturated liquid (*vf* = 0), and two-phase, single-component (0 < *vf* < 1) streams.

Select Equipment Parameters

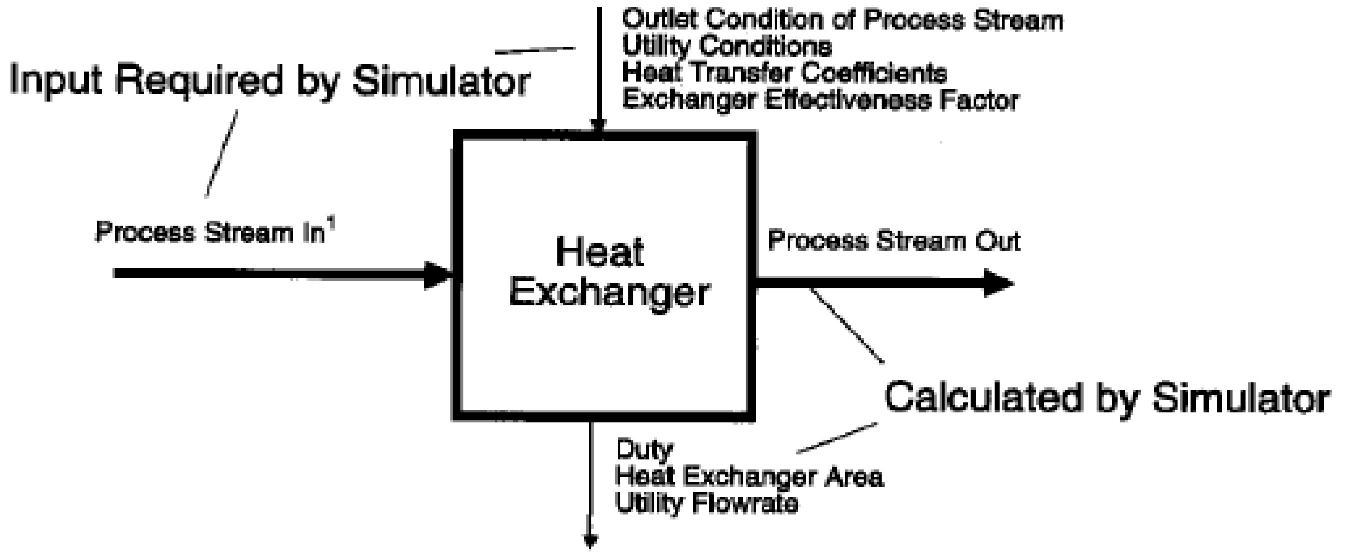
When first simulating a process, input only the data required to perform the material and energy balances for the process.

Select Equipment Parameters (cont.)



Select Equipment Parameters (cont.)

(b) Level 2 Simulation—Design/Perfomance



[1] This information may come from the preceding unit operation and thus would be supplied automatically by the simulator.

Figure 11.4 Information Required for Different Levels of Simulation

Select Equipment Parameters (cont.)

Information Required for Level 1 Simulation

- **Pumps**
  - Discharge Pressure or ΔP.
- **Compressors and Turbines**
  - Pressure of leaving stream or ΔP
  - Mode of compression or expansion
    - Adiabatic
    - Isothermal
    - Polytropic

Select Equipment Parameters (cont.)

Information Required for Level 1 Simulation

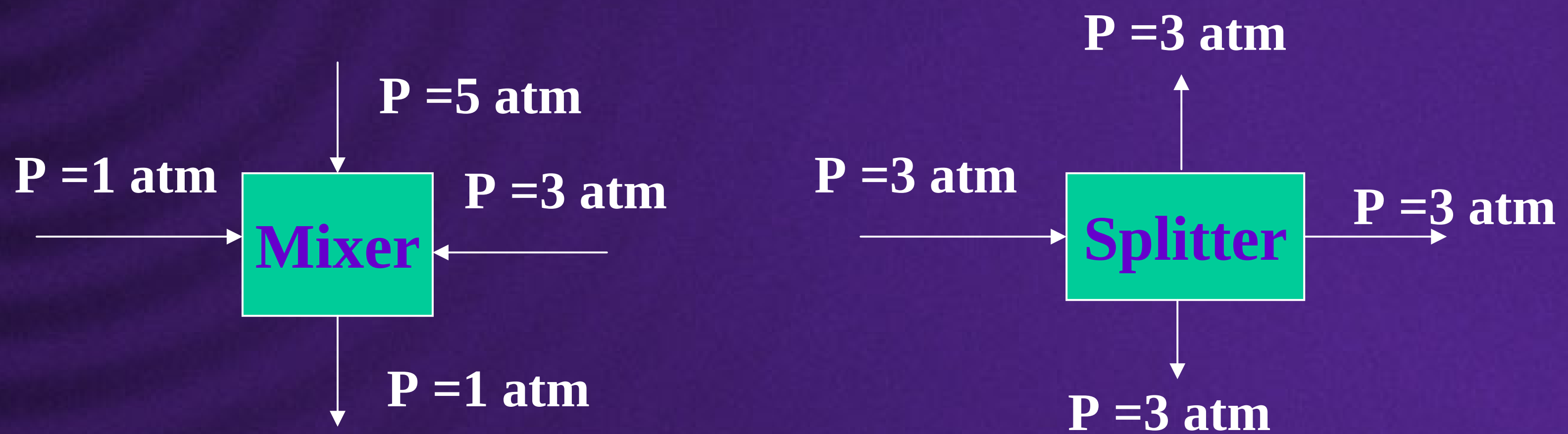
- **Heat Exchangers (single process stream) and Fired Heaters**
  - **Condition of exit process stream.**
    - **T & P (single-phase exit condition)**
    - **P & vf (two-phase exit condition)**

- **Heat Exchangers (Multiple process streams)**
  - **Exit conditions of both streams**
  - **Beware of temperature crosses**

Select Equipment Parameters (cont.)

Information Required for Level 1 Simulation

- **Mixers and Splitters**
  - Either outlet pressure or ΔP across device.
  - Usually ΔP is assumed to be zero.
  - For splitters, information on relative flow of the output streams is needed.



Select Equipment Parameters (cont.)

Information Required for Level 1 Simulation

- **Valves**
  - Either outlet pressure or ΔP across device.

- **Reactors:**
  - Stoichiometric Reactor
    - Number and stoichiometry of reactions, T, P, Conversion of the limiting reactant.
  - Kinetic Reactor (PFR or CSTR)
    - Number and stoichiometry of reactions, Kinetics contants and Rate law.
  - Equilibrium Reactor
    - Number and stoichiometry of reactions, Fractional approch to equilibrium, Equilibrium constants.

Select Equipment Parameters (cont.)

Information Required for Level 1 Simulation

- **Flash Units**
  - Two parameters must be specified: Either
    - T & P .
    - T and heat load
    - P and V/L ratio

- **Distillation Column**
  - Short-cut Module
    - Identification of key components
    - Fractional recovery of key components in the overhead product
    - Colum pressure and pressure drop
    - Ratio of actual to minimum reflux ratio
  - Rigorous Module
    - Number of theroretical plates
    - Condenser and reboiler type
    - Column pressure and pressure drop
    - Feed tray and side products locations
    - NOTE: Total number of specifications = Number of products produced

Example 11.2

Example 11.2

Consider the benzene recovery column in the toluene hydrodealkylation process shown in Figure 1.5. This column is redrawn in Figure E11.2. The purpose of the column is to separate the benzene product from unreacted toluene, which is recycled to the front end of the process. The desired purity of the benzene product is 99.6 mol%. The feed and the top and bottom product streams are presented in the following table, which is taken from Table 1.5.

There are many ways to specify the parameters needed by the rigorous column algorithm used to simulate this tower. We give two examples:

1. We identify the key components for the main separation as benzene and toluene. We specify the composition of the top product to be 99.6 mole% benzene and that the recovery of toluene in the bottom product is 0.98.

2. We specify the top composition to be 99.6 mol% benzene and that the recovery of benzene in the bottom product is 0.01.

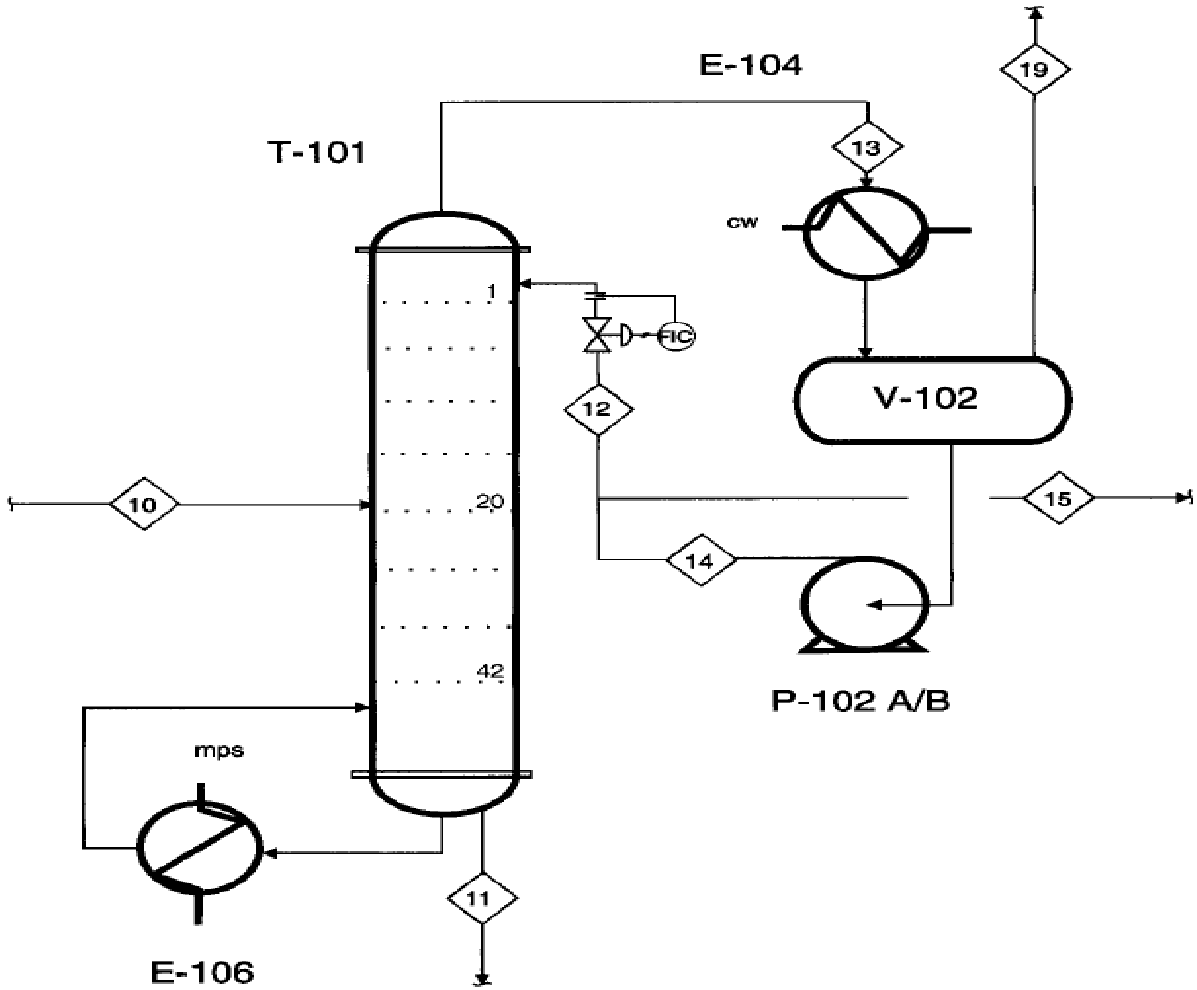


Figure E11.2 Benzene Column in Toluene Hydrodealkylation Process (from Figure 1.5)

Example 11.2 (cont.)

Component	Stream 10	Stream 15	Stream 19	Stream 11
Hydrogen	0.02	—	0.02	—
Methane	0.88	—	0.88	—
Benzene	106.3	105.2	—	1.1
Toluene	35.0	0.4	—	34.6

Example 11.2 (cont.)

The first specification violates the material balance whereas the second specification does not. Looking at the first specification we see that if 98% of the toluene in the feed is recovered in the bottom product, then 2% or 0.7 kmol/h must leave with the top product. Even if the recovery of benzene in the top product were 100%, this would yield a top composition of 106.3 kmol/h benzene and 0.7 kmol/h of toluene. This corresponds to a mole fraction of 0.993. Therefore, the desired mole fraction of 0.996 can never be reached. Thus, by specifying the recovery of toluene in the bottom product, we automatically violate the specification for the benzene purity.

Looking at the second specification, we see that we can achieve both specifications and not violate the material balance. The top product contains 99% of the feed benzene (105.2 kmol/h) and 0.4 kmol/h toluene, which gives a top composition of 99.6 mol% benzene. The bottom product contains 1.0% of the feed benzene (1.1 kmol/h) and 34.6 kmol/h of toluene.

When giving the top and bottom specifications for a distillation column, make sure that the specifications do not violate the material balance.

Select Equipment Parameters (cont.)

Information Required for Level 1 Simulation

- **Absorbers and Strippers**
  - Simulated using rigorous distillation module
  - Main differences with distillation:
    - No condenser and reboiler
    - Two feeds to the unit: One feed enters at the top and the other at the bottom.
- **Liquid-Liquid Extractors**
  - Simulated using rigorous tray-tray module
  - Thermodynamic model must be capable of predicting two-liquid phases.

Selection of Output Display Options

- Report profile can be generated and customized to include wide variety of steam and equipment information.

- The followings can also be generated
  - Simulation flowsheet
  - T-Q diagram for heat exchangers
  - Vapor and liquid flows
  - Temperature and composition profiles (tray-by-tray)
  - Various types of phase diagrams

Selection of Convergence Criteria

- Most important criteria.
  - Number of iterations
  - Tolerance
- Note: Unless specific problems arise, use default values set in the simulator.

If the simulation has not converged, the results do not represent a valid solution and should not be used.

Selection of Convergence Criteria (cont.)

Reasons for non-convergence

- The problem has been ill-poised.
- The tolerance for the solution has been set too tightly.
- The number of iterations is not sufficient for convergence.

> The most common reason for the failure of a simulation to converge is the use of incorrect or impossible equipment specifications.