Analysis, Synthesis, and Design of Chemical Processes

Fifth Edition

Richard Turton | Joseph A. Shaeiwitz
Debangsu Bhattacharyya| Wallace B. Whiting

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To the memory of Richard (Dick) C. Bailie (1928–2014)
Colleague, Friend, and Mentor

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Preface

This book represents the culmination of many years of teaching experience in the senior design course at West Virginia University (WVU), Auburn University, and the University of Nevada, Reno. The program at WVU has evolved over the past 30 years and is still evolving, and the authors continue to integrate design throughout the undergraduate curriculum in chemical engineering.

We view design as the focal point of chemical engineering practice. Far more than the development of a set of specifications for a new chemical plant, design is the creative activity through which engineers continuously improve the operations of facilities to create products that enhance the quality of life. Whether developing the grassroots plant, proposing and guiding process modifications, or troubleshooting and implementing operational strategies for existing equipment, engineering design requires a broad spectrum of knowledge and intellectual skills to be able to analyze the big picture and the minute details and, most important, to know when to concentrate on each.

Our vehicle for helping students develop and hone their design skills is process design covering synthesis of the entire chemical process through topics relating to the preliminary sizing of equipment, flowsheet optimization, economic evaluation of projects, and the operation of chemical processes. The purpose of this text is to assist chemical engineering students in making the transition from solving well-posed problems in a specific subject to integrating all the knowledge that they have gained in their undergraduate education and applying this information to solving open-ended process problems.

In the fifth edition, we have replaced the majority of Section IV, Analysis of Process Performance. In previous editions, process performance was explained through a series of increasingly complex case studies. The approach adopted in the fifth edition is to provide a more logical pedagogy for the design of basic process equipment including pipes, pumps, and compressors (Chapter 19); heat exchangers (Chapter 20); separation equipment (Chapter 21); reactors (Chapter 22); and process vessels and steam ejectors (Chapters 23). Each chapter starts out with the design procedure and basic equations needed to design the equipment. At the end of each chapter, examples of performance (or rating) problems are given. The purpose of these chapters is to review the key concepts needed in the design and then show how to analyze systems in which the equipment already exists. It may be tempting to solve the performance of existing equipment using the process simulator, but using steady-state simulators to model these changes in equipment performance can be difficult. Dynamic simulators are the preferred method for simulating performance changes but are rarely used in the undergraduate curriculum. Therefore, we regard the material on equipment performance included in Section IV to be an essential part of the undergraduate design

experience and encourage educators to adopt some if not all of this material in the design course or courses in each specific area that are often taught in the junior year. The content for Chapters 19–23 is taken from the book *Chemical Process Equipment Design* by Turton and Shaeiwitz (ISBN-13: 978-0-13-380447-8).

In addition to the changes in Chapters 19–23, a section on advanced optimization has been added to the chapter on advanced concepts in steady-state simulation (Chapter 16).

The arrangement of chapters into the six sections of the book is similar to that adopted in the fourth edition. These sections are as follows:

- Section I—Conceptualization and Analysis of Chemical Processes
- Section II—Engineering Economic Analysis of Chemical Processes
- Section III—Synthesis and Optimization of Chemical Processes
- Section IV—Chemical Equipment Design and Performance
- Section V—The Impact of Chemical Engineering Design on Society
- Section VI—Interpersonal and Communication Skills

In Section I, the student is introduced first to the principal diagrams that are used to describe a chemical process. Next, the evolution and generation of different process configurations are covered. Key concepts used in evaluating batch processes are included in Chapter 3, and the concepts of product design are given in Chapter 4. Finally, the analysis of existing processes is covered. In Section II, the information needed to assess the economic feasibility of a process is covered. This includes the estimation of fixed capital investment and manufacturing costs, the concepts of the time value of money and financial calculations, and finally the combination of these costs into profitability measures for the process. Section III covers the synthesis of a chemical process. The minimum information required to simulate a process is given, as are the basics of using a process simulator. The choice of the appropriate thermodynamic model to use in a simulation is covered, and the choice of separation operations is covered. Process optimization (including an introduction to optimization of batch processes) and heat integration techniques are covered in this section. In addition, advanced concepts using steady-state process simulators (Chapter 16), the use of dynamic simulators (Chapter 17), and process regulation (Chapter 18) are included in Section III. In Section IV, the analysis of the design of process equipment and the performance of existing process equipment is covered. The presentation of this material has changed substantially from all previous editions and was discussed previously. In Section V, the impact of chemical engineering design on society is covered. The role of the professional engineer in society is addressed. Separate chapters addressing ethics and professionalism, health, safety, and the environment, and green engineering are included. Finally, in Section VI, the interpersonal skills required by the engineer to function as part of a team and to communicate both orally and in written form are covered. An entire chapter is devoted to addressing some of the common mistakes that students make in written reports.

Finally, three appendices are included. Appendix A gives a series of cost charts for equipment. This information is embedded in the CAPCOST program for evaluating fixed capital investments and process economics. Appendix B gives the preliminary design information for 15 chemical processes: dimethyl ether, ethylbenzene, styrene, drying oil, maleic anhydride, ethylene oxide, formalin, batch manufacture of amino acids, acrylic acid, acetone, heptenes production, shift reaction, acid-gas removal by a physical solvent, the removal of H_2S from a gas stream using the Claus process, and finally coal gasification. This information is used in many of the end-of-chapter problems in the book. These processes can also be used as the starting point for more detailed analyses—for example, optimization studies. Other projects, given in Appendix C, are

also included. The reader (faculty and students) is also referred to our Web site at https://richardturton.faculty.wvu.edu/projects, where a variety of design projects for sophomore-through senior-level chemical engineering courses is provided. In addition, a revised CAPCOST program is also available at https://richardturton.faculty.wvu.edu/publications/analysis-synthesis-and-design-of-chemical-processes-5th-edition as well as the HENSAD program and the virtual plant tour. It should be noted that revisions to the CAPCOST program will appear periodically on the Web site.

The structure of the senior-year design course obviously varies with each instructor. However, the following coverage of materials is offered as suggestions. For a one-semester design course, we recommend including the following core:

- Section I—Chapters 1 through 6
- Section III—Chapters 11, 12, and 13
- Section V—Chapters 25 and 26

For programs in which engineering economics is not covered in a separate course, Section II (Chapters 7–10) should also be included. If students have previously covered engineering economics, Chapters 14 and 15 covering optimization and pinch technology could be substituted. Similarly, for programs that have separate courses on process safety and/or where engineering ethics is treated elsewhere, Chapters 14 and 15 could be substituted.

For the second term of a two-term sequence, we recommend Chapters 19 through 23 (and Chapters 14 and 15 if not included in the first design course) plus a design project. Chapters 19 through 23 could also be the basis for an equipment design course that might precede a process design course. Alternatively, advanced simulation techniques in Chapters 16 and 17 could be covered. If time permits, we also recommend Chapter 18 (Regulation and Control of Chemical Processes with Applications Using Commercial Software) and Chapter 24 (Process Troubleshooting and Debottlenecking), because these tend to solidify as well as extend the concepts of Chapters 19 through 23, that is, what an entry-level process engineer will encounter in the first few years of employment at a chemical process facility. For an environmental emphasis, Chapter 27 could be substituted for Chapters 18 and 24; however, it is recommended that supplementary material be included.

We have found that the most effective way both to enhance and to examine student progress is through oral presentations in addition to the submission of written reports. During these oral presentations, individual students or a student group defends its results to a faculty panel, much as a graduate student defends a thesis or dissertation.

Because design is at its essence a creative, dynamic, challenging, and iterative activity, we welcome feedback on and encourage experimentation with this design textbook. We hope that students and faculty will find the excitement in teaching and learning engineering design that has sustained us over the years.

Finally, we would like to thank those people who have been instrumental to the successful completion of this book. Many thanks are given to all undergraduate chemical engineering students at West Virginia University over the years, particularly the period 1992–2018, and the undergraduate chemical engineering students at Auburn University from 2013–2018. We also acknowledge the many colleagues who have provided, both formally and informally, feedback about this text. In particular, our thanks go to Dr. Susan Montgomery (University of Michigan) and Dr. John Hwalek (University of Maine) for their extensive review of Chapters 19–23 and Dr. Fernando Lima (West Virginia University) for his review of the optimization material in Chapter 16. Finally, RT would like to

thank his wife, Becky; JAS would like to thank his wife, Terry; and DB would like to thank his parents, Sambhunath and Gayatri, wife Pampa, and son Swagat for their continued support, love, and patience during the preparation of this fifth edition.

R.T.
J.A.S.
D.B
W.B.W.

About the Authors

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List of Nomenclature

Symbol	Definition	SI Units
a	Stoichiometric Coefficient	
a	Interfacial, Mass Transfer Area	m^2
a	Mean Ionic Diameter of an Electrolyte	m
a'	Interface Area per Unit Volume	m^2/m^3
A	Equipment Cost Attribute	
A	Area, Heat Transfer Surface Area	m^2
A	Absorption Factor	
A	Annuity Value	\$/time
A	Constant in Antoine's Equation	
$A/F, i, n$	Sinking Fund Factor	
$A/P, i, n$	Capital Recovery Factor	
A_b	Bubbling Area	m^2
A_c	Cross-Sectional Area	m^2
A_t	Total Cross-Sectional Area of Packed Bed	m^2
b	Fin Spacing	m
B	Constant in Antoine's Equation	°C
BC	Baffle Cut (% of Shell Diameter)	
B_o	Boiling Number	
BV	Book Value	\$
C	Constant in Antoine's Equation	°C
C	Molar Density	mol/m^3
C	Equipment Cost	\$
C or c	Molar Concentration	$kmol/m^3$
$C_{sb,f}$	Parameter in Flooding Calculation	m/s
CA	Corrosion Allowance	m
CBM	Bare Module Cost	\$
C_D	Drag Coefficient	
C_f	Material Constant for Surfaces Used in Boiling Heat Transfer	
COM	Cost of Manufacture	\$/time
cop	Coefficient of Performance	
C_p, C_v	Heat Capacities (Constant Pressure, Constant Volume)	kJ/kg°C or kJ/kmol°C

CCP	Cumulative Cash Position	$
CCR	Cumulative Cash Ratio	
D, D_{AB}	Diffusivity, Diffusion Coefficient of Solute A in Solution B	m^2/s
d, D	Diameter	m
D^*	Dimensionless Diameter	
D	Amount Allowed for Depreciation	$
D	Distillate Product Flowrate	kmol/time
d	Yearly Depreciation Allowance	$/yr
$DCFROR$	Discounted Cash Flow Rate of Return	
DMC	Direct Manufacturing Cost	$/time
$DPBP$	Discounted Payback Period	years
$\overline{D}$	Average Diffusivity	m^2/s
D_0	Diffusivity at Infinite Dilution	m^2/s
D_p, D_S	Particle Diameter, Sphere Diameter	m
$\boldsymbol{d}$	Vector of Disturbance Inputs	
d_s	Average Solvent Density	kg/m^3
e	Elementary Charge	Columb
e	Pipe Roughness Factor	m
e_f	Energy Dissipated by Friction	J/kg
E	Money Earned	$
E	Weld Efficiency	
$E(t)$	Residence Time Distribution in Reactor	s^{-1}
E_{act} or E	Activation Energy	kJ/kmol
E_o	Overall Column Efficiency	
$EAOC$	Equivalent Annual Operating Cost	$/yr
ECC	Equivalent Capitalized Cost	$
f	Fraction of Stream	
$f,$	Friction Factor	
f	Rate of Inflation	
f	Factor Used in Convective Boiling Correlation	
f_q	Quantity Factors for Trays	
F	Faraday's Constant	Columb/kmol
F	Future Value	$
F	Molar Flowrate	kmol/s, kmol/h
F	Equipment Module Cost Factor	
F	Correction for Multipass Heat Exchangers	
F	Force	N
F	Packing Factor in Packed Beds	
F_{lv}	Parameter in Flooding Calculation	
F_d, F_g, F_p	Drag, Gravitational, and Pressure Force	N/m^2 or kPa
F_x, F_y	Mass Transfer Coefficients for Liquid (x) or Vapor (y) Phase	m/s
$F/A, i, n$	Uniform Series Compound Amount Factor	
FCI	Fixed Capital Investment	$
$F/P, i, n$	Single Payment Compound Amount Factor	
FMC	Fixed Manufacturing Costs	$/time
F_{Lang}	Lang Factor	
f_i	Fugacity of Pure Component i	bar or kPa

$\hat{f}_i$	Fugacity of Component *i* in Mixture	bar or kPa
$\boldsymbol{f}$	System of Equations (vector)	
g	Acceleration Due to Gravity	m/s^2
g_c	Unit Conversion of 32.2 ft $lb/lb_f/sec^2$	ft $lb/lb_f/sec^2$
G, G'	Superficial Mass Velocity	$kg/m^2/s$
G	Gibbs Free Energy	kJ
G	Gas Flowrate	kg/s, kmol/s
GE	General Expenses	\$/time
h	Individual Heat Transfer Coefficient	$W/m^2/K$
H, H_A	Henry's Law Constant	bar or kPa in Equation (13.5), but can be different elsewhere
H, h	Enthalpy, Specific Enthalpy	kJ or kJ/kg
H *or* h	Height or Head	m
H, HTU	Height of Transfer Unit	m
$HETP$	Height Equivalent of a Theoretical Plate	m
h_f	Height of Froth on a Tray	m
h_{mf}	Bed Height at Minimum Fluidization	m
$\boldsymbol{I}$	Identity Matrix	
I	Ionic Concentration	$kmol/m^3$
I_x	Ionic Strength on a Mole Fraction Basis	
I	Cost Index	
i	Compound Interest	
i'	Effective Interest Rate Including Inflation	
$INPV$	Incremental Net Present Value	\$
$IPBP$	Incremental Payback Period	years
$\boldsymbol{J}$	Jacobian Matrix	
k	Thermal Conductivity	W/m K
k	Ratio of Specific Heat Capacities of a Gas	
k_o, K	Preexponential Factor for Reaction Rate Constant	Depends on molecularity of reaction
K	Loss Coefficient for Elbows, Fittings, etc.	
K_p	Equilibrium Constant	Depends on reaction stoichiometry
k_B	Boltzmann Constant	kJ/K
$\overline{k}_m$	Average Mass Transfer Coefficient	m/s
k_{reac} *or* k_i	Reaction Rate Constant	Depends on molecularity of reaction
k_{SB}	Souders-Brown Constant	m/s
K	Geometric Factor for Elliptical Heads	
K_c	Proportional Gain	
K_{cu}	Ultimate Controller Gain	
K_{eq}	Equilibrium Constant of a Chemical Reaction	
K_i	Vapor-Liquid Equilibrium Ratio of Species *i*	
K_x, K_y	Mass Transfer Coefficient (*x* is Liquid Phase, *y* is Vapor Phase)	$kmol/m^2/s$
L	Lean Stream Flowrate	kg/s

L	Length (also Baffle Spacing), Characteristic Length of a Catalyst Particle	m
L_{eq}	Equivalent Length of Pipe	m
$L, \overline{L}$	Liquid Flowrate (Over Bar signifies Below Feed in Distillation Column)	kg/s or kmol/s
$\dot{m}$	Mass Flowrate	kg/s
m	Equilibrium/Partition Coefficient (y/x)	
m	Molality	kmol/kg
m	Parameter Used in Fin Effectiveness, $m = (2h / \delta k)^{1/2}$ for Rectangular Fins, etc.	
m, M	Ratio of Tube Side and Shell Side Flows in Performance Problems	
M, mw	Molecular Weight	kg/kmol
M	Mass	kg
M	Stress Intensity Factor for Dished Heads	
M_T	Thiele Modulus	
n	Life of Equipment	years
n	Years of Investment	years
n	Number of Batches	
n_c	Number of Campaigns	
N	Number of Streams, Trays, Stages, Transfer Units, Shells, etc.	
N_u	Nusselt Number	
N	Molar Flowrate or Molar Flux	kmol/s or kmol/m^2/s
$NPSH_A$ $NPSH_R$	Net Positive Suction Head (Available, Required)	m of liquid (or Pa)
NPV	Net Present Value	$
N_{toG}	Number of Transfer Units	
N	Molar Holdup	kmol
OBJ, OF	Objective Function	usually $ or $/time
p	Tube Pitch (Distance between Centers of Adjacent Tubes)	m
p	Price	$
p_i	Partial Pressure	Pa
P	Dimensionless Temperature Approach Used in Log-Mean Temperature Correction Factor	
P, p	Pressure and Partial Pressure	bar or kPa
P	Present Value	$
P^*	Vapor Pressure	bar or kPa
P_i	Membrane Permeability of Component i	m^3/m^2/s/kPa
$P/A, i, n$	Uniform Series Present Worth Factor	
PBP	Payback Period	year
PC	Project Cost	$
$P/F, i, n$	Single Payment Present Worth Factor	
PVR	Present Value Ratio	
$P(x)$	Probability Density Function of x	
Pr	Prandtl Number	
P_u	Ultimate Period of Oscillation	s
Q *or* q	Rate of Heat Transfer or Heat Duty	W or MJ/h
q	Fraction of Liquid in Distillation Column Feed	

$\dot{Q}$	Heat Transfer Rate	W or MJ/h
r	Radius	m
r	Reaction Rate	kmol/m^3 or kmol/kg cat s
r	Rate of Production	kg/h
r_k	Knuckle Radius for Dished Heads	m
R	Gas Constant	kJ/kmol K
R	Ratio of Heat Capacities Used in Log-Mean Temperature Correction Factor	
R	Residual Funds Needed	$
R	Reflux Ratio	
R	Heat Transfer Resistance	m^{2}K/W
R	Restoring Force to Keep Elbow (pipe fitting) Stationary	N
Re	Reynolds Number	
Re_{emf}	Reynolds Number at Minimum Fluidization	
Re_t	Reynolds Number at Terminal Velocity	
R	Rich Stream Flowrate	kg/s
Rand	Random Number	
ROROI	Rate of Return on Investment	% p.a.
ROROII	Rate of Return on Incremental Investment	% p.a.
s	Suppression Factor Used in Convective Boiling Correlation	
S	Entropy	kJ/K
S	Salvage Value	$
S	Maximum Allowable Working Pressure	bar
S	Salt Concentration Factor	
S	Sensitivity	
S	Interfacial Surface Area	m^2
S	Stripping Factor	
SF	Stream Factor	
t	Thickness of Wall	m
t	Time	s, min, h, yr
$\overline{t}$	Average Time Spent in Reactor	s
t_m	Membrane Thickness	m
T_m	Melting Temperature	K
T	Total Time for a Batch	s, min, h, yr
T	Temperature	K, R, °C, or °F
U	Internal Energy	kJ
$\boldsymbol{u}$	Vector of Manipulated Inputs	
u	Flow Velocity	m/s
u_t^*	Dimensionless Terminal Velocity	
u_s	Superficial Velocity in Packed or Fluidized Bed	m/s
u_t	Terminal Velocity of a Particle	m/s
U	Overall Heat Transfer Coefficient	W/m^{2}K
U	Internal Energy	J
v	Molar Volume	m^3/mol
V	Volume	m^3
V, $\overline{V}$	Vapor Flow Rate (Over Bar is Below Feed in Distillation Column)	kmol/h
v_{react}	Specific Volume of Reactor	m^3/kg of product

v_p	Velocity	m/s
$\dot{v}$	Volumetric Flowrate	m^3/s
W	Weight	kg
W	Total Moles of a Component	kmol
W	Width of Heat Transfer Fin	m
W or W_S	Work or Shaft Work	kJ/kg
$\dot{W}_s$	Shaft Power	W
WC	Working Capital	$
$\boldsymbol{X}$	Matrix of Independent Variables	
$\boldsymbol{x}$	Vector of Variables	
x	Mole or Mass Fraction	
x	Wall or Film Thickness	m
x	Mole Faction in Liquid Phase	
X	Conversion	
X	Base-Case Ratio	
X_{tp}	Martinelli's Two-Phase Flow Parameter	
y	Mole or Mass Fraction (in Vapor Phase)	
Y	Yield	
YOC	Yearly Operating Cost	$/yr
YS	Yearly Cash Flow (Savings)	$/yr
z	Valence of Ions	
z	Solids Mole Fraction, Mole Fraction in Feed Stream	
z	Distance or level	m
z	Coordinate in Direction Opposite Gravity	M

Greek Symbols

α	Multiplication Cost Factor	
α_{AB}	Relative Volatility or Relative Permeability (between Species A and B)	
α	NRTL Nonrandomness Factor	
α	Parameter in Calculating Pressure Drop in Packed Bed	
β	Parameter in Calculating Pressure Drop in Packed Bed	
β	Orifice Diameter/Pipe Diameter	
δ	Thickness of the Ion-Free Layer below	
δ	(Condensing) Film Thickness or Fin Thickness	m
ε	Void Fraction	
ε	Pump Efficiency	
ε	Tolerance, Error	
ε	Emissivity	
ε	Effectiveness (for fins)	
ε_{ij}	Lennard-Jones Energy Parameter between Species *i* and *j*	kJ/kmol
ε_r	Relative Permittivity of the Solvent	
ε_r'	Relative Permittivity of the Vapor Phase	
ε_s	Permittivity of the Solvent	$Columb^2/kJ\ m$
ϕ	Fugacity Coefficient	
$\hat{\phi}$	Fugacity Coefficient in Mixture	
ϕ^*	Fugacity Coefficient of Saturated Vapor	
γ	Activity Coefficient	

γ	Ratio of Heat Capacities = C_p/C_v	
γ^{∞}	Activity Coefficient in the Mixture at Infinite Dilution	
$\gamma_{\pm}$	Mean Ionic Activity Coefficient	
κ	Inverse of Debye-Hückel Length	m^{-1}
η	Catalyst Effectiveness Factor	
η	Selectivity	
$\eta, \eta_c, \eta_f, \eta_p, \eta_t$	Efficiency for Compressor, Separator, Pump, Turbine	
λ	Heat of Vaporization	kJ/kg
λ	Eigenvalue	
λ	Heat of Vaporization/Condensation	kJ/kg
λ	Lagrangian Multiplier Vector	
λ_0	Thermal Conductivity of Pure Solvent	W/m K
μ	Viscosity	kg/m s
μ_c	Chemical Potential	kJ
μ_0	Viscosity of Pure Solvent	kg/m s
ν	Stoichiometric Coefficient	
$\boldsymbol{\theta}$	Parameter Vector	
θ	Ratio of Species Concentration to That of Limiting Reactant	
θ	Angle	° or rad
θ	Stage Cut in Gas Permeation Membrane	
σ	Statistical Variance	
σ	Collision Diameter	m
σ	Surface Tension	N/m (dyne/cm^2)
σ	Stefan-Boltzmann Constant	$W/m^2/K^4$
ξ	Selectivity	
ρ, ρ_s	Density, Solid (Particle) Density	kg/m^3
Θ	Stoichiometric Parameter	
Θ	Cycle Time	s
τ	Space Time	s
$\boldsymbol{\tau}$	NRTL Binary Interaction Energy Parameter	
τ_D	Derivative Time Constant	s
τ_I	Integral Time Constant	s
ψ	Density of Water/Density of Liquid in Packed Bed	
Ψ	Sphericity	
Ψ	Inertial Separation Parameter	
Ω	Overall Catalyst Effectiveness (Including Internal and External Resistances)	
Ω	Collision Integral	

Subscripts

1	Base Time, Base Case, or Inlet Condition
2	Desired Time, New Case, or Outlet Condition
a	Required Attribute
air-leak	Air Leak Due to Vacuum Conditions
A, B, R, S	Designating Components A, B, R, S
ACT, actual	Actual
Active	Refers to Active Column Area

Aux	Auxiliary Buildings
a, a′	Anion
b	Base Attribute, Baffle
b	Bulk or Bubble Phase
bare	Bare Fin
base	Fin Base
B	Bottoms of Distillation Column
BM	Bare Module
c, c′	Cation
c	Cold, Corrected, Critical, Coolant
cb	Convective Boiling
cat	Catalyst
clean	Cleaning
cocurrent	Designating a Cocurrent Arrangement for an S-T Heat Exchanger
countercurrent	Designating a Countercurrent Arrangement for an S-T Heat Exchanger
Cont	Contingency
C	Refers to Condenser
cv	Control Volume
cw	Cooling Water
cycle	Cycle
d	Without Depreciation
dished	Dished Vessel Head
elliptical	Elliptical Vessel Head
D, d	Demand
D	Distillate
E	Emulsion Phase
E	Contractor Engineering Expenses
eff	Effective
eq	Equivalent
el	Electrolyte(s)
eq	Metal in the Equipment
f	Flooding Conditions
fb	Film Boiling
fin	Fin
film	Film
F,f	Feed
Fee	Contractor Fee
FTT	Transportation, etc.
g	Gas
GR	Grass Roots
h	Hot
H	Hydraulic
i	Species
i	Index, Inside, or Interface
in	Inlet or Inner
int	Internal
k	Year
lm	Log-Mean
l-h	Liquid Holdup
l, L	Liquid

L	Installation Labor
L	Lean Streams
L	Without Land Cost
LF	Long-Range Force
m	Molality Scale
m	Mass Transfer
m	Molecular Species
m	Heating/Cooling Medium or Membrane
m	Number of Years
M	Materials for Installation
M	Material Cost Factor
max	Maximum
MC	Matching Costs
mesh	Mesh
min	Minimum
n	Index for Time Instant
nom	Nominal Interest
o	Outside
out	Outlet
O or *OH*	Construction Overhead
Off	Offsites and Utilities
OL	Operating Labor
OL, OV, ov	Overall Liquid and Overall Vapor Transfer Units or Height of Transfer Unit, Respectively
opt	Optimum
p	Production
p	Process Stream or Permeate Stream
pb	Pool Boiling
P	Equipment at Manufacturer's Site (Purchased), Pressure Cost Factor, Process or Particle
P&I	Piping and Instrumentation
rev	Reversible
rxn, r	Reaction
r	Reduced (Pressure)
r	Retenate Stream
rad	Radiation
R	Rich Stream, Reboiler, Reference
RM	Raw Materials
s	All Nonwater Solvents, Simple Interest, Surface, or Stream
sat	Saturated
s, shell	Shell (Side) of Heat Exchanger
S	Supply
SB	Souders-Brown
Site	Site Development
SF	Short-Range Force
sph	Spherical or Equivalent Spherical
t, tube	Tube (Side) of Heat Exchanger
t	Terminal
tp	Tube Passes
TM	Total Module

UT	Utilities
V, v	Vapor
vap	Vaporization
ves	Vessel
wire	Wire
WT	Waste Treatment
w	Water or Wall
y	Designation for Type in Effectiveness Factor for Heat Exchangers, y = 1-2, 2-4, 3-6, etc.
z	Distance Along Reactor or Tube
+	Cation
−	Anion

Superscripts

α, β	Powers of Coefficients in Langmuir-Hinshelwood Kinetics
a, b	Powers in Simple Rate Laws
DB	Double Declining Balance Depreciation
E or ex	Excess Property
L	Lower Limit
L, l	Liquid
*	Equilibrium Value
o	Cost for Ambient Pressure Using Carbon Steel
s	Solid
SL	Straight Line Depreciation
SOYD	Sum of the Years Depreciation
U	Upper Limit
v	Vapor
∞	Aqueous Infinite Dilution
′	Includes Effect of Inflation on Interest
‴	Signifies Reaction Rate Per Unit Mass of Catalyst

Additional Nomenclature

Table 1.2	Convention for Specifying Process Equipment
Table 1.3	Convention for Specifying Process Streams
Table 1.7	Abbreviations for Equipment and Materials of Construction
Table 1.10	Convention for Specifying Instrumentation and Control Systems

Note: In this book, matrices are denoted by boldface, uppercase, italicized letters and vectors are denoted by boldface, lowercase, italicized letters.

CHAPTER

0

Outcomes Assessment

If you are reading this chapter, you are either a student about to begin the design class that culminates your chemical engineering training or you are a professor planning to teach that same class. The design class is often called the *capstone* class, because not only is it the ultimate class in the chemical engineering curriculum, but also it is where students are expected to apply knowledge gained earlier in the curriculum to the solution of a comprehensive chemical engineering design problem.

Outcomes assessment is the process of determining whether students have learned what the faculty expects them to have learned. The term *learned* is used in this context to include both subject matter (math, chemistry, fluid mechanics, etc.) and skills (report writing, oral presentations, teamwork). Outcomes assessment can be understood by analogy to process control. In process control, a process has a set point—temperature, for example. If the exit temperature is measured and it is not at the desired value, there may be a feedback loop that alters, for example, the flowrate of a cooling water stream in a heat exchanger to bring the temperature to the desired value, that is, the set point. In outcomes assessment, the faculty determines the knowledge and skills (learning outcomes) it expects graduates to have mastered. This is the set point. Then the faculty measures the level of mastery of the desired knowledge and skills, and, if the measurement is not at the set point, there should be feedback to students to ensure that the deficiencies are corrected for the current students. In addition, there should be changes made to the curriculum to ensure that future students are closer to the desired set point. This process is analogous to feedback control and is illustrated in Figure 0.1. Several nested feedback loops are illustrated, because assessment results can be obtained from alumni, from seniors about to graduate, and at any point in the curriculum. Before the advent of outcomes assessment, the traditional model for higher education was more analogous to feed-forward control, as illustrated in Figure 0.2. In this model, the outcomes are assumed based on the content of the curriculum. The weakness of feed-forward control is that the output is assumed based on a model of the process (curriculum, in this example), but prediction of the correct output is completely dependent on the validity of the model.

So what is done with outcomes assessment results? As discussed above, one possibility is feedback to improve student learning. This is termed *formative assessment*. Another possibility is to use the results to prove that students have achieved the desired outcomes. This is termed *summative assessment*. Both forms of assessment are necessary. Summative assessment is necessary to satisfy current accreditation requirements and, particularly at state-supported institutions, to satisfy the requirements of governing bodies (e.g., boards of trustees). Formative assessment is necessary to improve student learning to ensure that the desired learning outcomes are achieved.

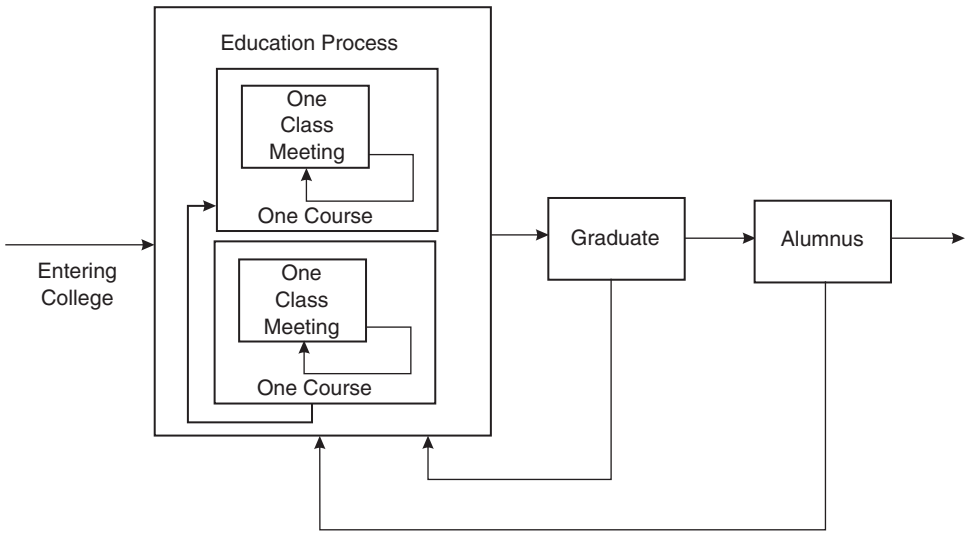

Figure 0.1 Feedback Model for Higher Education

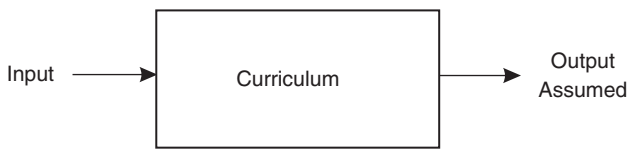

Figure 0.2 Feed-Forward Model of Higher Education

So why include this topic in a process design textbook? There are two reasons. One is that accreditation of all engineering programs by ABET is now based on outcomes assessment [1]. The second reason is that it is believed that the capstone design class is one of the most logical places in the curriculum for outcomes assessment. Both the faculty and students can perform assessment in the capstone design class. Because this is the class that culminates a student's undergraduate experience and it is the class in which students are expected to apply what they have learned earlier in the curriculum, there is no better opportunity to assess learning outcomes before students graduate. By performing this assessment before graduation, there is opportunity for feedback to students, possibly in the form of remedial instruction, in case any of the desired outcomes are not met.

In what follows, students will first be shown how to assess themselves, followed by methods that instructors can use to assess student outcomes in the design class.

0.1 STUDENT SELF-ASSESSMENT

There are two ways to describe what you should have learned before receiving your chemical engineering degree. One is to list all of the skills and subject matter you should have learned. This is curriculum dependent, so the list in one department may differ from the list in another department, although the lists between departments will probably have at least 75% common material. However, accreditation requirements state that a department's objectives and outcomes must be published, so your department's expectations for you are probably easy to find on the Web. You can compare your current level of achievement to your department's expectations. As you proceed through the design class, if you encounter something you do not fully understand, you should take this opportunity to learn it. In many cases, it will be something that your instructor believes you

already know, so, by taking the time to catch up, you will be moving closer to the desired outcomes of your department. If it is something that was never covered in an earlier class, you should still take the time to learn it. After you graduate, you will encounter many aspects of chemical engineering that were not part of the undergraduate curriculum, and you will have to learn them on your own. It is better to practice this skill while in school. If you believe that you should be taught all aspects of chemical engineering in school, then you are either being unrealistic or you want a ten-year undergraduate degree! As are all professions, chemical engineering is ever changing. As professionals, chemical engineers are expected to continue to learn throughout their careers. Besides, one of your department's outcomes is undoubtedly that you should have the ability to educate yourself. Therefore, the capstone class often requires you to teach yourself new material—on purpose.

A second, more general method for describing what you have learned is known as Bloom's Taxonomy of educational objectives [2]. This is known as the **cognitive domain**, and it includes knowledge, thinking, and the application of knowledge, certainly the issues most applicable to chemical engineering education. (The other domain is known as the **affective domain**, and it includes attitudes and values. This domain will not be discussed here.)

Bloom's Taxonomy has six levels:

1. **Knowledge:** In this context, knowledge means facts, definitions, technical jargon, and so on. Knowledge is most often tested using multiple-choice questions. The primary skill necessary to be successful at this level is memorization, which, by now, you know is not sufficient to be successful as a chemical engineer. If you know that mass and energy are always conserved, or if you know that the ideal gas law is $PV = nRT$, you have demonstrated this level of cognitive achievement.
2. **Comprehension:** Comprehension means that you understand what something means. The simplest way to demonstrate comprehension is to explain something in your own words. For example, if you can explain the meaning of each term in the Navier-Stokes equations, you have reached this level of cognitive achievement. For the ideal gas law, if you can explain its meaning in your own words, including the assumptions of noninteracting molecules and molecules that have no volume, you are at the comprehension level of cognitive achievement. Comprehension is most often tested with short answer and essay questions.
3. **Application:** Application means that you can apply the knowledge mastered at levels 1 and 2 to solve problems. If you have reached the capstone design class, then you most certainly have achieved this level of cognitive achievement. Achievement of application is the minimum standard to pass lower-level engineering classes. Problems must be solved, and the problems you have been solving at the end of textbook chapters for the past few years demonstrate application. If you can solve a problem that requires use of the ideal gas law (without specifically being told to use it), then you have reached this level of cognitive achievement. Most of the problems in this book in Section II (engineering economics) and Section II (process equipment design and performance) are at this level.
4. **Analysis:** Analysis is generally described as the ability to break a complex problem down into its component parts. The more difficult end-of-chapter problems you have been assigned are often at this level. For example, a problem that requires use of both material and energy balances, and requires you to determine when to use each one, is an analysis problem. The problems in this book in Section I, Chapters 5–6, and some in Section IV, particularly those in Chapter 24, are at this level, because these problems require you to break down a process flowsheet into its component parts.
5. **Synthesis:** Synthesis is putting pieces of a problem together to make a whole. It is possible that you have not yet been given this challenge. In Section III, Chapters 12 and 13, where a chemical process is constructed (synthesized) from its component parts, you will meet this challenge. In completing a process design, the concept of a base case will be introduced.

A base case is a reasonable first estimate of a process design that has not yet been optimized. Construction of a base case involves synthesis.

6. **Evaluation:** Evaluation is the use of judgment when obtaining a problem solution. It is the use of judgment in choosing among alternatives. A simple example of evaluation might be checking someone else's work for errors. In the context of design, optimization, which is discussed in Chapter 14, is a very common mechanism of evaluation. In optimization, the "best" solution is sought using constraints and judgment. If you take the base-case design discussed above and improve it based on your engineering judgment, which may be based on optimization, experience, or heuristics, you are performing evaluation.

As a student, you can reflect on your undergraduate education using Bloom's Taxonomy and determine what level you believe that you have achieved to date, and you can trace your progress through level 6 before you graduate. By that time, you should have had experiences through level 6. It is levels 4–6 that are required for success with a company or in graduate school.

0.2 ASSESSMENT BY FACULTY

The capstone class is one of the most logical opportunities for program assessment, because it is where students are expected to apply previously learned knowledge. Another advantage is that the capstone design experience is something that is already being done; therefore, outcomes assessment can be performed with only an incremental effort. The question is how to measure learning outcomes. Several methods are suggested below, many of which the authors have used successfully.

One measure that the authors have used is a classroom assessment technique related to the memory matrix or categorizing grid [3]. On the first day of the design class, students are told that this is the class where they apply what they have learned thus far, and they are asked to enumerate the concepts they believe they have learned prior to the design class. Quite often, the initial response is to list the names of all classes taken in the chemical engineering curriculum. At that point, those classes are listed on the board and students are asked to fill in what they learned in each class. The resulting list provides a good idea of what students believe they have learned. There are always topics that are omitted. If you believe a key topic has been omitted, ask the class about it. If they all agree that it was their omission that is a good sign. If they all disclaim any knowledge of the topic, or even its definition, that is a sign that you may want to include this topic somewhere in the design class, especially if you think it is important. This provides feedback to students. If you think this topic was omitted from the syllabus or not learned by students in an earlier class, then you should consider finding a method to ensure that it is learned in the future. This is a delicate matter, of course, but it is made somewhat easier by the accreditation requirement that course objectives be included in the syllabus. One result of this requirement is that many faculties now discuss course content more than they did in the past. The authors can send interested instructors results of this exercise from our classes.

Another method for obtaining assessment results from capstone experiences is to develop a rubric containing attributes expected from a design project and evaluate the finished product within its context. In this situation, the term *rubric* means a procedure. The advantage of a well-defined rubric is that it makes it easier to obtain consistency in evaluation between multiple evaluators. A portion of a rubric that can be used for evaluating the technical content of design reports is shown in Figure 0.3. A composite score, which must be an integer, is entered only for the attribute in bold. It is an average of the characteristics under each attribute. If the average of all scores is significantly less than 3, it is believed that feedback is required, both to current students in the form of remedial work and into the curriculum to improve the performance of students when they are assigned a similar design project. An updated version of this complete rubric, as well as others currently used by the authors for oral presentations, written reports, and laboratory reports, is

Attribute	1–Not Acceptable	2–Below Expectations	3–Meets Expectations	4–Exceeds Expectations	Score
Design of equipment, analysis of performance of existing equipment, understand interrelationship between equipment in process					
Design of individual equipment	Major errors in individual equipment design	Some errors in equipment design	Equipment designed correctly	Unique aspects of equipment design enhance result	
Understand interrelationship between equipment on flowsheet	No understanding of equipment interrelationship	Minimum understanding of equipment interrelationship	Clear understanding of equipment interrelationship	Exploitation of equipment interrelationship to enhance result	
Constraints/limitations of individual equipment and flowsheet understood	Constraints/ limitations not understood	Not all constraints/ limitations understood	Constraints/ limitations clearly understood	Exploitation of constraints/ limitations to enhance result	
Response to questions indicates understanding of chemical engineering principles	Response to questions demonstrates lack of understanding	Response to questions shows gaps in understanding	Response to questions shows clear understanding	Response to questions shows superior understanding	
Significance of conclusions understood	Lack of understanding	Gaps in understanding	Clear understanding	Superior understanding	

Figure 0.3 Portion of a Rubric for Evaluating Design Projects

available at http://cbe.statler.wvu.edu/che-accreditation-assessment. By using a rubric for assessment purposes, it is possible to determine the success in student achievement of each attribute considered to be an important component of the whole. By merely assigning a grade, only a composite evaluation is obtained. This method reveals the details and can also be used to make subjective evaluation of design projects more objective.

One of the authors' favorite methods for obtaining assessment results is from the questions and follow-up questions after oral design report presentations [4]. Students' responses to questions and follow-up questions can reveal their true understanding of what they did and the principles they applied to arrive at the solution to the problem. In many ways, this is similar to a Ph.D. dissertation defense. The chemical engineering department at West Virginia University uses a series of projects over the senior year for assessment purposes. From these, feedback can be provided several times over the senior year. For a program that has only one project, another way to get similar information is from interim presentations or interim review meetings in which students are asked to explain their thought patterns. Students will always make errors; after all, they are still students. However, if a significant number of students make the same error or have the same misconception, then it is a significant result and should be noted. Documentation of questions asked (to the instructor or to a TA) can reveal the same type of information.

An important assessment principle is that skills should be developed over time, so students may demonstrate improvement after receiving feedback. Design is one such skill, as are oral presentations, written reports, teamwork, and so on. The capstone design class usually requires all of these experiences. It is difficult to argue that students have developed any of these skills if they have only one such experience while an undergraduate. Therefore, it is recommended that students receive multiple experiences to develop these skills, with feedback after each experience. One way to do this is by integrating these experiences throughout the curriculum. If this is not possible, then it is suggested that there be multiple experiences with feedback in the capstone experience.

0.3 SUMMARY

The capstone design class, the class for which this book is written, is a logical place for outcomes assessment, because it is where students apply knowledge learned earlier in the curriculum and because, given that the capstone experience already exists, only incremental effort is required. Students can assess their own progress using Bloom's Taxonomy or by comparing their progress to the educational objectives and/or learning outcomes published by their department. Several methods have been described here that the faculty can use to obtain program assessment results.

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SECTION

I

Conceptualization and Analysis of Chemical Processes

The purpose of this section of the book is to introduce the tools necessary to understand, interpret, synthesize, and create chemical processes. The basis of interpreting chemical processes lies with understanding the principal diagrams that are routinely used to describe chemical processes, most important of which is the process flow diagram (PFD). Although PFDs are unique for each chemical product, they possess many of the same characteristics and attributes. Moreover, the conditions (pressure, temperature, and concentration) at which different equipment operate are unique to the chemical product and processing route chosen. In order for process engineers to understand a given process or to be able to synthesize and optimize a new process, they must be able to apply the principles outlined in this section.

Chapter 1: Diagrams for Understanding Chemical Processes
The technical diagrams commonly used by chemical engineers are presented. These diagrams include the block flow diagram (BFD), the process flow diagram (PFD), and the piping and instrumentation diagram (P&ID). A standard method for presenting a PFD is given and illustrated using a process to produce benzene via the catalytic hydrodealkylation of toluene. The 3-D topology of chemical processes is introduced, and some basic information on the spacing and elevation of equipment is presented. These concepts are further illustrated in the Virtual Plant Tour AVI file on the webpage for this book given in the preface. Finally, operator training (OTS) and 3-D immersive training simulators (ITS) are discussed and their role in training and educating engineers is covered.

Chapter 2: The Structure and Synthesis of Process Flow Diagrams
The evolutionary process of design is investigated. This evolution begins with the process concept diagram that shows the *input/output* structure of all processes. From this simple starting point, the engineer can estimate the gross profit margins of competing processes and of processes that use different chemical synthesis routes to produce the same product. In this chapter, it is shown that all processes have a similar input/output structure whereby raw materials enter a process and are reacted to form products and by-products. These products are separated from unreacted feed, which is usually recycled. The product streams are then purified to yield products that are acceptable to the marketplace. All equipment in a process can be categorized into one of the six elements of the generic block flow process diagram.

The development of the process design continues by building preliminary flowsheets from these basic functional elements that are common to all processes.

Chapter 3: Batch Processing
In this chapter, key issues relating to the production of chemical products using batch processes are explored. The major difference between continuous and batch processes is that unsteady-state operations are normal to batch plants whereas steady state is the norm for continuous processes. The chapter starts with an example illustrating typical calculations required to design a sequence of batch operations to produce a given product. The remainder of the chapter is devoted to how best to sequence the different operations required to produce multiple chemical products using a fixed amount of equipment. The concepts of Gantt charts, cycle times, batch campaigning, intermediate and final product storage, and parallel operations are covered.

Chapter 4: Chemical Product Design
Chemical product design is defined to include application of chemical engineering principles to the development of new devices, development of new chemicals, development of new processes to produce these new chemicals, and development of marketable technology. The design hierarchy for chemical product design is presented. The necessity of considering customer needs in chemical product design and the need to develop interdisciplinary teams are discussed.

Chapter 5: Tracing Chemicals through the Process Flow Diagram
In order to gain a better understanding of a PFD, it is often necessary to follow the flow of key chemical components through the diagram. This chapter presents two different methods to accomplish this. The tracing of chemicals through the process reinforces understanding of the role that each piece of equipment plays. In most cases, the major chemical species can be followed throughout the flow diagram using simple logic without referring to the flow summary table.

Chapter 6: Understanding Process Conditions
Once the connectivity or topology of the PFD has been understood, it is necessary to understand why a piece of equipment is operated at a given pressure and temperature. The idea of conditions of special concern is introduced. These conditions are either expensive to implement (due to special materials of construction and/or the use of thick-walled vessels) or use expensive utilities. The reasons for using these conditions are introduced and explained.

CHAPTER

1

Diagrams for Understanding Chemical Processes

WHAT YOU WILL LEARN

- Different types of chemical process diagrams
- How these diagrams represent process views at different scales
- One consistent method for drawing process flow diagrams
- The information to be included in a process flow diagram
- The purpose of operator training simulators and recent advances in 3-D representation of different chemical processes

The chemical process industry (CPI) is involved in the production of a wide variety of products that improve the quality of our lives and generate income for companies and their stockholders. In general, chemical processes are complex, and chemical engineers in industry encounter a variety of chemical process flow diagrams. These processes often involve substances of high chemical reactivity, high toxicity, and high corrosivity operating at high pressures and temperatures. These characteristics can lead to a variety of potentially serious consequences, including explosions, environmental damage, and threats to people's health. It is essential that errors or omissions resulting from missed communication between persons and/or groups involved in the design and operation do not occur when dealing with chemical processes. Visual information is the clearest way to present material and is least likely to be misinterpreted. For these reasons, it is essential that chemical engineers be able to formulate appropriate process diagrams and be skilled in analyzing and interpreting diagrams prepared by others.

The most effective way of communicating information about a process is through the use of flow diagrams.

This chapter presents and discusses the more common flow diagrams encountered in the chemical process industry. These diagrams evolve from the time a process is conceived in the laboratory through design, construction, and the many years of plant operation. The most important of these diagrams are described and discussed in this chapter.

The following narrative is taken from Kauffman [1] and describes a representative case history related to the development of a new chemical process. It shows how teams of engineers work together to provide a plant design and introduces the types of diagrams that will be explored in this chapter.

> *The research and development group at ABC Chemicals Company worked out a way to produce alpha-beta souptol (ABS). Process engineers assigned to work with the development group have pieced together a continuous process for making ABS in commercial quantities and have tested key parts of it. This work involved hundreds of* ***block flow diagrams****, some more complex than others. Based on information derived from these block flow diagrams, a decision was made to proceed with this process.*
>
> *A process engineering team from ABC's central office carries out the detailed process calculations, material and energy balances, equipment sizing, etc. Working with their drafting department, they produced a series of* ***PFDs (Process Flow Diagrams)*** *for the process. As problems arise and are solved, the team may revise and redraw the PFDs. Often the work requires several rounds of drawing, checking, and revising.*
>
> *Specialists in distillation, process control, kinetics, and heat transfer are brought in to help the process team in key areas. Some are company employees and others are consultants.*
>
> *Since ABC is only a moderate-sized company, it does not have sufficient staff to prepare the 120* ***P&IDs (Piping and Instrumentation Diagrams)*** *needed for the new ABS plant. ABC hires a well-known engineering and construction firm* ***(E&C Company)****, DEFCo, to do this work for them. The company assigns two of the ABC process teams to work at DEFCo to coordinate the job. DEFCo's process engineers, specialists, and drafting department prepare the P&IDs. They do much of the detailed engineering (pipe sizes, valve specifications, etc.) as well as developing the necessary computer aided design (CAD) and process drawings. The job may take two to six months. Every drawing is reviewed by DEFCo's project team and by ABC's team. If there are disagreements, the engineers and specialists from the companies must resolve them.*
>
> *Finally, all the PFDs and the P&IDs are completed and approved. ABC can now go ahead with the construction. They may extend their contract with DEFCo to include this phase, or they may go out for construction bids from a number of other companies.*

This narrative describes a typical sequence of events taking a project from its initial stages through plant construction. If DEFCo had carried out the construction, ABC could go ahead and take over the plant or DEFCo could be contracted to carry out the start-up and to commission the plant. Once satisfactory performance specifications have been met, ABC would take over the operation of the plant and commercial production would begin.

From conception of the process to the time the plant starts up, two or more years will have elapsed and millions of dollars will have been spent with no revenue from the plant. The plant must operate successfully for many years to produce sufficient income to pay for all plant operations and to repay the costs associated with designing and building the plant. During this operating period, many unforeseen changes are likely to take place. The quality of the raw materials used by the plant may change, product specifications may be raised, production rates may need to be increased, the equipment performance will decrease because of wear, the development of new and better catalysts will occur, the costs of utilities will change, new environmental regulations may be introduced, or improved equipment may appear on the market.

As a result of these unplanned changes, plant operations must be modified. Although the operating information on the original process diagrams remains informative, the actual performance taken from the operating plant will be different. The current operating conditions will appear on updated versions of the various process diagrams, which will act as a primary basis for understanding the changes taking place in the plant. These process diagrams are essential to

an engineer who has been asked to diagnose operating problems, solve problems in operations, debottleneck systems for increased capacity, and predict the effects of making changes in operating conditions. All these activities are essential in order to maintain profitable plant operation.

In this chapter, the focus is on three diagrams that are important to chemical engineers: block flow, process flow, and piping and instrumentation diagrams. Of these three diagrams, the most useful to chemical engineers is the PFD. The understanding of the PFD represents a central goal of this textbook.

1.1 BLOCK FLOW DIAGRAM (BFD)

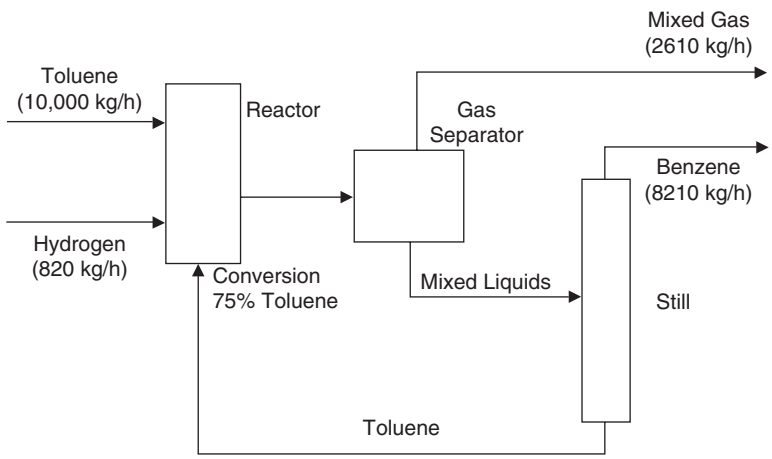
Block flow diagrams are introduced early in the chemical engineering curriculum. For example, in the first course in material and energy balances, often an initial step is to convert a word problem into a simple block diagram. This diagram consists of a series of blocks representing different equipment or unit operations that are connected by input and output streams. Important information such as operating temperatures, pressures, conversions, and yield are included on the diagram along with flowrates and some chemical compositions. However, the diagram does not include any details of equipment within any of the blocks.

The block flow diagram can take one of two forms. First, a block flow diagram may be drawn for a single process. Alternatively, a block flow diagram may be drawn for a complete chemical complex involving many different chemical processes. These two types of diagrams are differentiated by calling the first a block flow process diagram and the second a block flow plant diagram.

1.1.1 Block Flow Process Diagram

An example of a block flow process diagram is shown in Figure 1.1, and the illustrated process is described below.

Toluene and hydrogen are converted in a reactor to produce benzene and methane. The reaction does not go to completion, and excess toluene is required. The noncondensable gases are separated and discharged. The benzene product and the unreacted toluene are then separated by distillation. The toluene is then recycled back to the reactor and the benzene removed in the product stream.



Reaction : $C_7H_8 + H_2 \rightarrow C_6H_6 + CH_4$

Figure 1.1 Block Flow Process Diagram for the Production of Benzene

Table 1.1 Conventions and Format Recommended for Laying Out a Block Flow Process Diagram

1. Operations shown by blocks.
2. Major flow lines shown with arrows giving direction of flow.
3. Flow goes from left to right whenever possible (recycles go right to left).
4. Light stream (gases) toward top with heavy stream (liquids and solids) toward bottom.
5. Critical information unique to process supplied.
6. If lines cross, then the horizontal line is continuous and the vertical line is broken (hierarchy for all drawings in this book).
7. Simplified material balance provided.

This block flow diagram gives a clear overview of the production of benzene, unobstructed by the many details related to the process. Each block in the diagram represents a process function and may, in reality, consist of several pieces of equipment. The general format and conventions used in preparing block flow process diagrams are presented in Table 1.1.

Although much information is missing from Figure 1.1, it is clear that such a diagram is very useful for "developing a feel" for the process. Block flow process diagrams often form the starting point for developing a PFD. They are also very helpful in conceptualizing new processes and explaining the main features of the process without getting bogged down in the details.

1.1.2 Block Flow Plant Diagram

An example of a block flow plant diagram for a complete chemical complex is illustrated in Figure 1.2. This block flow plant diagram is for a coal to higher alcohol fuels plant. Clearly, this is a complicated process in which there are a number of alcohol fuel products produced from a feedstock of coal. Each block in this diagram represents a complete chemical process (compressors and turbines are also shown as trapezoids), and a block flow process diagram could be drawn for each block in Figure 1.2. The advantage of a diagram such as Figure 1.2 is that it allows a complete picture to be obtained of what this plant does and how all the different processes interact. On the other hand, in order to keep the diagram relatively uncluttered, only limited information is available about each process unit. The conventions for drawing block flow plant diagrams are similar to Table 1.1.

Both types of block flow diagrams are useful for explaining the overall operation of chemical plants. For example, consider that you have just joined a large chemical manufacturing company that produces a wide range of chemical products from the site to which you have been assigned. You would most likely be given a *block flow plant diagram* to orient you to the products and important areas of operation. Once assigned to one of these areas, you would again likely be provided with a *block flow process diagram* describing the operations in your particular area.

In addition to the orientation function described earlier, block flow diagrams are used to sketch out and screen potential process alternatives. Thus, they are used to convey information necessary to make early comparisons and eliminate competing alternatives without having to make detailed and costly comparisons.

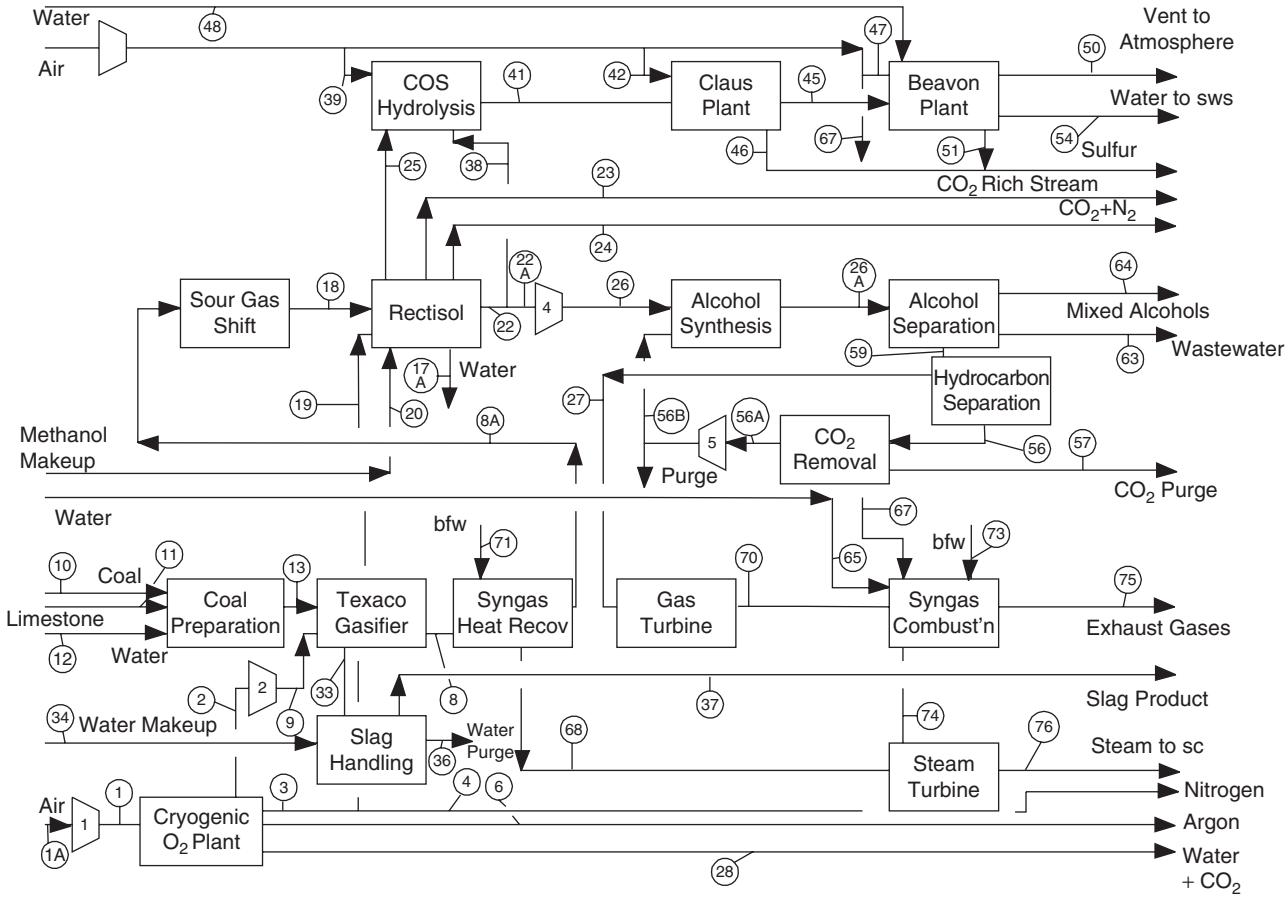


Figure 1.2 Block Flow Plant Diagram of a Coal to Higher Alcohol Fuels Process

1.2 PROCESS FLOW DIAGRAM (PFD)

The process flow diagram (PFD) represents a quantum step up from the BFD in terms of the amount of information that it contains. The PFD contains the bulk of the chemical engineering data necessary for the design of a chemical process. For all of the diagrams discussed in this chapter, there are no universally accepted standards. The PFD from one company will probably contain slightly different information from the PFD for the same process from another company. Having made this point, it is fair to say that most PFDs convey very similar information. A typical commercial PFD will contain the following information:

1. All the major pieces of equipment in the process will be represented on the diagram along with a description of the equipment. Each piece of equipment will have a unique equipment number and a descriptive name.
2. All process flow streams will be shown and identified by a number. A description of the process conditions and chemical composition of each stream will be included. These data will be either displayed directly on the PFD or included in an accompanying flow summary table.
3. All utility streams supplied to major equipment that provide a process function will be shown.
4. Basic control loops, illustrating the control strategy used to operate the process during normal operations, will be shown.

It is clear that the PFD is a more complex diagram than a BFD requiring a substantial effort to prepare. It is essential that it should remain uncluttered and be easy to follow, to avoid errors in presentation and interpretation. Often PFDs are drawn on large sheets of paper (for example, size D: 24 in × 36 in), and several connected sheets may be required for a complex process. Because of the page size limitations associated with this text, complete PFDs cannot be presented here. Consequently, certain liberties have been taken in the presentation of the PFDs in this text. Specifically, certain information will be presented in accompanying tables, and only the essential process information will be included on the PFD. The resulting PFDs will retain clarity of presentation, but the reader must refer to the flow summary and equipment summary tables in order to extract all the required information about the process.

Before the various aspects of the PFD are discussed, it should be noted that the PFD and the process that is described in this chapter will be used throughout the book. The process is the hydrodealkylation of toluene to produce benzene. This is a well-studied and well-understood commercial process still used today. The PFD presented in this chapter for this process is technically feasible but is in no way optimized. In fact, many improvements to the process technology and economic performance can be made. Many of these improvements will become evident when the appropriate material is presented. This allows the techniques provided throughout this text to be applied both to identify technical and economic problems in the process and to make the necessary process improvements. Therefore, throughout the text, weak spots in the design, potential improvements, and a path toward an optimized process flow diagram will be identified.

The basic information provided by a PFD can be categorized into one of the following:

1. Process topology
2. Stream information
3. Equipment information

Each aspect of the PFD will be considered separately. After each of the three topics has been addressed, all the information will be gathered and presented in the form of a PFD for the benzene process.

1.2.1 Process Topology

Figure 1.3 is a skeleton process flow diagram for the production of benzene (see also the block flow process diagram in Figure 1.1). This skeleton diagram illustrates the location of the major

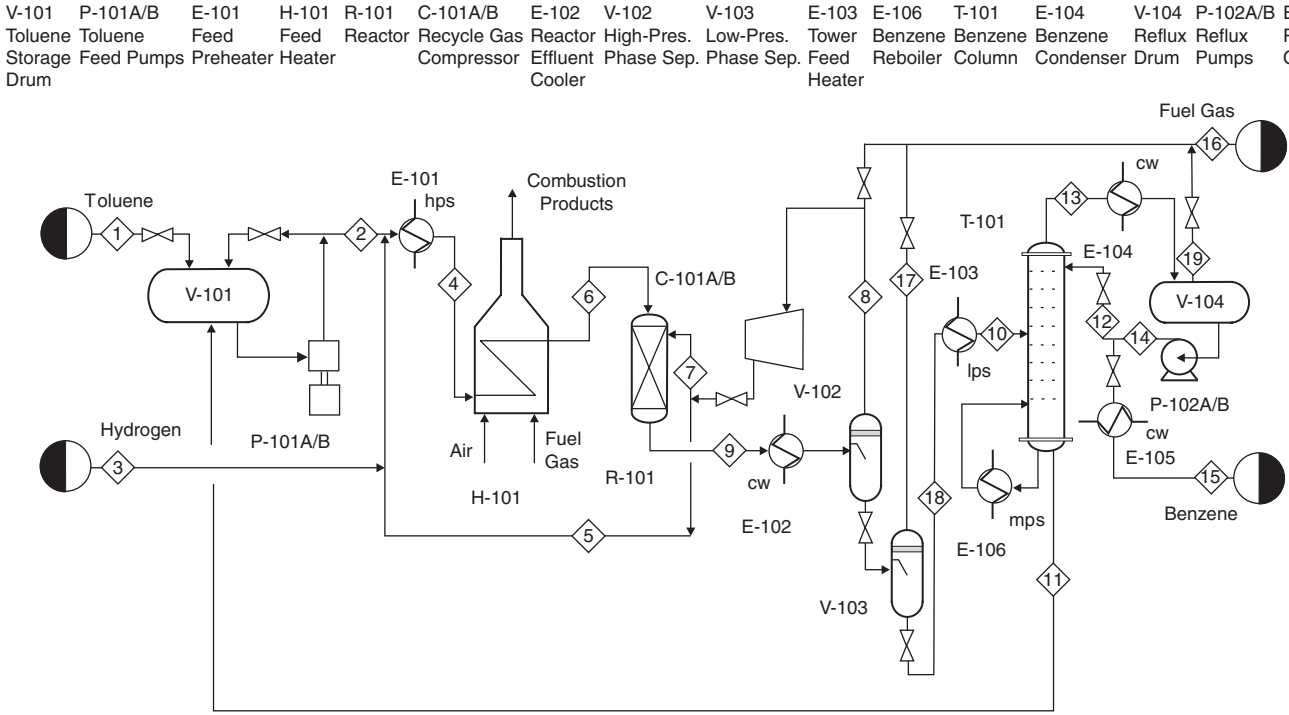


Figure 1.3 Skeleton Process Flow Diagram (PFD) for the Production of Benzene via the Hydrodealkylation of Toluene

pieces of equipment and the connections that the process streams make between equipment. The location of and interaction between equipment and process streams are referred to as the process topology.

Equipment is represented symbolically by "icons" that identify specific unit operations. Although the American Society of Mechanical Engineers (ASME) [2] publishes a set of symbols to use in preparing flowsheets, it is common for companies to use in-house symbols. A comprehensive set of symbols is also given by Austin [3]. Whatever set of symbols is used, there is seldom a problem in identifying the operation represented by each icon. Figure 1.4 contains a list of the symbols used in process diagrams presented in this text. This list covers more than 90% of those needed in fluid (gas or liquid) processes.

Figure 1.3 shows that each major piece of process equipment is identified by a number on the diagram. A list of the equipment numbers along with a brief descriptive name for the equipment is printed along the top of the diagram. The location of these equipment numbers and names roughly corresponds to the horizontal location of the corresponding piece of equipment. The convention for formatting and identifying the process equipment is given in Table 1.2. This table provides the information necessary for the identification of the process equipment icons shown in a PFD. As an example of how to use this information, consider the unit operation P-101A/B and what each number or letter means.

P-101A/B identifies the equipment as a pump.

P-**1**01A/B indicates that the pump is located in area 100 of the plant.

P-1**01**A/B indicates that this specific pump is number 01 in unit 100.

P-101**A/B** indicates that a backup pump is installed. Thus, there are two identical pumps, P-101A and P-101B. One pump will be operating while the other is idle.

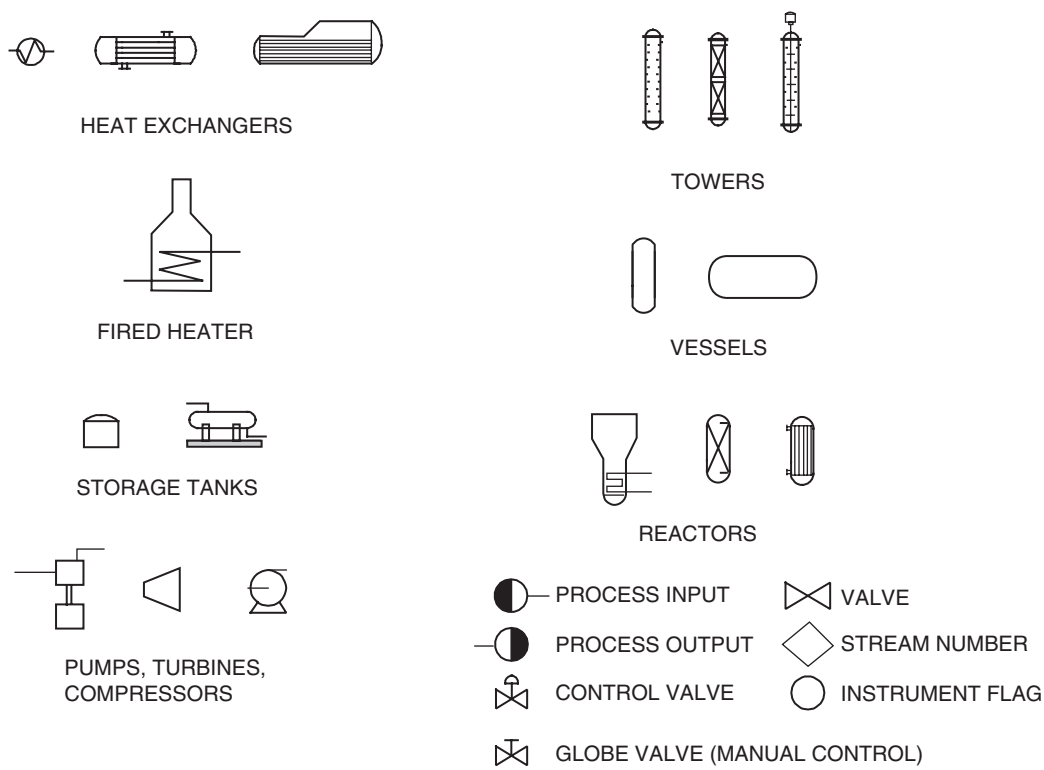


Figure 1.4 Symbols for Drawing Process Flow Diagrams

Table 1.2 Conventions Used for Identifying Process Equipment

General Format XX-YZZ A/B
XX are the identification letters for the equipment classification
C – Compressor or Turbine
E – Heat Exchanger
H – Fired Heater
P – Pump
R – Reactor
T – Tower
TK – Storage Tank
V – Vessel
Y designates an area within the plant
ZZ is the number designation for each item in an equipment class
A/B identifies parallel units or backup units not shown on a PFD
Additional description of equipment is given on top of PFD

The 100 area designation will be used for the benzene process throughout this text. Other processes presented in the text will carry other area designations. Along the top of the PFD, each piece of process equipment is assigned a descriptive name. From Figure 1.3 it can be seen that Pump P-101 is called the "toluene feed pump." This name will be commonly used in discussions about the process and is synonymous with P-101.

During the life of the plant, many modifications will be made to the process; often it will be necessary to replace or eliminate process equipment. When a piece of equipment wears out and is replaced by a new unit that provides essentially the same process function as the old unit, then it is not uncommon for the new piece of equipment to inherit the old equipment's name and number (often an additional letter suffix will be used, e.g., H-101 might become H-101A). On the other hand, if a significant process modification takes place, then it is usual to use new equipment numbers and names. The key point here is that when an engineer looks for information about a piece of equipment there should be no ambiguity. For example, if they find data on a piece of equipment named E-103 then there should be no confusion to what heat exchanger this documentation refers. If the original E-103 had been replaced with a different exchanger also designated E-103 then clearly a lot of confusion, wasted time, and potential safety issues could result by using the data for the old exchanger to modify and/or evaluate the new exchanger. Example 1.1, taken from Figure 1.3, illustrates this concept.

Example 1.1

Operators report frequent problems with E-102, which are to be investigated. The PFD for the plant's 100 area is reviewed, and E-102 is identified as the "Reactor Effluent Cooler." The process stream entering the cooler is a mixture of condensable and noncondensable gases at 654°C that are partially condensed to form a two-phase mixture. The coolant is water at 30°C. These conditions characterize a complex heat transfer problem. In addition, operators have noticed that the pressure drop across E-102 fluctuates wildly at certain times, making control of the process difficult. Because of the frequent problems with this exchanger, it is recommended that E-102 be replaced by two separate heat exchangers. The first exchanger cools the effluent gas and generates steam needed in the plant. The second exchanger uses cooling water to reach the desired exit temperature of 38°C. These exchangers are to be designated as E-107 (reactor effluent boiler) and E-108 (reactor effluent condenser).

In reviewing Example 1.1, the E-102 designation is retired and not reassigned to the new equipment. There can be no mistake that E-107 and E-108 are new units in this process and that E-102 no longer exists.

1.2.2 Stream Information

Referring back to Figure 1.3, it can be seen that each of the process streams is identified by a number in a diamond box located on the stream. The direction of the stream is identified by one or more arrowheads. The process stream numbers are used to identify streams on the PFD, and the type of information that is typically given for each stream is discussed in the next section.

Also identified in Figure 1.3 are utility streams. Utilities are needed services that are available at the plant. Chemical plants are provided with a range of central utilities that include electricity, compressed air, cooling water, refrigerated water, steam, condensate return, inert gas for blanketing, chemical sewer, wastewater treatment, and flares. A list of the common services is given in Table 1.3, which also provides a guide for the identification of process streams.

Each utility is identified by the initials provided in Table 1.3. As an example, locate E-102 in Figure 1.3. The notation, cw, associated with the nonprocess stream flowing into E-102 indicates that cooling water is used as a coolant.

Table 1.3 Conventions for Identifying Process and Utility Streams

Process Streams	
All conventions shown in Table 1.1 apply.	
Diamond symbol located in flow lines.	
Numerical identification (unique for that stream) inserted in diamond.	
Flow direction shown by arrows on flow lines.	
Utility Streams	
lps	Low-Pressure Steam: 3–5 barg (sat)*
mps	Medium-Pressure Steam: 10–15 barg (sat)*
hps	High-Pressure Steam: 40–50 barg (sat)*
htm	Heat Transfer Media (Organic): to 400°C
cw	Cooling Water: From Cooling Tower 30°C Returned at Less than 45°C†
wr	River Water: From River 25°C Returned at Less than 35°C
rw	Refrigerated Water: In at 5°C Returned at Less than 15°C
rb	Refrigerated Brine: In at −45°C Returned at Less than 0°C
cs	Chemical Wastewater with High COD
ss	Sanitary Wastewater with High BOD, etc.
el	Electric Heat (Specify 220, 440, 660V Service)
bfw	Boiler Feed Water
ng	Natural Gas
fg	Fuel Gas
fo	Fuel Oil
fw	Fire Water

*These pressures are set during the preliminary design stages and typical values vary within the ranges shown.

†Above 45°C, significant scaling occurs and the usual return temperature is 40°C.

Electricity used to power motors and generators is an additional utility that is not identified directly on the PFD or in Table 1.3 but is treated separately. Most of the utilities shown are related to equipment that adds or removes heat within the process in order to control temperatures. This is common for most chemical processes.

From the PFD in Figure 1.3, the identification of the process streams is clear. For small diagrams containing only a few operations, the characteristics of the streams such as temperatures, pressures, compositions, and flowrates can be shown directly on the figure, adjacent to the stream. This is not practical for a more complex diagram. In this case, only the stream number is provided on the diagram. This indexes the stream to information on a flow summary or stream table, which is often provided below the process flow diagram. In this text the flow summary table is provided as a separate attachment to the PFD.

The stream information that is normally given in a flow summary table is given in Table 1.4. It is divided into two groups—required information and optional information—that may be important to specific processes. The flow summary table, for Figure 1.3, is given in Table 1.5 and contains all the required information listed in Table 1.4.

With information from the PFD (Figure 1.3) and the flow summary table (Table 1.5), problems regarding material balances and other problems are easily analyzed. Examples 1.2 and 1.3 are provided to offer experience in working with information from the PFD.

Table 1.4 Information Provided in a Flow Summary

Required Information
Stream Number
Temperature (°C)
Pressure (bar)
Vapor Fraction
Total Mass Flowrate (kg/h)
Total Mole Flowrate (kmol/h)
Individual Component Flowrates (kmol/h)
Optional Information
Component Mole Fractions
Component Mass Fractions
Individual Component Flowrates (kg/h)
Volumetric Flowrates (m^3/h)
Significant Physical Properties Density Viscosity Other
Thermodynamic Data Heat Capacity Stream Enthalpy *K*-values
Stream Name

Example 1.2

Check the overall material balance for the benzene process shown in Figure 1.3.

Solution

From the figure, identify the input streams as Stream 1 (toluene feed) and Stream 3 (hydrogen feed) and the output streams as Stream 15 (product benzene) and Stream 16 (fuel gas). From the flow summary table, these flows are listed as (units are in $(10^3$ kg)/h):

Input:		Output:	
Stream 3	0.82	Stream 15	8.21
Stream 1	10.00	Stream 16	2.61
Total	10.82×10^3 kg/h	Total	10.82×10^3 kg/h

This confirms that the overall material balance is achieved.

Example 1.3

Determine the conversion per pass of toluene to benzene in R-101 in Figure 1.3.

Solution

Conversion is defined as

X = (benzene produced in reactor)/(total toluene fed to reactor)

From the PFD, the input streams to R-101 are shown as Stream 6 (reactor feed) and Stream 7 (recycle gas quench), and the output stream is Stream 9 (reactor effluent stream). From the information in Table 1.5 (units are kmol/h):

Toluene fed to reactor = 144 (Stream 6) + 0.04 (Stream 7) = 144.04 kmol/h
Benzene produced in reactor = 116 (Stream 9) – 7.6 (Stream 6) – 0.37 (Stream 7)
= 108.03 kmol/h

$$X = 108.03/144.04 = 0.75$$

Alternatively, the following can be written:

Moles of benzene produced in reactor = Toluene in – Toluene out = 144.04 – 36.00
= 108.04 kmol/h

$$X = 108.04/144.04 = 0.75$$

Table 1.5 Flow Summary Table for the Benzene Process Shown in Figure 1.3 (and Figure 1.5)

Stream Number	1	2	3	4	5	6	7	8
Temperature (°C)	25	59	25	225	41	600	41	38
Pressure (bar)	1.90	25.8	25.5	25.2	25.5	25.0	25.5	23.9
Vapor Fraction	0.0	0.0	1.00	1.0	1.0	1.0	1.0	1.0
Mass Flow (tonne/h)	10.0	13.3	0.82	20.5	6.41	20.5	0.36	9.2
Mole Flow (kmol/h)	108.7	144.2	301.0	1204.4	758.8	1204.4	42.6	1100.8
Component Flowrates (kmol/h)								
Hydrogen	0.0	0.0	286.0	735.4	449.4	735.4	25.2	651.9
Methane	0.0	0.0	15.0	317.3	302.2	317.3	16.95	438.3
Benzene	0.0	1.0	0.0	7.6	6.6	7.6	0.37	9.55
Toluene	108.7	143.2	0.0	144.0	0.7	144.0	0.04	1.05

1.2.3 Equipment Information

The final element of the PFD is the equipment summary. This summary provides the information necessary to estimate the purchase costs of equipment and furnish the basis for the detailed design of equipment. Table 1.6 provides the information needed for the equipment summary for most of the equipment encountered in fluid processes.

The information presented in Table 1.6 is used in preparing the equipment summary portion of the PFD for the benzene process. The equipment summary for the benzene process is presented in Table 1.7, and details of how to estimate and choose various equipment parameters are discussed in Chapter 11.

1.2.4 Combining Topology, Stream Data, and Control Strategy to Give a PFD

Up to this point, the amount of process information displayed on the PFD has been kept to a minimum. A more representative example of a PFD for the benzene process is shown in Figure 1.5. This diagram includes all of the elements found in Figure 1.3, some of the information found in Table 1.5, plus additional information on the major control loops used in the process.

Stream information may be added to the diagram by attaching "information flags." The shape of the flags indicates the specific information provided on the flag. Figure 1.6 illustrates all the flags used in this text. These information flags play a dual role. They provide information needed in the plant design leading to plant construction and in the analysis of operating problems during the life of the plant. Flags are mounted on a staff connected to the appropriate process stream. More than one flag may be mounted on a staff. Example 1.4 illustrates the different information displayed on the PFD.

Example 1.4

Locate Stream 1 in Figure 1.5 and note that immediately following the stream identification diamond a staff is affixed. This staff carries three flags containing the following stream data:

1. Temperature of 25°C
2. Pressure of 1.9 bar
3. Mass flowrate of 10.0×10^3 kg/h

The units for each process variable are indicated in the key provided at the left-hand side of Figure 1.5.

9	10	11	12	13	14	15	16	17	18	19
654	90	147	112	112	112	38	38	38	38	112
24.0	2.6	2.8	3.3	2.5	3.3	2.3	2.5	2.8	2.9	2.5
1.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	0.0	1.0
20.9	11.6	3.27	14.5	22.7	22.7	8.21	2.61	0.07	11.5	0.01
1247.0	142.2	35.7	185.2	291.6	290.7	105.6	304.2	4.06	142.2	0.90
652.6	0.02	0.0	0.0	0.02	0.0	0.0	178.0	0.67	0.02	0.02
442.3	0.88	0.0	0.0	0.88	0.0	0.0	123.05	3.10	0.88	0.88
116.0	106.3	1.1	184.3	289.46	289.46	105.2	2.85	0.26	106.3	0.0
36.0	35.0	34.6	0.88	1.22	1.22	0.4	0.31	0.03	35.0	0.0

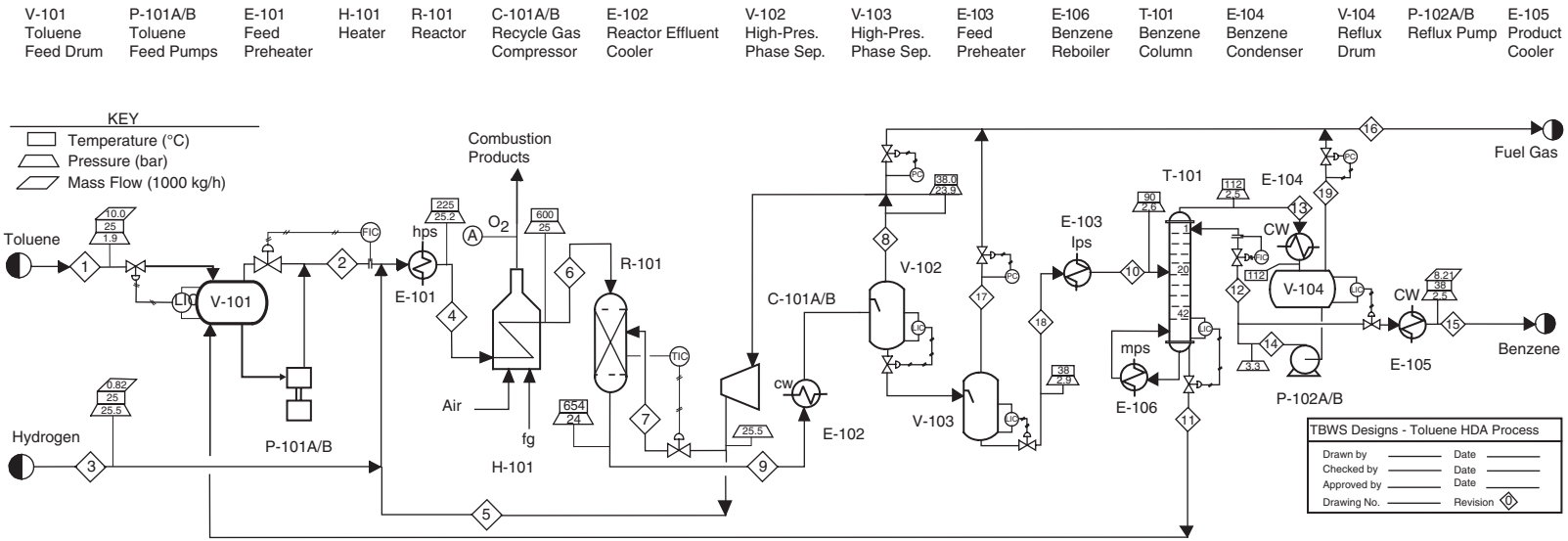


Figure 1.5 Benzene Process Flow Diagram (PFD) for the Production of Benzene via the Hydrodealkylation of Toluene

Table 1.6 Equipment Descriptions for PFD and P&IDs

Equipment Type
Description of Equipment
Towers
Size (height and diameter), Pressure, Temperature Number and Type of Trays Height and Type of Packing Materials of Construction
Heat Exchangers
Type: Gas-Gas, Gas-Liquid, Liquid-Liquid, Condenser, Vaporizer Process: Duty, Area, Temperature, and Pressure for Both Streams Number of Shell and Tube Passes Materials of Construction: Tubes and Shell
Tanks and Vessels
Height, Diameter, Orientation, Pressure, Temperature, Materials of Construction
Pumps
Flow, Discharge Pressure, Temperature, ΔP, Driver Type, Shaft Power, Materials of Construction
Compressors
Actual Inlet Flowrate, Temperature, Pressure Inlet and Outlet, Driver Type, Shaft Power, Materials of Construction
Heaters (Fired)
Type, Tube Pressure, Tube Temperature, Duty, Fuel, Material of Construction
Other
Provide Critical Information

With the addition of the process control loops and the information flags, the PFD starts to become cluttered. Therefore, in order to preserve clarity, it is necessary to limit what data are presented with these information flags. Fortunately, flags on a PFD are easy to add, remove, and change, and even temporary flags may be provided from time to time.

The information provided on the flags is also included in the flow summary table. However, often it is far more convenient when analyzing the PFD to have certain data directly on the diagram.

Not all process information is of equal importance. General guidelines for what data should be included in information flags on the PFD are difficult to define. However, at a minimum, information critical to the safety and operation of the plant should be given. This includes temperatures and

Table 1.7 Equipment Summary for Toluene Hydrodealkylation PFD

Heat Exchangers	**E-101**	**E-102**	**E-103**	**E-104**	**E-105**	**E-106**
Type	Fl.H.	Fl.H.	MDP	Fl.H.	MDP	Fl.H.
Area (m^2)	36	763	11	35	12	80
Duty (MJ/h)	15,190	46,660	1055	8335	1085	9045
Shell						
Temp. (°C)	225	654	160	112	112	185
Pres. (bar)	26	24	6	3	3	11
Phase	Vap.	Par. Cond.	Cond.	Cond.	l	Cond.
MOC	316SS	316SS	CS	CS	CS	CS
Tube						
Temp. (°C)	258	40	90	40	40	147
Pres. (bar)	42	3	3	3	3	3
Phase	Cond.	l	l	l	l	Vap.
MOC	316SS	316SS	CS	CS	CS	CS
Vessels/Tower/ Reactors	**V-101**	**V-102**	**V-103**	**V-104**	**T-101**	**R-101**
Temperature (°C)	55	38	38	112	147	660
Pressure (bar)	2.0	24	3.0	2.5	3.0	25
Orientation	Horizontal	Vertical	Vertical	Horizontal	Vertical	Vertical
MOC	CS	CS	CS	CS	CS	316SS
Size						
Height/Length (m)	5.9	3.5	3.5	3.9	29	14.2
Diameter (m)	1.9	1.1	1.1	1.3	1.5	2.3
Internals		s.p.	s.p.		42 sieve trays 316SS	Catalyst packed bed-10m
Pumps/Compressors	**P-101 (A/B)**	**P-102 (A/B)**	**C-101 (A/B)**	**Heater**		**H-101**
Flow (kg/h)	13,000	22,700	6770	Type		Fired
Fluid Density (kg/m^3)	870	880	8.02	MOC		316SS
Power (shaft) (kW)	14.2	3.2	49.1	Duty (MJ/h)		27,040
Type/Drive	Recip./ Electric	Centrf./ Electric	Centrf./ Electric	Radiant Area (m^2)		106.8
Efficiency (Fluid Power/ Shaft Power)	0.75	0.50	0.75	Convective Area (m^2)		320.2

(*continued*)

Table 1.7 Equipment Summary for Toluene Hydrodealkylation PFD (*Continued*)

Pumps/Compressors	P-101 (A/B)	P-102 (A/B)	C-101 (A/B)	Heater	H-101
MOC	CS	CS	CS	Tube P (bar)	26.0
Temp. (in) (°C)	55	112	38		
Pres. (in) (bar)	1.2	2.2	23.9		
Pres. (out) (bar)	27.0	4.4	25.5		

Key:

MOC	Materials of construction	Par	Partial
316SS	Stainless steel type 316	F.H.	Fixed head
CS	Carbon steel	Fl.H.	Floating head
Vap	Stream being vaporized	Rbl	Reboiler
Cond	Stream being condensed	s.p.	Splash plate
Recipr.	Reciprocating	l	Liquid
Centrf.	Centrifugal	MDP	Multiple double pipe

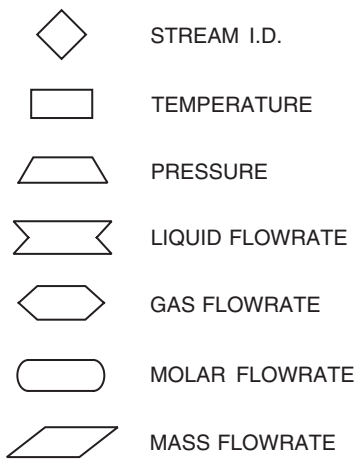


Figure 1.6 Symbols for Stream Identification

pressures associated with the reactor, flowrates of feed and product streams, and stream pressures and temperatures that are substantially higher than the rest of the process. Additional needs are process specific. Examples 1.5–1.7 illustrate where and why information should be included directly on a PFD.

Example 1.5

Acrylic acid is temperature sensitive and polymerizes at 90°C when present in high concentration. It is separated by distillation and leaves from the bottom of the tower. In this case, a temperature and pressure flag would be provided for the stream leaving the reboiler.

Example 1.6

In the benzene process, Figure 1.5, the feed to the reactor is substantially hotter than to the rest of the equipment and is crucial to the operation of the process. In addition, the reaction is

exothermic, and the reactor effluent temperature must be carefully monitored. For this reason Stream 6 (entering) and Stream 9 (leaving) have temperature flags.

Example 1.7

The pressures of the streams to and from R-101 in the benzene process are also important. The difference in pressure between the two streams gives the pressure drop across the reactor. This, in turn, gives an indication of any maldistribution of gas through the catalyst beds. For this reason, pressure flags are also included on Streams 6 and 9 in Figure 1.5.

Of secondary importance is the fact that flags are useful in reducing the size of the flow summary table. For pumps, compressors, and heat exchangers, the mass flows are the same for the input and output streams, and complete entries in the stream table are not necessary. If the input (or output) stream is included in the stream table, and a flag is added to provide the temperature (in the case of a heat exchanger) or the pressure (in the case of a pump) for the exit stream, then there is no need to present this stream in the flow summary table. Example 1.8 illustrates this point.

Example 1.8

Follow Stream 13 leaving the top of the benzene column in the benzene PFD given in Figure 1.5 and in Table 1.5. This stream passes through the benzene condenser, E-104, into the reflux drum, V-104. The majority of this stream then flows into the reflux pump, P-102, and leaves as Stream 14, while the remaining noncondensables leave the reflux drum in Stream 19. The mass flowrate and component flowrates of all these streams are given in Table 1.5. The stream leaving E-104 is not included in the stream table. Instead, a flag giving the temperature (112°C) is provided on the diagram (indicating condensation without subcooling). An additional flag, showing the pressure following the pump, is also shown. In this case the entry for Stream 14 could be omitted from the stream table, because it is simply the sum of Streams 12 and 15, and no information would be lost.

More information could be included in Figure 1.5 had space for the diagram not been limited by text format. It is most important that the PFD remain uncluttered and easy to follow in order to avoid errors and misunderstandings. Adding additional material to Figure 1.5 risks sacrificing clarity.

The flow table presented in Table 1.5, the equipment summary presented in Table 1.7, and Figure 1.5 taken together constitute all the information contained on a commercially produced PFD.

The PFD is the first comprehensive diagram drawn for any new plant or process. It provides all of the information needed to understand the chemical process. In addition, sufficient information is given on the equipment, energy, and material balances to establish process control protocol and to prepare cost estimates to determine the economic viability of the process.

Many additional drawings are needed to build the plant. However, all the process information required can be taken from this PFD. As described in the narrative at the beginning of this chapter, the development of the PFD is most often carried out by the operating company. Subsequent activities in the design of the plant are often contracted out.

The value of the PFD does not end with the construction of the plant. It remains the document that best describes the process, and it is used in the training of operators and new engineers. It is consulted regularly to diagnose operating problems that arise and to predict the effects of changes on the process. Finally as changes are made to the process the PFD is updated to reflect the current operating conditions and process performance.

1.3 PIPING AND INSTRUMENTATION DIAGRAM (P&ID)

The piping and instrumentation diagram (P&ID), also known as the mechanical flow diagram (MFD), provides information needed by engineers to begin planning for the construction of the plant. The P&ID includes every mechanical aspect of the plant except the information given in Table 1.8. The general conventions used in drawing P&IDs are given in Table 1.9.

Each PFD will require many P&IDs to display all the necessary data. Figure 1.7 is a representative P&ID for the distillation section of the benzene process shown in Figure 1.5. The P&ID presented in Figure 1.7 provides information on the piping, and this is included as part of the diagram. As an alternative, each pipe can be numbered, and the specifics of every pipe/line can be provided

Table 1.8 Exclusions from Piping and Instrumentation Diagram

1. Operating Conditions *T, P*
2. Stream Flows
3. Equipment Locations
4. Pipe Routing
a. Pipe Lengths
b. Pipe Fittings (elbows, tee, etc., are not shown but valves and instrument connections above a certain minimum size are normally shown)
5. Supports, Structures, and Foundations

Table 1.9 Conventions in Constructing Piping and Instrumentation Diagrams

For Equipment—Show Every Piece Including
Spare Units
Parallel Units
Summary Details of Each Unit
For Piping—Include All Lines Including Drains and Sample Connections, and Specify
Size (Use Standard Sizes)
Schedule (Thickness)
Materials of Construction
Insulation (Thickness and Type)
For Instruments—Identify
Indicators
Recorders
Controllers
Show Instrument Lines
For Utilities—Identify
Entrance Utilities
Exit Utilities
Exit to Waste Treatment Facilities

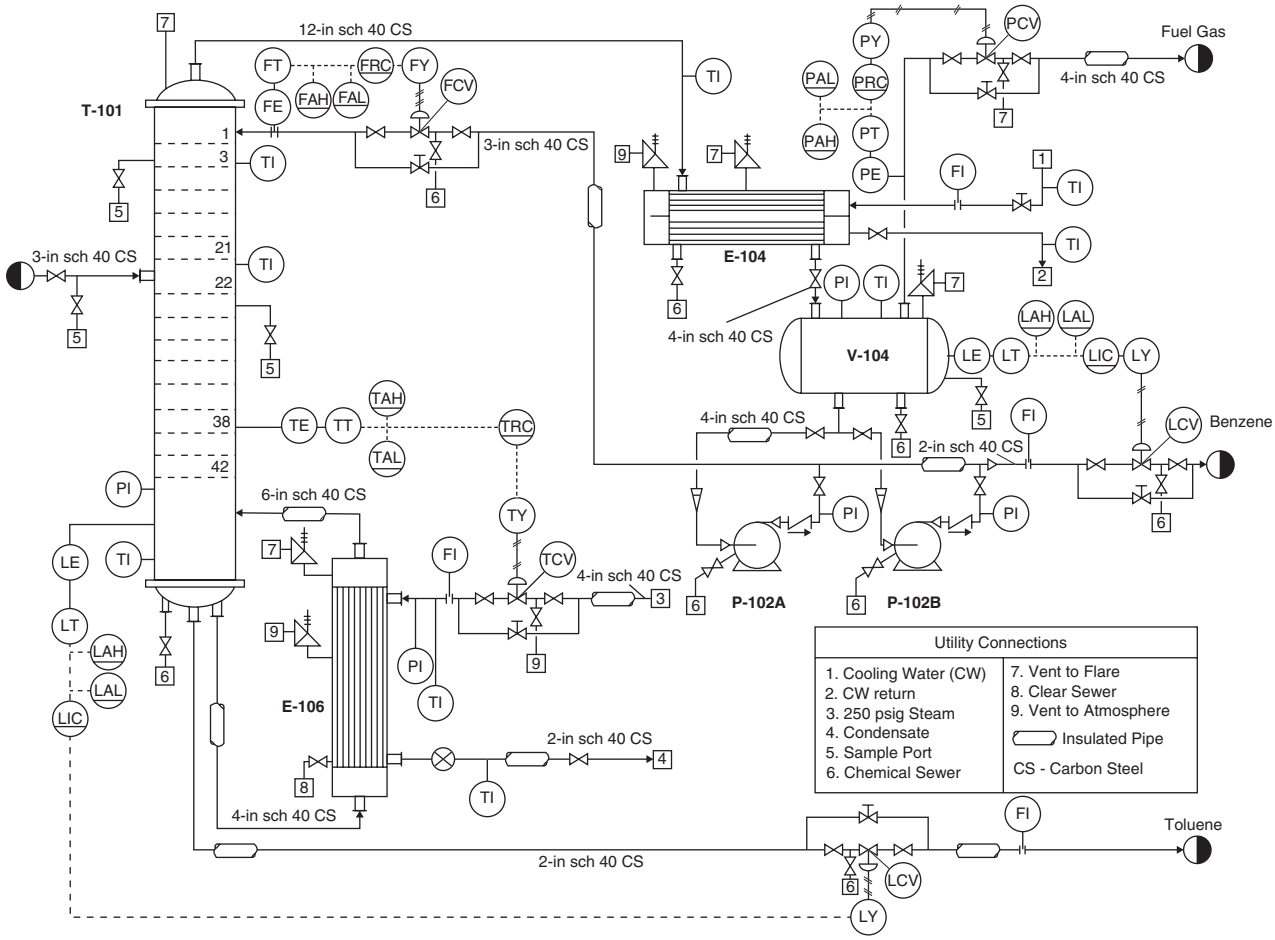


Figure 1.7 Piping and Instrumentation Diagram for Benzene Distillation (adapted from Kauffman, D., *Flow Sheets and Diagrams, AIChE Modular Instruction, Series G: Design of Equipment,* series editor J. Beckman, AIChE, New York, 1986, vol. 1, Chapter G.1.5, AIChE copyright © 1986 AIChE, all rights reserved)

in a separate table accompanying this diagram. When possible, the physical size of the larger-sized equipment is reflected by the size of the symbol in the diagram.

Utility connections are identified by a numbered box in the P&ID. The number within the box identifies the specific utility. The key identifying the utility connections is shown in a table on the P&ID.

All process information that can be measured in the plant is shown on the P&ID by circular flags. This includes the information to be recorded and used in process control loops. The circular flags on the diagram indicate where the information is obtained in the process and identify the measurements taken and how the information is used. Table 1.10 summarizes the conventions used to identify information related to instrumentation and control. Example 1.9 illustrates the interpretation of instrumentation and control symbols.

Example 1.9

Consider the benzene product line leaving the right-hand side of the P&ID in Figure 1.7. The flowrate of this stream is controlled by a control valve that receives a signal from a level measuring element placed on V-104. The sequence of instrumentation is as follows:

A level sensing element (LE) is located on the reflux drum V-104. A level transmitter (LT) also located on V-104 sends an electrical signal (designated by a dashed line) to a level indicator and controller (LIC). This LIC is located in the control room on the control panel or console (as indicated by the horizontal line under LIC) and can be observed by the operators. From the LIC, an electrical signal is sent to an instrument (LY) that computes the correct valve position and in turn sends a pneumatic signal (designated by a solid line with cross hatching) to activate the control valve (LCV). In order to warn operators of potential problems, two alarms are placed in the control room. These are a high-level alarm (LAH) and a low-level alarm (LAL), and they receive the same signal from the level transmitter as does the controller.

This control loop is also indicated on the PFD of Figure 1.5. However, the details of all the instrumentation are condensed into a single symbol (LIC), which adequately describes the essential process control function being performed. The control action that takes place is not described explicitly in either drawing. However, it is a simple matter to infer that if there is an increase in the level of liquid in V-104, the control valve will open slightly and the flow of benzene product will increase, tending to lower the level in V-104. For a decrease in the level of liquid, the valve will close slightly.

The details of the other control loops in Figures 1.5 and 1.7 are left to problems at the end of this chapter. It is worth mentioning that in virtually all cases of process control in chemical processes, the final control element is a valve. Thus, all control logic is based on the effect that a change in a given flowrate has on a given variable. The key to understanding the control logic is to identify which flowrate is being manipulated to control a given variable. Once this has been done, it is a relatively simple matter to see in which direction the valve should change in order to make the desired change in the control variable. The response time of the system and type of control action used—for example, proportional, integral, or differential—are left to the instrument engineers and are given in a typical process control course but are not covered in this text.

The final control element in nearly all chemical process control loops is a valve.

Table 1.10 Conventions Used for Identifying Instrumentation on P&IDs (ISA standard ISA-S5-1, [4])

Location of Instrumentation	
◯	Instrument Located in Plant
⊖	Instrument Located on Front of Panel in Control Room
⊖ (dashed)	Instrument Located on Back of Panel in Control Room

Meanings of Identification Letters (XYY)		
	First Letter (X)	Second or Third Letter (Y)
A	Analysis	Alarm
B	Burner Flame	
C	Conductivity	Control
D	Density or Specific Gravity	
E	Voltage	Element
F	Flowrate	
H	Hand (Manually Initiated)	High
I	Current	Indicate
J	Power	
K	Time or Time Schedule	Control Station
L	Level	Light or Low
M	Moisture or Humidity	Middle or Intermediate
O		Orifice
P	Pressure or Vacuum	Point
Q	Quantity or Event	
R	Radioactivity or Ratio	Record or print
S	Speed or Frequency	Switch
T	Temperature	Transmit
V	Viscosity	Valve, Damper, or Louver
W	Weight	Well
Y		Relay or Compute
Z	Position	Drive

Identification of Instrument Connections	
———	Capillary
—// ———	Pneumatic
·····	Electrical

The generation of the final P&ID is one of the last stages of the design process and this diagram serves as a guide for those who will be responsible for the final design and construction. Based on this diagram,

1. Mechanical engineers and civil engineers will design and install the various pieces of process equipment.
2. Instrument engineers will specify, install, and check control systems.
3. Piping engineers will develop plant layout, piping isometrics, and elevation drawings.
4. Project engineers will develop plant and construction schedules.

Before final acceptance, the P&IDs serve as a checklist in the construction phase against which each item in the plant is checked.

The P&ID is also used to train operators. Once the plant is built and is operational, there are limits to what operators can do. About all that can be done to correct or alter performance of the plant is to open, close, or change the position of a valve. Part of the training would pose situations and require the operators to be able to describe what specific valve should be changed, how it should be changed, and what to observe in order to monitor the effects of the change. Plant simulators (similar to flight simulators) are often used in operator training. These programs are sophisticated, real-time process simulators that show a trainee operator how quickly changes in controlled variables propagate through the process. It is also possible for such programs to display scenarios of process upsets so that operators can receive training in recognizing and correcting such situations. These types of programs are very useful and cost-effective in initial operator training. However, the use of P&IDs is still very important in this regard.

The P&ID is particularly important for the development of start-up procedures when the plant is not under the influence of the installed process control systems. An example of a start-up procedure is given in Example 1.10.

Example 1.10

Consider the start-up of the distillation column shown in Figure 1.7. What sequence would be followed?

Solution

The procedure is beyond the scope of this text, but it would be developed from a series of questions such as

a. What valve should be opened first?
b. What should be done when the temperature of...reaches...?
c. To what value should the controller be set?
d. When can the system be put on automatic control?

These last three sections have followed the development of a process from a simple BFD through the PFD and finally to the P&ID. Each step showed additional information. This can be seen by following the progress of the distillation unit as it moves through the three diagrams described.

1. **Block Flow Diagram (BFD) (see Figure 1.1):** The column was shown as a part of one of the three process blocks.
2. **Process Flow Diagram (PFD) (see Figure 1.5):** The column was shown as the following set of individual equipment: a tower, condenser, reflux drum, reboiler, reflux pumps, and associated process controls.
3. **Piping and Instrumentation Diagram (P&ID) (see Figure 1.7):** The column was shown as a comprehensive diagram that includes additional details such as pipe sizes, utility streams, sample taps, numerous indicators, and so on. It is the only unit operation on the diagram.

The value of these diagrams does not end with the start-up of the plant. The design values on the diagram are changed to represent the actual values determined under normal operating conditions. These conditions form a "base case" and are used to compare operations throughout the life of the plant.

1.4 ADDITIONAL DIAGRAMS

During the planning and construction phases of a new project, many additional diagrams are needed. Although these diagrams do not possess additional process information, they are essential to the successful completion of the project. Computers are being used more and more to do the tedious work associated with all of these drawing details. The creative work occurs through the development of the concepts provided in the BFD and the process development required to produce the PFD. The computer can help with the drawings but cannot create a new process. Computers are valuable in many aspects of the design process where the size of equipment to do a specific task is to be determined. Computers are also used when considering performance problems that deal with the operation of existing equipment. However, steady-state simulations are limited when dealing with diagnostic problems that are required throughout the life of the plant and operational experience is important in diagnosing problems within the process.

The diagrams presented here are in both American Engineering and SI units. The most noticeable exception is in the sizing of piping, where pipes are specified in inches and pipe schedule. This remains the way they are produced and purchased in the United States. A process engineer today must be comfortable with SI, conventional metric, and American (formerly British, who now use SI exclusively) Engineering units.

These additional diagrams are discussed briefly below.

A **utility flowsheet** may be provided that shows all the headers for utility inputs and outputs available along with the connections needed to the process. It provides information on the flows and characteristics of the utilities used by the plant. In particular, it is common to perform utility balances (steam balance, cooling water balance, etc.) in order to check the total utilities required and to ensure that the design of the facilities to produce the utilities are sized correctly.

Vessel sketches, logic ladder diagrams, wiring diagrams, site plans, structural support diagrams, and many other drawings are routinely used but add little to our understanding of the basic chemical processes that take place.

Additional drawings are necessary to locate all of the equipment in the plant. **Plot plans** and **elevation diagrams** are provided that locate the placement and elevation of all of the major pieces of equipment such as towers, vessels, pumps, heat exchangers, and so on. When constructing these drawings, it is necessary to consider and provide for access for repairing equipment, removing

tube bundles from heat exchangers, replacement of units, and so on. What remains to be shown is the addition of the structural support and piping.

Piping isometrics are drawn for every piece of pipe required in the plant. These drawings are 3-D sketches of the pipe run, indicating the elevations and orientation of each section of pipe. An example of a piping isometric for the liquid return line from V-104 to T-101 is illustrated in Figure 1.8. Note that the drawing has all the information needed to estimate the frictional losses in the pipe at a given flowrate (see Chapter 19). In addition, there is enough information for a piping engineer/technician to construct and route the pipe through the plant. In the past, it was also common to build a **scale model (prior to 1980)** for comprehensive plants so the process could be viewed in three dimensions and modified to remove any potential problems. Over the past thirty or more years, scale models have been replaced by three-dimensional **computer aided design (CAD)** programs that are capable of representing the plant as-built in three dimensions. They provide an opportunity to view the local equipment topology from any angle at any location inside the plant. One can actually "walk through" the plant and preview what will be seen when the plant is built. The ability to "view" the plant before construction is made even more realistic with the development and implementation of **virtual reality software**. With this relatively new tool, it is possible for an avatar operated by an engineer to not only to walk through the plant but also to "touch" the equipment, turn valves, "climb" to the top of distillation columns, and so on. In the next section, the information needed to complete a preliminary plant layout design is reviewed, and the logic used to locate the process units in the plant and how the elevations of different equipment are determined are briefly explained.

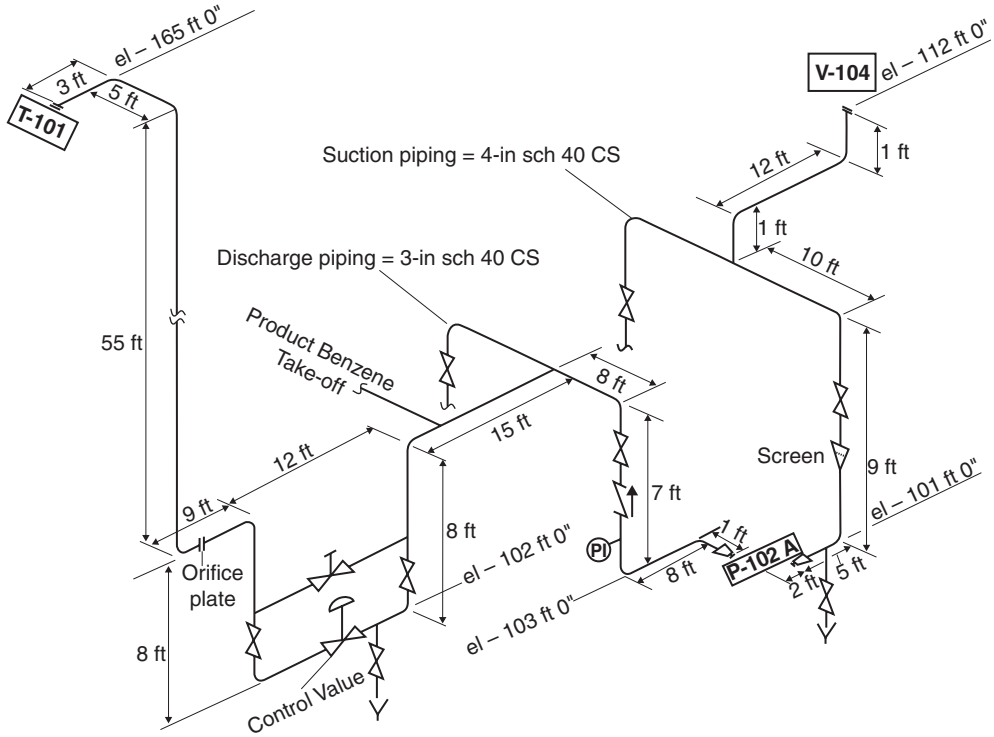


Figure 1.8 Piping Isometric for the Liquid Line from the Overhead Reflux Drum (V-104) to the Distillation Tower (T-101)

1.5 THREE-DIMENSIONAL REPRESENTATION OF A PROCESS

As mentioned earlier, the major products of design work, both chemical and mechanical, are recorded on two-dimensional diagrams (PFD, P&ID, etc.). However, when it comes to the construction of the plant, there are many issues that require a three-dimensional representation of the process. For example, the location of shell-and-tube exchangers must allow for tube bundle removal for cleaning and repair. Locations of pumps must allow for access for maintenance and replacement. For compressors, this access may also require that a crane be able to remove and replace a damaged drive. Control valves must be located at elevations that allow operator access. Sample ports and instrumentation must also be located conveniently. For anyone who has toured a moderate-to-large chemical facility, the complexity of the piping and equipment layout is immediately apparent. Even for experienced engineers, the review of equipment and piping topology is far easier to accomplish in 3-D than 2-D. Due to the rapid increase in computer power and advanced software, such representations are now done routinely using the computer. In order to "build" an electronic representation of the plant in 3-D, all the information in the previously mentioned diagrams must be accessed and synthesized. This in itself is a daunting task, and a complete accounting of this process is well beyond the scope of this text. However, in order to give the reader a flavor of what can now be accomplished using such software, a brief review of the principles of plant layout design will be given. A more detailed account involving a virtual plant tour of the dimethyl ether (DME) plant (Appendix B.1) can be found on the website.

For a complete, detailed analysis of the plant layout, all equipment sizes, piping sizes, PFDs, P&IDs, and all other information should be known. However, for this description, a preliminary plant layout based on information given in the PFD for the DME process (Figure B.1.1) in Appendix B is considered. Using this figure and the accompanying stream tables and equipment summary table (Tables B.1.1 and B.1.3), the following steps are followed:

1. *The PFD is divided into logical subsystems.* For the DME process, there are three logical subsections, namely, the feed and reactor section, the DME purification section, and the methanol separation and recycle section. These sections are shown as dotted lines on Figure 1.9.
2. *For each subsystem, a preliminary plot plan is created.* The topology of the plot plan depends on many factors, the most important of which are discussed below.

   In general, the layout of the plot plan can take one of two basic configurations: the grade-level, horizontal, in-line arrangement and the structure-mounted vertical arrangement [5]. The grade-level, horizontal, in-line arrangement will be used for the DME facility. In this arrangement, the process equipment units are aligned on either side of a pipe rack that runs through the middle of the process unit. The purpose of the pipe rack is to carry piping for utilities, product, and feed to and from the process unit. Equipment is located on either side of the pipe rack, which allows for easy access. In addition, vertical mounting of equipment is usually limited to a single level. This arrangement generally requires a larger "footprint" and, hence, more land than does the structure-mounted vertical arrangement. The general arrangement for these layout types is shown in Figure 1.10.

   The minimum spacing between equipment should be set early on in the design. These distances are set for safety purposes and should be set with both local and national codes in mind. A comprehensive list of the recommended minimum distances between process equipment is given by Bausbacher and Hunt [5]. The values for some basic process equipment are listed in Table 1.11.

   The sizing of process equipment should be completed and the approximate location on the plot plan determined. Referring to Table B.1.3 for equipment specifications gives some

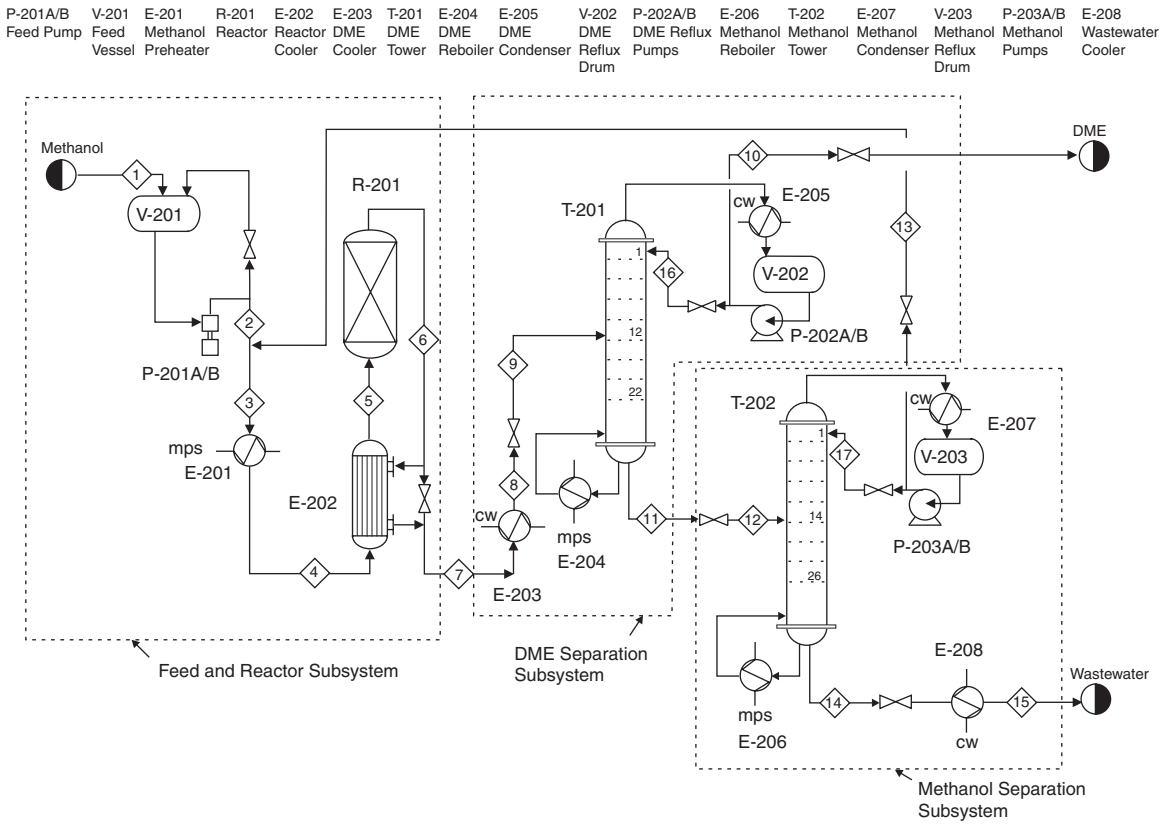


Figure 1.9 Subsystems for Preliminary Plan Layout for DME Process

Table 1.11 Recommended Minimum Spacing (in Feet) between Process Equipment for Refinery, Chemical, and Petrochemical Plants

	Pumps	Compressors	Reactors	Towers and Vessels	Exchangers
Pumps	M	25	M	M	M
Compressors		M	30	M	M
Reactors			M	15	M
Towers				M	M
Exchangers					M

M = minimum for maintenance access

Source: Process Plant Layout and Piping Design, by E. Bausbacher and R. Hunt, © 1994, reprinted by permission of Pearson Education, Inc., Upper Saddle River, NJ

idea of key equipment sizes. For example, the data given for the reflux drums V-202 and V-203, reactor R-201, and towers T-201 and T-202 are sufficient to sketch these units on the plot plan. However, pump sizes must be obtained from vendors or previous jobs, and additional calculations for heat exchangers must be done to estimate their required footprint on the plot plan. Calculations to illustrate the estimation of equipment footprints are given in Example 1.11.

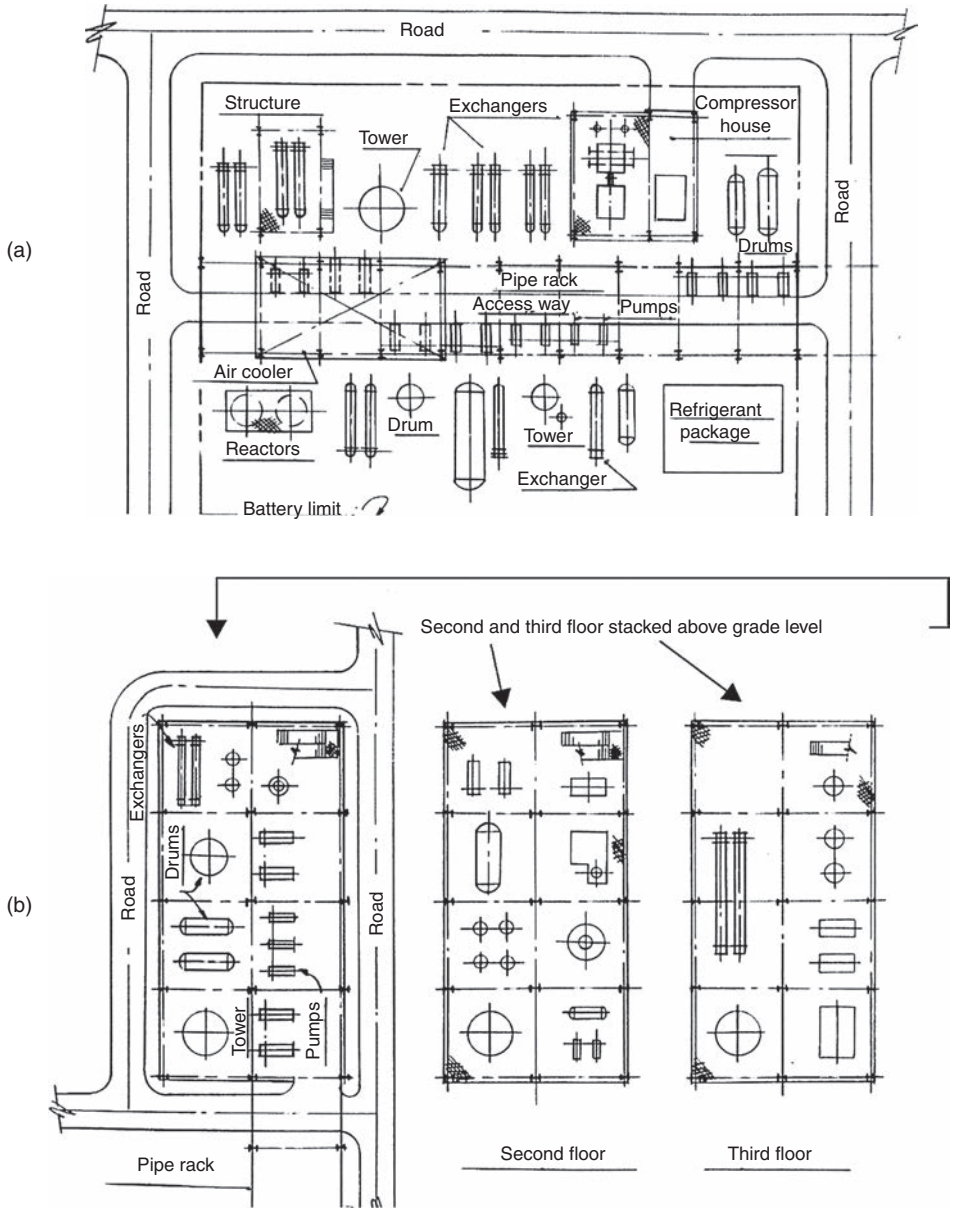


Figure 1.10 Different Types of Plant Layout: (a) Grade-Mounted, Horizontal, In-line Arrangement, and (b) Structure-Mounted Vertical Arrangement

(*Source: Process Plant Layout and Piping Design*, by E. Bausbacher and R. Hunt, © 1994, reprinted by permission of Pearson Education, Inc., Upper Saddle River, NJ)

Example 1.11

Estimate the footprint for E-202 in the DME process.
From Table B.1.3 the following information can be found:

Floating-Head Shell-and-Tube design
Area = 171 m^2
Hot Side—Temperatures: in at 364°C and out at 281°C
Cold Side—Temperatures: in at 154°C and out at 250°C
Choose a two-shell pass and four-tube pass exchanger
Area per shell = 171/2 = 85.5 m^2
Using 12 ft, 1-in OD tubes, 293 tubes per shell are needed

Assuming the tubes are laid out on a ¼-in square pitch, a 27-in ID shell is required, see Table 20.6.

Assume that the front and rear heads (where the tube fluid turns at the end of the exchanger) are 30-in in diameter and require 2 ft of length each (including flanges), and that the two shells are stacked on top of each other. The footprint of the exchanger is given in Figure E1.11.

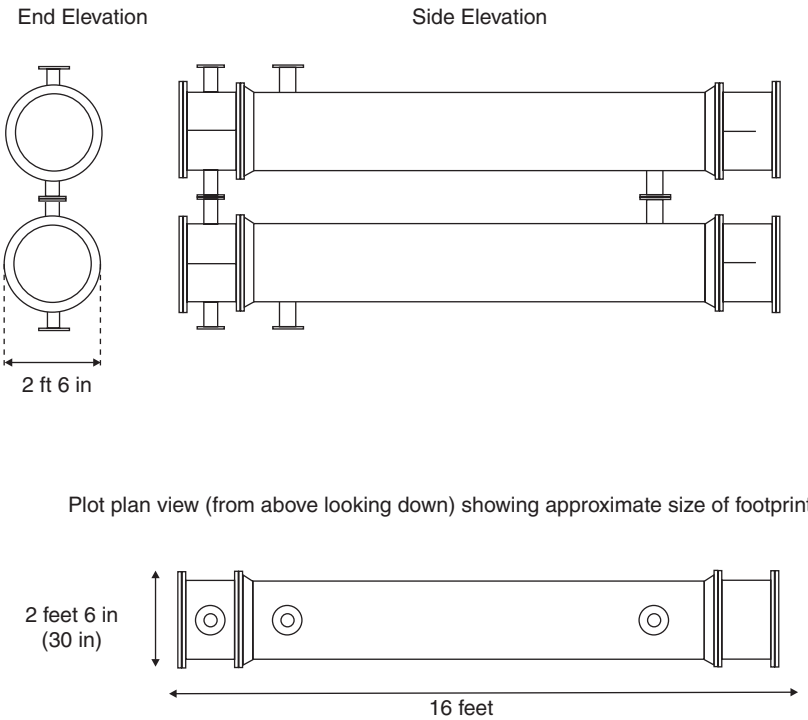


Figure E1.11 Approximate Dimensions and Footprint of Exchanger E-202

3. *Estimates of major process pipe sizes are made*. In order to estimate these pipe sizes, it is necessary to use some heuristics. A heuristic is a simple algorithm or hint that allows an approximate answer to be calculated. The preliminary design of a piece of equipment might well use many such heuristics, and some of these might conflict with each other. Like any simplifying procedure, the result from a heuristic must be reviewed carefully. For preliminary purposes, the heuristics from Chapter 11 can be used to estimate approximate pipe sizes. Example 1.12 illustrates the heuristic for calculating pipe size.

Example 1.12

Consider the suction line to P-202 A/B; what should the pipe diameter be?

Solution

From Table 11.8, 1(b) for liquid pump suction, the recommended liquid velocity and pipe diameter are related by $u = (1.3 + D\ (\text{in})/6)$ ft/s.
From Table B.1.1, the mass flowrate of the stream entering P-202,
$\dot{m}$ = Stream 16 + Stream 10 = 2170 + 5970 = 8140 kg/h and the density is found to be 800 kg/m^3.
The volumetric flowrate is 8140/800 = 10.2 m^3/h = 0.00283 m^3/s = 0.0998 ft^3/s.
The procedure is to calculate the velocity in the suction line and compare it to the heuristic. Using this approach, Table E1.12 is constructed:

Table E1.12 Actual Velocities and Velocities from Heuristic for the Suction Line to P-202 A/B

Nominal Pipe Diameter (inch)	Velocity (ft/s) = Vol Flow/Flow Area	Velocity (ft/s) from $u = (1.3 + D/6)$
1.0	18.30	1.47
1.5	8.13	1.55
2.0	4.58	1.63
3.0	2.03	1.80
4.0	1.14	1.97

The data in Table E1.12 are plotted in Figure E1.12 and show that the pipe diameter satisfying both the heuristic and the continuity equation lies between 3 and 4 inches. Taking a conservative estimate, a 4-in suction line is chosen for P-202.

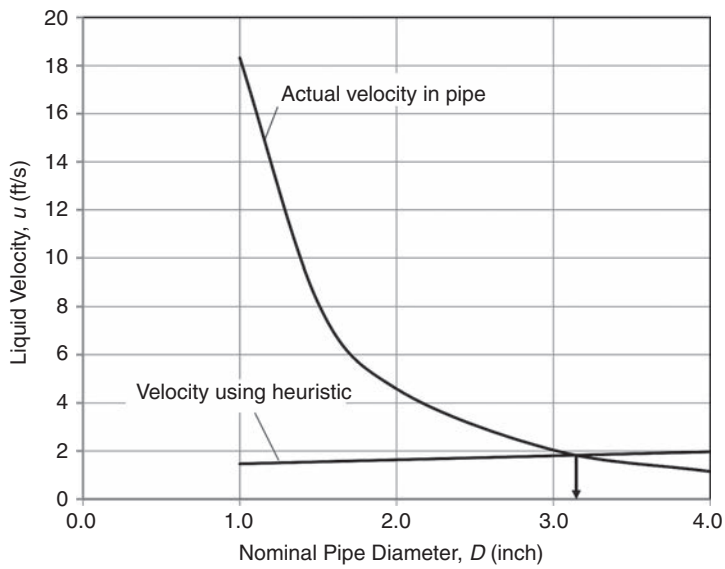


Figure E1.12 Suction Line Velocity and Velocity Using Heuristic as a Function of Nominal Pipe Diameter

4. *Placement of equipment within the plot plan*. Equipment placement must be made considering the required access for maintenance of the equipment and also the initial installation. Although this step may seem elementary, there are many cases [5] where the incorrect placement of equipment subsequently led to considerable cost overruns and major problems both during the construction of the plant and during maintenance operations. Consider the example shown in Figure 1.11(a), where a vessel, two towers, and a heat exchanger are shown in the plot plan. Clearly, T-901 blocks the access to the exchanger's tube bundle, which often requires removal to change leaking tubes or to remove scale on the outside of the tubes. With this arrangement, the exchanger would have to be lifted up vertically and placed somewhere where there was enough clearance so that the tube bundle could be removed. However, vessel, V-903, and tower T-902 are located such that crane access is severely limited and a very tall (and expensive) crane would be required. The relocation of these same pieces of equipment, as shown in Figure 1.11(b), alleviates both these problems. There are too many considerations of this type to cover in detail in this text, and the reader is referred to Bausbacher and Hunt [5] for more in-depth coverage of these types of problems. Considering the DME facility, a possible arrangement for the feed and reactor subsection is shown in Figure 1.12.
5. *The elevation of all major equipment is established*. In general, equipment located at grade (ground) level is easier to access and maintain and is cheaper to install. However, there are circumstances that dictate that equipment be elevated in order to provide acceptable operation. For example, the bottoms product of a distillation column is a liquid at its bubble point. If this liquid is fed to a pump, then, as the pressure drops in the suction line due to friction, the liquid boils and causes the pumps to cavitate. To alleviate this problem, it is necessary to elevate the bottom of the column relative to the pump inlet, in order to increase the Net Positive Suction Head Available (for more detail about $NPSH_A$ see Chapter 19). This can be done by digging a pit below grade for the pump or by elevating the tower. Pump pits have a tendency to accumulate denser-than-air gases, and maintenance of equipment in such pits is

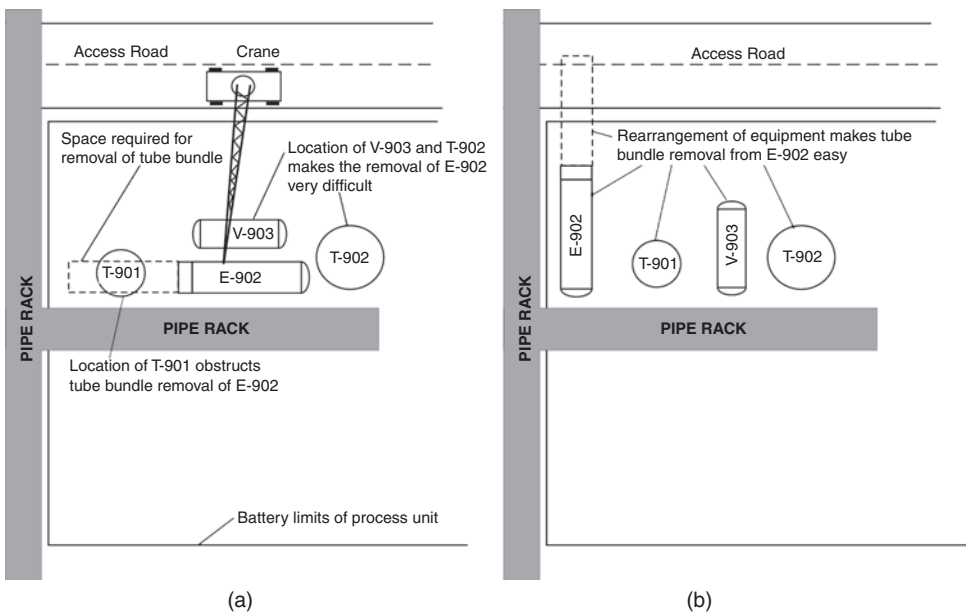


Figure 1.11 The Effect of Equipment Location on the Ease of Access for Maintenance, Installation, and Removal

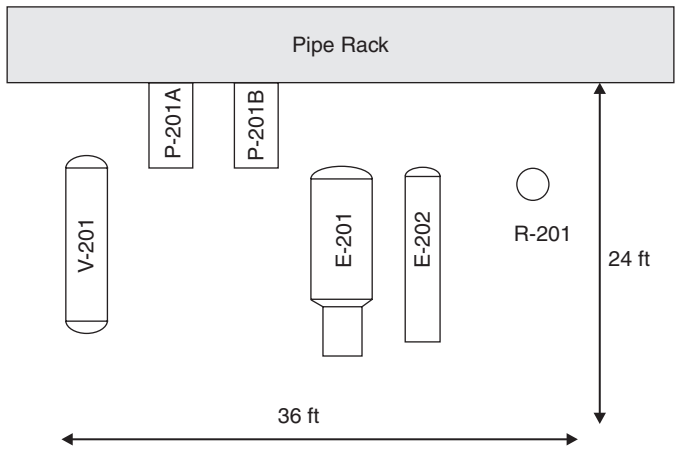


Figure 1.12 Possible Equipment Arrangement for the Reactor and Feed Section of DME Facility, Unit 200

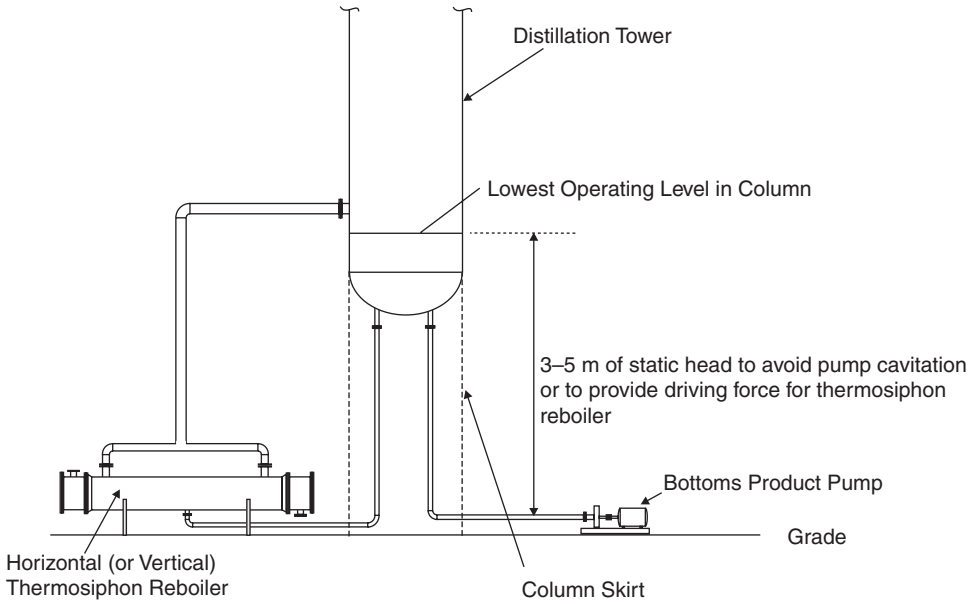


Figure 1.13 Sketch Illustrating Reasons for Elevating Distilling Column

dangerous due to the possibility of suffocation and poisoning (if the gas is toxic). For this reason, towers are generally elevated between 3 and 5 m (10 and 15 ft) above ground level by using a "skirt." This is illustrated in Figure 1.13. Another reason for elevating a distillation column is also illustrated in Figure 1.13. Often a thermosiphon reboiler is used. These reboilers use the difference in density between the liquid fed to the reboiler and the two-phase mixture (saturated liquid-vapor) that leaves the reboiler to "drive" the circulation of bottoms liquid through the reboiler. In order to obtain an acceptable driving force for this circulation, the static head of the liquid must be substantial, and a 3–5 m height differential between the liquid level in the column and the liquid inlet to the reboiler is typically sufficient. Examples showing when equipment elevation is required are given in Table 1.12.

Table 1.12 Reasons for Elevating Equipment

Equipment to Be Elevated	Reason for Elevation
Columns or vessels	When the NPSH available ($NPSH_A$) is too low to avoid cavitation in the discharge pump, equipment must be elevated.
Columns	To provide driving head for thermosiphon reboilers.
Any equipment containing suspended solids or slurries	To provide gravity flow of liquids containing solids that avoids the use of problematic slurry pumps.
Contact barometric condensers	This equipment is used to produce vacuum by expanding high-pressure steam through an ejector. The condensables in the vapor are removed by direct contact with a cold-water spray. The tail pipe of such a condenser is sealed with a 34-foot leg of water.
Critical fire-water tank (or cooling water holding tank)	In some instances, flow of water is absolutely critical, for example, in firefighting or critical cooling operations. The main water supply tank for these operations may be elevated to provide enough water pressure to eliminate the need for feed pumps.

6. *Major process and utility piping are sketched in*. The final step in this preliminary plant layout is to sketch in where the major process (and utility) pipes (lines) go. Again, there are no set rules to do this. However, the most direct route between equipment that avoids clashes with other equipment and piping is usually desirable. It should be noted that utility lines originate and usually terminate in headers located on the pipe rack. When process piping must be run from one side of the process to another, it may be convenient to run the pipe on the pipe rack. All control valves, sampling ports, and major instrumentation must be located conveniently for the operators. This usually means that they should be located close to grade or on a steel access platform. This is also true for equipment isolation valves.

1.6 THE 3-D PLANT MODEL

The best way to see how all the above elements fit together is to view the Virtual Plant Tour AVI file on the website for this book. The quality and level of detail that 3-D software is capable of giving depend on the system used and the level of detailed engineering that is used to produce the model. Figures 1.14–1.16 were generated for the DME facility using the PDMS software package from Cadcentre, Inc. (These figures and the Virtual_Plant_Tour.AVI file are presented here with permission of Cadcentre, Inc.) In Figure 1.14, an isometric view of the DME facility is shown. All major process equipment, major process and utility piping, and basic steel structures are shown. The pipe rack is shown running through the center of the process, and steel platforms are shown where support of elevated process equipment is required. The distillation sections are shown to the rear of the figure on the far side of the pipe rack. The reactor and feed section is shown on the near side of the pipe rack. The elevation of the process equipment is better illustrated in Figure 1.15, where the piping and structural steel have been removed. The only elevated equipment apparent from this figure are the overhead condensers and reflux drums for the distillation columns. The overhead condensers are located vertically above their respective reflux drums to allow for the gravity flow of condensate from the exchangers to the drums. Figure 1.16 shows the arrangement of process

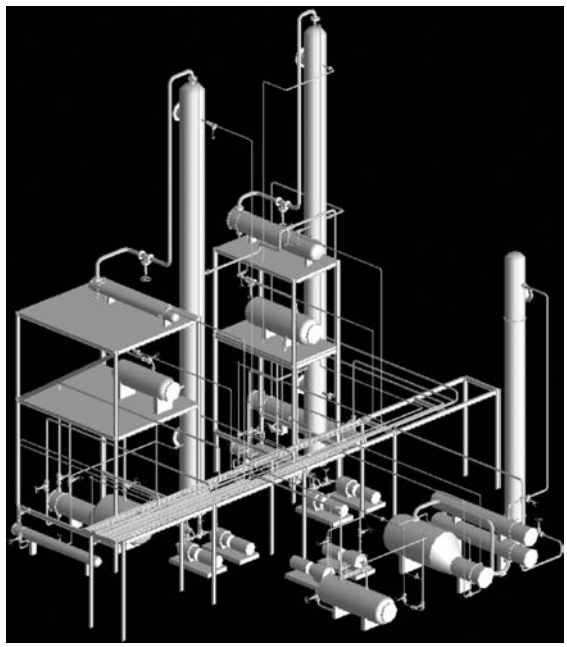


Figure 1.14 Isometric View of Preliminary 3-D Plant Layout Model for DME Process (Reproduced by Permission of Cadcentre, an Aveva Group Company, from their Vantage/PDMS Software)

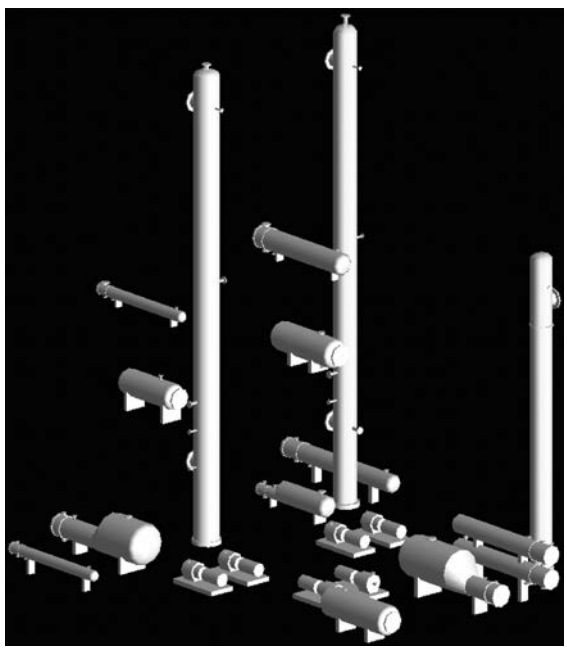


Figure 1.15 3-D Representation of Preliminary Equipment Layout for the DME Process (Reproduced by Permission of Cadcentre, an Aveva Group Company, from their Vantage/PDMS Software)

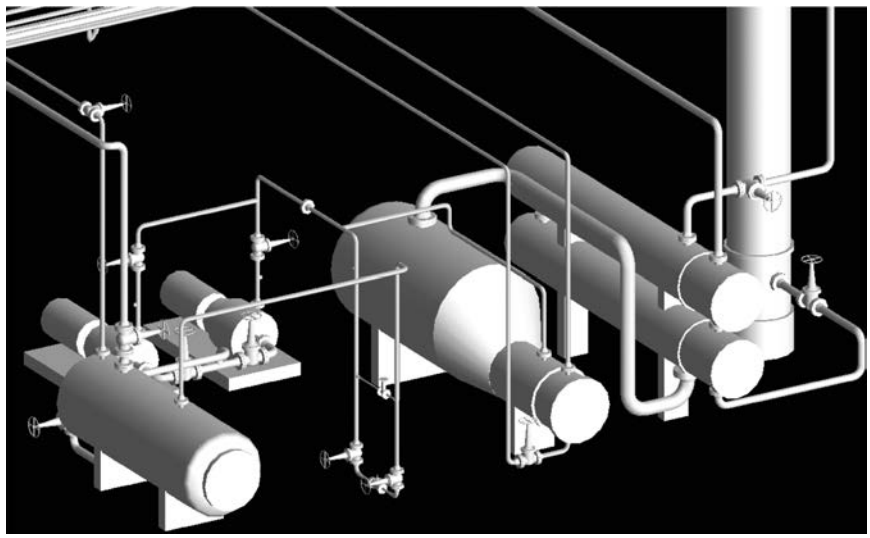


Figure 1.16 3-D Representation of the Reactor and Feed Sections of the DME Process Model (Reproduced by Permission of Cadcentre, an Aveva Group Company, from their Vantage/PDMS Software)

equipment and piping for the feed and reactor sections. The layout of equipment corresponds to that shown in Figure 1.12. It should be noted that the control valve on the discharge of the methanol feed pumps is located close to grade level for easy access.

1.7 OPERATOR AND 3-D IMMERSIVE TRAINING SIMULATORS

1.7.1 Operator Training Simulators (OTS)

Up to this point in the chapter, the different elements and diagrams used in the specification and description of a process have been covered. The means by which the material balances, energy balances, and design calculations for the various unit operations, required to specify all the design conditions, have been carried out has not been covered. Indeed, the simulation of chemical processes using programs such as CHEMCAD, Aspen Plus, PRO/II, HYSIS, and others is not addressed until much later, in Chapter 13. Nevertheless, it should be clear that extensive simulation of the process will be required to determine and to specify all of the conditions needed in the design. Typically, these simulations are carried out under steady-state conditions and represent a single design operating point, although simulations for several different operating points might also be made. The steady-state simulation of the process is clearly very important from the standpoint of defining the design conditions and specifying the equipment parameters, such as vessel sizes, heat-exchanger areas and duties, pipe sizes, and so on. However, once the plant has been built, started up, and commissioned, it is rare that the process will operate at that design condition for any given period of time. Moreover, how the process can be started up or run at, for example, 65% or 110% of design capacity is not evident from the original design. Nevertheless, the plant will be run at off-design conditions throughout its life. In order to help operators and engineers understand how to start up and shut down the process, deal with emergencies, or operate at off-design conditions, an operator training simulator (OTS) may be built.

The foundation of an OTS is a dynamic simulation (model) of the process to which a human machine interface (HMI) is connected. The HMI, in its simplest form, is a pictorial representation of the

process that communicates with the dynamic model, and through it, process variables are displayed. The HMI also displays all the controls for the process; an operator can control the process by changing these controls. An example of an HMI is shown in Figure 1.17. This particular example shows a portion of an acid-gas recovery (AGR) unit for an OTS developed by the Department of Energy to simulate an IGCC (Integrated Gasification Combined Cycle) coal-fed power plant. Process variables calculated by the dynamic model are displayed in boxes throughout the HMI. Operators can monitor the change in these variables with time just as they would in a control room situation. The only difference is that the process is simulated rather than actually operating. In general terms, the OTS functions for an operator just as a flight simulator does for a pilot or astronaut. Therefore, operators and engineers can gain operational experience and understanding about a process or plant through the OTS but with the added benefit that any mistakes or errors can be identified and corrected during training sessions without exposing personnel to any risks that might occur if training were to be done on the actual plant.

The starting point for developing an OTS is the steady-state simulation, the equipment information, and instrumentation and control data. In general, the P&IDs are used as the starting point for the generation of the HMIs since they contain all the necessary information for the controls and instrumentation. The dynamic model is developed so that the steady-state design condition will be simulated when all the inputs (feeds) are at their design values. Details of how dynamic simulators are used in process design are included in Chapter 17. Needless to say, the development of a

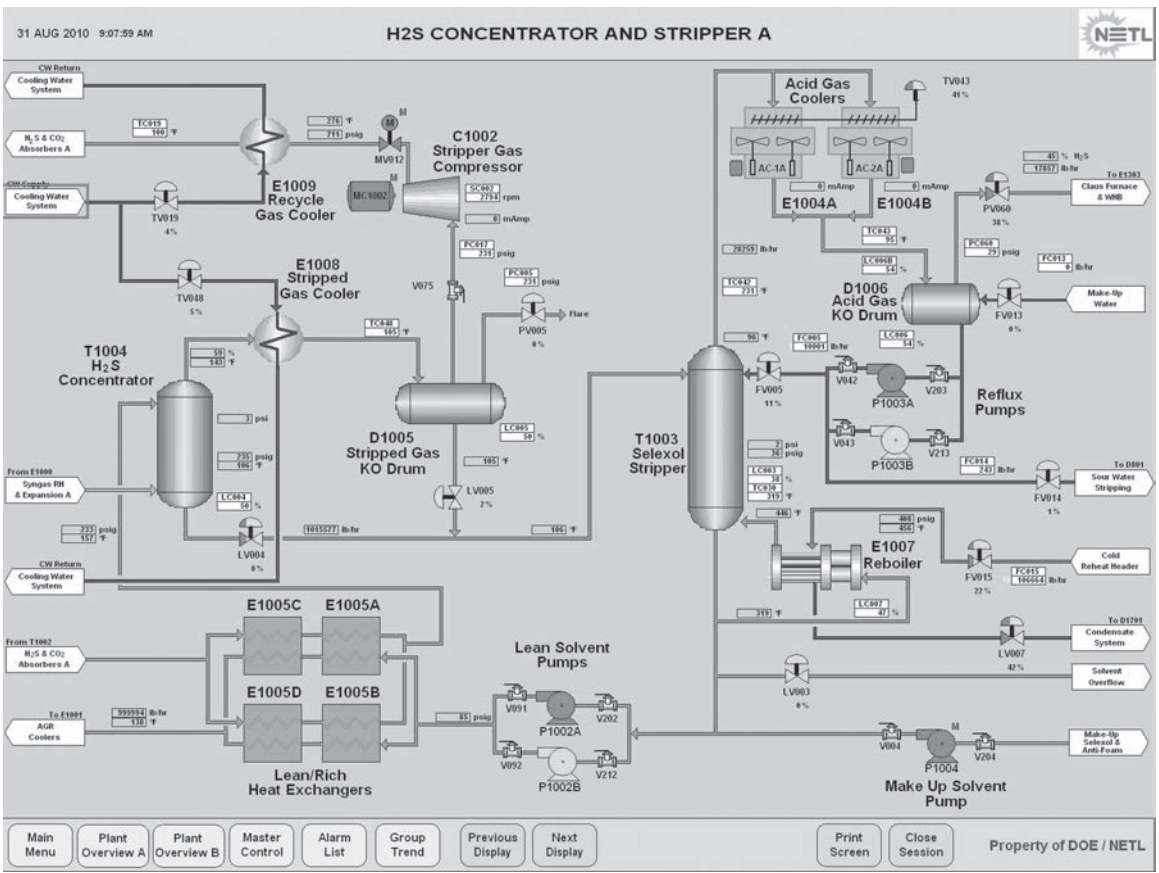


Figure 1.17 Example of an HMI Interface for an OTS (Reproduced by Permission of the DOE's National Energy Technical Laboratory and Invensys Systems Inc., Property and Copyright of Invensys plc, UK)

fully functioning dynamic model for a process that accurately reflects all the controls and valves in the process is a substantial task that takes a team of engineers many months to accomplish.

1.7.2 3-D Immersive Training Simulators (ITS)

In Section 1.6, the concept of a 3-D plant model was introduced. Such models are "constructed" with specialized software using precise design data on the size, location and elevation (*x*-, *y*-, and *z*-coordinates), and orientation of each piece of equipment. In addition, the piping arrangement and location of valves, nozzles, instruments, sample ports, drains, and so forth are all specified. Such a representation allows the engineer and operator to evaluate the accessibility of critical process components and to obtain a feel for how the plant will look (and operate) when constructed. The engineer may access this information through either a 2-D viewer or a 3-D virtual environment (for example, using 3-D goggles). However, no matter how the information is viewed, the resulting images are essentially static and are generally of low to medium fidelity. Therefore, when viewing a 3-D plant model, it will always be clear to the viewer that it is just a model, and that the representation of the 3-D object is crude.

The visual enhancement of 3-D models using sophisticated imaging software and overlaying photorealistic images on top of a skeleton of the 3-D representation are now not only possible but commonplace for higher-end video games. Computer-generated graphics are now so advanced that, as any movie fan will attest, it is often difficult to determine what is "real" and what is animated. This technology is now being applied to develop 3-D immersive training simulators (ITS) for chemical plants. As can be seen from Figure 1.18, the quality and realism captured by computer-generated graphics are excellent. Furthermore, the use of avatars to represent plant operators makes it possible for a user to navigate through, interact with, and be truly immersed in the virtual plant.

Figure 1.18 An Example of a Computer-Generated Image of a Horizontal Drum (Reproduced by Permission of the DOE's National Energy Technical Laboratory and Invensys Systems Inc., Property and Copyright of Invensys plc, UK)

1.7.3 Linking the ITS with an OTS

The potential for education and training of engineers, operators, and students using both the OTS and ITS appears to be limitless. Indeed, these two systems can be linked together such that they can communicate, and the real-time operation of the process, both in the control room and outside in the plant, can be simulated in the virtual environment. Consider the following scenario that might occur during the start-up of a chemical process:

> *Feed to a distillation column from an on-site storage drum has begun. The feed pump has been started and the flow through the pump has been confirmed from the HMI display in the control room. The liquid feed flows into the top of the tower, and the liquid levels on the distillation trays start to increase. The process appears to be working as described in the start-up manual that the operator is following. However, approximately 30 minutes after the start of the feed pumps, a low-level alarm sounds on the on-site storage drum. The operator monitors the level in the drum from the control room and determines that it is continuing to fall and will cause the feed pump to vapor lock (cavitate) if the situation is not remedied. In reviewing the start-up procedure, the operator determines that there is a remote function valve (one that cannot be operated remotely from the control room) that connects the on-site storage drum to the off-site storage tank, and that this valve may have been closed inadvertently. She then contacts an operator in the field by wireless communication and asks him to check the status of the remote function valve. The field operator walks to the storage drum, identifies the tag name on the valve, and confirms that the valve is indeed closed. The control room operator then instructs the field operator to open the valve, which he does. The control room operator then confirms that the level in the drum has started to go back up and thanks the field operator for his help.*

This scenario might well represent an actual incident occurring during a scheduled plant start-up. However, this scenario could just as easily be simulated in the virtual environment. The control room operator would be sitting in front of the HMI screen that is connected to the OTS. A field operator could be sitting in the room next door with a cell phone and wearing 3-D goggles connected to the ITS. The field operator would move his avatar to the location of the on-site storage drum and locate the remote function valve. The field operator using his avatar would then note the setting of the valve and after receiving instructions from the control room operator would open the valve. At this point, the ITS would communicate to the OTS that a valve had been opened, and this would then allow the flow of product to continue to the drum; that is, the dynamic model of the process would respond to the valve being opened and model the flow to the drum. The control room operator, monitoring the HMI, would see the result of the flow of product as an increase in the drum level.

Clearly, any number of scenarios involving control room operators and field operators could be implemented. Moreover, maintenance operations, safety training, and a whole host of other operator functions could be simulated—all in the virtual plant.

Augmented Reality. From the previous example it is clear that any feasible scenario that might occur in the actual plant can be simulated in the virtual environment. However, a series of cases can be simulated that would be almost impossible to simulate in the actual plant but are easily accomplished in virtual reality. For example, it might be helpful to show a young engineer how a particular piece of equipment works by showing him or her the details of the internals of that equipment. In the actual plant, this opportunity might not be available until a scheduled plant shutdown occurs, and that might not happen for one or two years. However, in the virtual environment, the operation of a given piece of equipment can be easily displayed. In fact, the avatar can move into the plant and simply "strip away" the outer wall of a piece of equipment and look inside to see what is happening. This additional feature is sometimes referred to as augmented reality (AR). As an example of AR, the operation of a reboiler and a distillation column is illustrated in Figures 1.19(a) and (b), respectively.

(a) (b)

Figure 1.19 Augmented Reality in ITS: (a) Reboiler, (b) Bubble-Cap Distillation Column (Reproduced by Permission of the DOE's National Energy Technical Laboratory and Invensys Systems Inc., Property and Copyright of Invensys plc, UK)

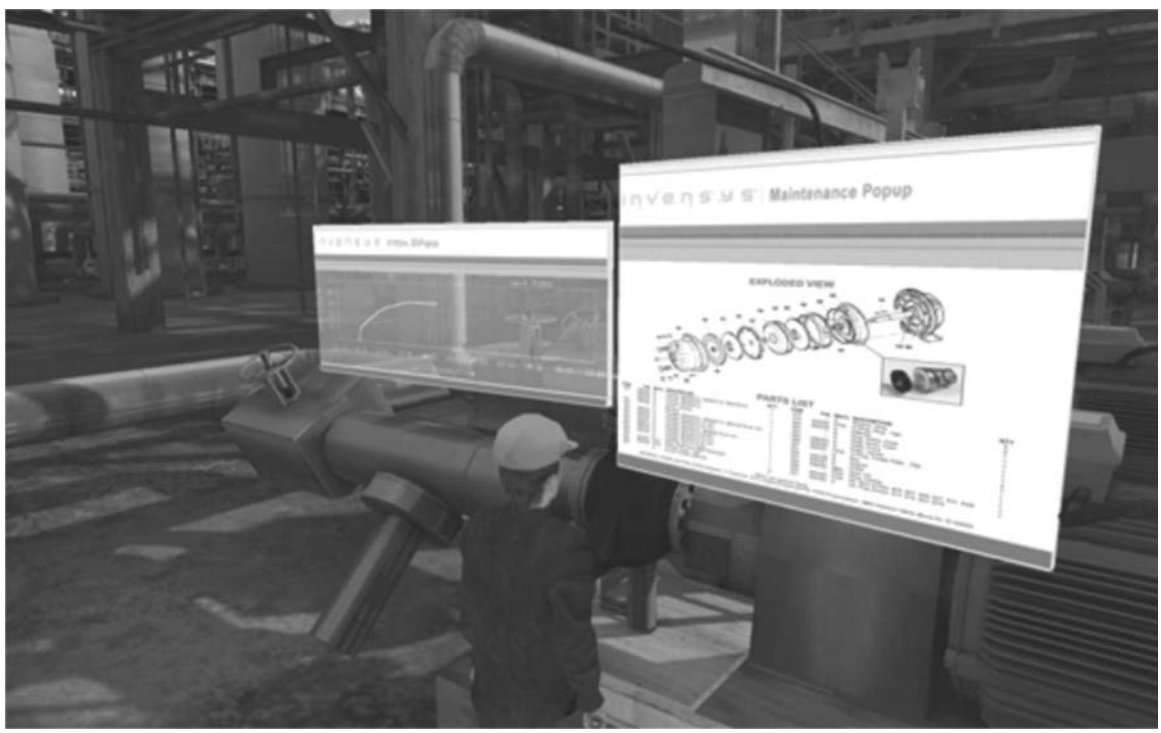


Figure 1.20 An Avatar Can Access Process Trends and Observe Equipment Schematics in AR (Reproduced by Permission of Invensys Systems Inc., Property and Copyright of Invensys plc, UK)

Another example of AR is the display of process data in the virtual plant. For example, if an operator wanted to check on the trend of a certain process variable, say, the temperature in a reactor, or look at a schematic of a pump, the avatar can simply click on a piece of equipment and display that trend, as shown in Figure 1.20. Clearly, in the virtual environment, there are very few limitations on what information the operator (avatar) can access.

Training for Emergencies, Safety, and Maintenance. The possibilities for training operators and engineers in the virtual plant environment are unlimited. Of particular importance are the areas of safety, emergency response, and routine maintenance. For example, the response of an operator or team of operators to an emergency situation can be monitored, recorded, and played back in the virtual plant. Any mistakes made by the operator(s) can be analyzed, feedback given, and then the exercise can be repeated until the correct response is achieved. Although such training does not absolutely guarantee that when a real emergency arises in the plant the operators will respond correctly, it nevertheless provides crucial emergency training under realistic conditions without the fear of actual harm to personnel and equipment. Furthermore, the more often such scenarios are rehearsed, the more likely are operators to respond correctly when real emergencies occur in the plant.

Corresponding scenarios for safety and maintenance training can also be implemented. Often these activities must follow well-defined procedures, and again, the virtual environment offers a perfect venue to record, analyze, and provide feedback to personnel as they perform these various tasks.

In summary, the use of the virtual plant environment (ITS linked to an OTS) provides unlimited opportunities to a new generation of engineers and operators to learn and to train as process plant personnel and to hone their respective skills in an environment that is both realistic and safe.

1.8 SUMMARY

In this chapter, the three principal types of diagrams used to describe the flow of chemical streams through a process were introduced, namely, the block flow diagram (BFD), the process flow diagram (PFD), and the piping and instrumentation diagram (P&ID). These diagrams describe a process in increasing detail.

Each diagram serves a different purpose. The block flow diagram is useful in conceptualizing a process or a number of processes in a large complex. Little stream information is given, but a clear overview of the process is presented. The process flow diagram contains all the necessary information to complete material and energy balances on the process. In addition, important information such as stream pressures, equipment sizes, and major control loops is included. Finally, the piping and instrumentation diagram contains all the process information necessary for the construction of the plant. These data include pipe sizes and the location of all instrumentation for both the process and utility streams.

In addition to the three diagrams, there are a number of other diagrams used in the construction and engineering phase of a project. However, these diagrams contain little additional information about the process.

The logic for equipment placement and layout within the process was presented. The reasons for elevating equipment and providing access were discussed, and a 3-D representation of a DME plant was presented. The concept of operator training simulators was presented and the role of 3-D immersive training systems was also introduced.

The PFD is the single most important diagram for the chemical or process engineer and will form the basis of much of the discussion covered in this book.

WHAT YOU SHOULD HAVE LEARNED

- The difference between and uses of the block flow diagram, the process flow diagram, the piping and instrumentation diagram, plot plans, elevation diagrams, and piping isometrics
- A method for drawing consistent process flow diagrams
- How operator training systems and 3-D graphic process representations are used to train operators and engineers

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SHORT ANSWER QUESTIONS

1. What are the three principal types of diagrams used by process engineers to describe the flow of chemicals in a process? On which of these diagrams would you expect to see the following items?
   a. The temperature and pressure of a process stream
   b. An overview of a multiple-unit process
   c. A major control loop
   d. A pressure indicator
   e. A pressure-relief valve
2. A problem has occurred in the measuring element of a level-indicating controller in a batch reactor. To what principal diagram should you refer in order to troubleshoot the problem?
3. Why is it important for a process engineer to be able to review a three-dimensional model (actual or virtual/electronic) of the plant prior to the construction phase of a project?
4. Name five things that would affect the locations of different pieces of equipment when determining the layout of equipment in a process unit.
5. Why are accurate plant models (made of plastic parts) no longer made as part of the design process? What function did these models play and how is this function now achieved?
6. In the context of process modeling tools, what do OTS and ITS stand for?
7. What is augmented reality? Give one example of it.
8. What are the two principle methods for the layout of process equipment in a chemical plant?
9. When is it appropriate to add a flag to a stream in a PFD rather than including the stream in the stream flow table?
10. What problems would you foresee in naming equipment in a process that had a unit number of 10 (for example, pumps starting with P-11, P-12, etc.)?
11. What diagram would you refer to in order to estimate the frictional loss through a certain piping run within a process?
12. In the vast majority of cases what is the final control element in a process control loop?
13. What is the most effective way of communicating information about a process?

14. Vessel V-307 is to be replaced in a plant with a vessel that is designed to withstand a higher pressure and which has a larger volume. Should this vessel be numbered V-307 to correspond with the vessel it is replacing? Explain your answer.

PROBLEMS

15. There are two common reasons for elevating the bottom of a tower by means of a "skirt." One reason is to provide enough $NPSH_A$ for bottoms product pumps to avoid cavitation. What is the other reason?
16. Which of the principal diagrams should be used to do the following:
    a. Determine the number of trays in a distillation column?
    b. Determine the top and bottom temperatures in a distillation column?
    c. Validate the overall material balance for a process?
    d. Check the instrumentation for a given piece of equipment in a "pre-start-up" review?
    e. Determine the overall material balance for a whole chemical plant?
17. What is the purpose(s) of a pipe rack in a chemical process?
18. When would a structure-mounted vertical plant layout arrangement be preferred over a grade-mounted, horizontal, in-line arrangement?
19. A process that is being considered for construction has been through several technical reviews; block flow, process flow, and piping and instrumentation diagrams are available for the process. Explain the changes that would have to be made to the three principal diagrams if during a final preconstruction review, the following changes were made:
    a. The efficiency of a fired heater had been specified incorrectly as 92% instead of 82%.
    b. A waste process stream flowrate (sent to a sludge pond) was calculated incorrectly and is now 30% greater than before.
    c. It has been decided to add a second (backup) drive for an existing compressor.
    d. The locations of several control valves have changed to allow for better operator access.
20. During a retrofit of an existing process, a vessel used to supply the feed pump to a batch reactor has been replaced because of excessive corrosion. The vessel is essentially identical to the original one, except it is now grounded differently to reduce the corrosion. If the function of the vessel (namely, to supply liquid to a pump) has not changed, answer the following questions:
    a. Should the new vessel have a new equipment number, or should the old vessel number be used again? Explain your answer.
    b. On which diagram or diagrams (BFD, PFD, or P&ID) should the change in the grounding setup be noted?
21. Draw a section of a P&ID diagram for a vessel receiving a process liquid through an insulated 4-in schedule-40 pipe. The purpose of the vessel is to store approximately 5 minutes of liquid volume and to provide "capacity" for a feed pump connected to the bottom of the vessel using a 6-in schedule-40 pipe. The diagram should include the following features:
    a. The vessel is numbered V-1402 and the pump(s) are P-1407 A/B.
    b. The discharge side of the pump is made of 4-in schedule-40 carbon steel pipe and all pipe is insulated.

c. A control valve is located in the discharge line of the pump, and a double block and bleed arrangement is used (see Problem 1.22 for more information).
d. Both pumps and vessel have isolation (gate) valves.
e. The pumps should be equipped with drain lines that discharge to a chemical sewer.
f. The vessel is equipped with local pressure and temperature indicators.
g. The vessel has a pressure-relief valve set to 50 psig that discharges to a flare system.
h. The tank has a drain valve and a sampling valve, both of which are connected to the tank through separate 2-in schedule-40 CS lines.
i. The tank level is used to control the flow of liquid out of the tank by adjusting the setting of the control valve on the discharge side of the pump. The instrumentation is similar to that shown for V-104 in Figure 1.7.

22. A standard method for instrumenting a control valve is termed the "double block and bleed," which is illustrated in Figure P1.22.

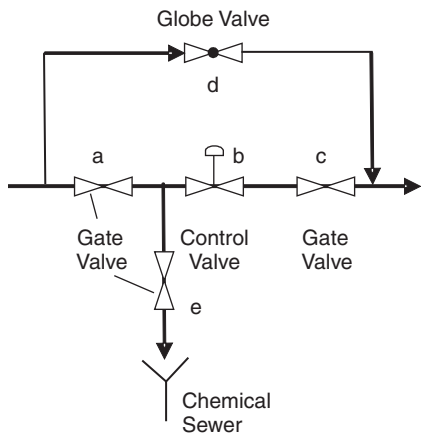

Figure P1.22 Double Block and Bleed Arrangement for Problem 1.22

Under normal conditions, valves a to c are open and valves d and e are closed. Answer the following:

a. Explain, carefully, the sequence of opening and closing valves required in order to change out the valve stem on the control valve (valve b).
b. What changes, if any, would you make to Figure P1.22 if the process stream did not contain a process chemical but contained process water?
c. It has been suggested that the bypass valve (valve d) be replaced with another gate valve to save money. Gate valves are cheap but essentially function as on-off valves. What do you recommend?
d. What would be the consequence of eliminating the bypass valve (valve d)?

23. Often, during the distillation of liquid mixtures, some noncondensable gases are dissolved in the feed to the tower. These noncondensables come out of solution when heated in the tower and may accumulate in the overhead reflux drum. In order for the column to operate satisfactorily, these vapors must be periodically vented to a flare or stack. One method to achieve this venting process is to implement a control scheme in which a process control

valve is placed on the vent line from the reflux drum. A pressure signal from the drum is used to trigger the opening or closing of the vent line valve. Sketch the basic control loop needed for this venting process on a process flow diagram representing the top portion of the tower.

24. Repeat Problem 1.23, but create the sketch as a P&ID to show all the instrumentation needed for this control loop.
25. Explain how each of the following statements might affect the layout of process equipment:
    a. A specific pump requires a large NPSH.
    b. The flow of liquid from an overhead condenser to the reflux drum is gravity driven.
    c. Pumps and control valves should be located for easy access and maintenance.
    d. Shell-and-tube exchanges may require periodic cleaning and tube bundle replacement.
    e. Pipes located at ground level present a tripping hazard.
    f. The prevailing wind is nearly always from the west.
26. Estimate the footprint for a shell-and-tube heat exchanger from the following design data:
    - Area = 145 m^2
    - Hot side temperatures: in at 300°C, out at 195°C
    - Cold side temperatures: bfw at 105°C, mps at 184°C
    - Use 12 ft, 1-in OD tubes on a 1-1/4-in square pitch, use a single shell-and-tube pass because of change of phase on shell side
    - Use a vapor space above boiling liquid = 3 times liquid volume
27. Make a sketch of a layout (plot plan only) of a process unit containing the following process equipment:
    - 3 reactors (vertical—diameter 1.3 m each)
    - 2 towers (1.3 and 2.1 m in diameter, respectively)
    - 4 pumps (each mounting pad is 1 m by 1.8 m)
    - 4 exchangers (footprints of 4 m by 1 m, 3.5 m by 1.2 m, 3 m by 0.5 m, and 3.5 m by 1.1 m)

    The two columns and the three reactors should all be aligned with suitable spacing and all the exchangers should have clearance for tube bundle removal.
28. Using the data from Table 1.7, estimate the footprints of all the equipment in the toluene HDA process.
    - For the shell-and-tube exchangers, assume 12 ft, 1.25-in tubes on a 1.5-in square pitch, and assume 2 ft additional length at either end of the exchanger for tube return and feed header.
    - For double pipe exchangers, assume an 8-in schedule-20 OD and a 6-in schedule-40 ID pipe with a length of 12 ft including u-bend.
    - For the footprints of pumps, compressors, and fired heater, assume the following:
      - P-101 use 2 m by 1 m, P-102 use 2 m by 1 m
      - C-101 (+D-101) use 4 m by 2 m
      - H-101 use 5 m by 5 m

29. With the information from Problem 1.28 and the topology given in Figure 1.5, accurately sketch a plant layout (plot plan) of the toluene HDA process using a grade-mounted, horizontal, in-line arrangement similar to the one shown in Figure 1.10. You should assume that the area of land available for this process unit is surrounded on three sides by an access road and that a pipe rack runs along the fourth side. Use the information in Table 1.11 as a guide to placing equipment.
30. A set of symbols seen on P&IDs are shown in Figure P1.30. Identify all the instrument types and instrument connections (electrical, pneumatic, capillary).

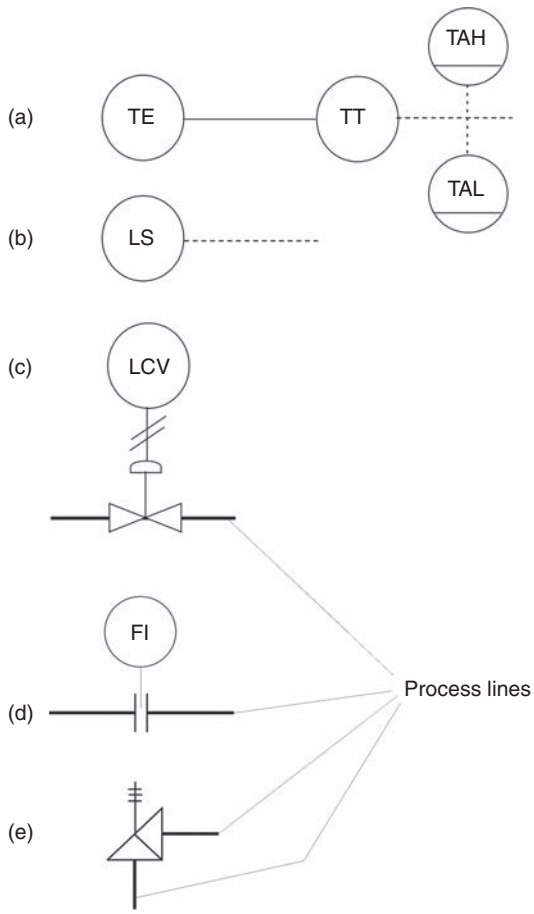

Figure P1.30 A Set of Symbols Seen on P&IDs, to Be Used in Problem 1.30

31. The P&ID shown in Figure P1.31 is for the feed section of a process in which a feed enters a tank and then is pumped through one of two pumps placed in parallel. The liquid then passes through a control valve that is used to regulate the level in the feed tank. Normally closed valves are shown shaded in black. Redraw this P&ID for the situation where the liquid level in the tank is used to regulate the flow into the tank and the discharge from the pumps is controlled through a flow controller using the signal from an orifice meter.

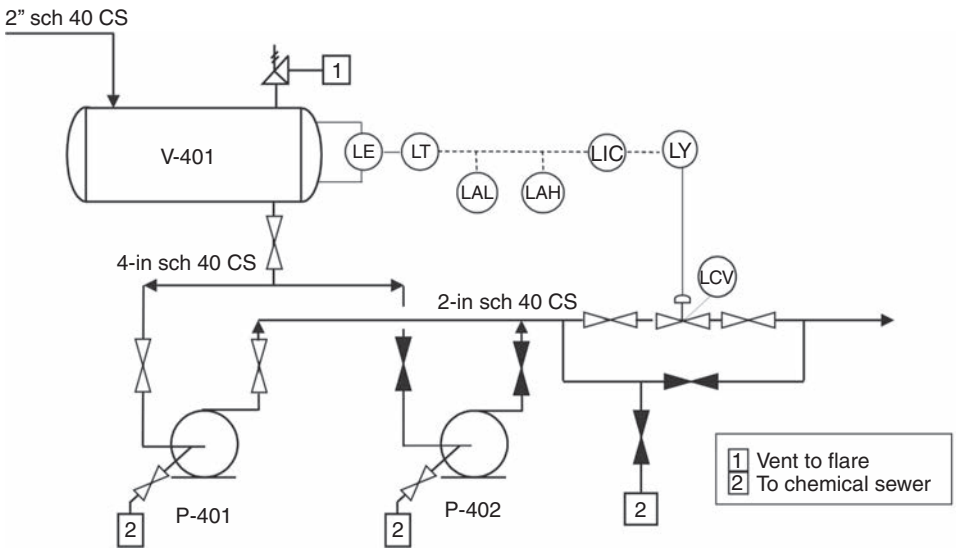

Figure P1.31 A Section of a P&ID to Be Used in Problem 1.31

32. Draw a section of a P&ID where a centrifugal pump receives feed from outside the plant and sends the feed through a furnace and then to a plug flow reactor. The fuel gas flow to the furnace is regulated to control the reactor inlet temperature. The pump discharge flowrate to the reactor is controlled at a desired value.
33. Draw a section of a P&ID where a vessel receives fuel oil and a positive displacement pump is used to send the fuel oil to a furnace. The fuel oil flow to the furnace is regulated to control the furnace temperature. You don't need to show the furnace, just the fuel oil line up to the furnace burner.
34. Draw a section of a P&ID where a gas is sent to a plug flow reactor through a heat exchanger. In the heat exchanger, a heating fluid is used to maintain the temperature of the gas at the inlet of the reactor. The gas flowrate to the reactor is controlled at a desired value.

CHAPTER

2

The Structure and Synthesis of Process Flow Diagrams

WHAT YOU WILL LEARN

- The hierarchy of chemical process design
- The structure of continuous chemical processes
- The differences between batch and continuous processes

When looking at a process flow diagram (PFD) for the first time, it is easy to be confused or overwhelmed by the complexity of the diagram. The purpose of this chapter is to show that the evolution of every process follows a similar path. The resulting processes will often be quite different, but the series of steps that have been followed to produce the final processes are similar. Once the path or evolution of the structure of processes has been explained and is understood, the procedure for understanding existing PFDs is also made simpler. Another important benefit of this chapter is to provide a framework to generate alternative PFDs for a given process.

2.1 HIERARCHY OF PROCESS DESIGN

Before discussing the steps involved in the conceptual design of a process, it should be noted that often the most important decision in the evolution of a process is the choice of which chemical syntheses or routes should be investigated to produce a desired product. The identification of alternative process chemistries should be done at the very beginning of any conceptual design. The conceptual design and subsequent optimization of a process are "necessary conditions" for any successful new process. However, the greatest improvements (savings) associated with chemical processes are most often due to changes, sometimes radical changes, to the chemical pathway used to produce the product. Most often, there are at least two viable ways to produce a given chemical. These alternative routes may require different raw materials and may produce different by-products. The cost of the raw materials, the value of the by-products, the complexity of the synthesis, and the environmental impact of any waste materials and pollutants produced must be taken into account when evaluating alternative synthesis routes.

Douglas [1, 2], among others, has proposed a hierarchical approach to conceptual process design. In this approach, the design process follows a series of decisions and steps. The order in which these decisions are made forms the hierarchy of the design process. These decisions are listed as follows:

1. Decide whether the process will be batch or continuous.
2. Identify the input/output structure of the process.
3. Identify and define the recycle structure of the process.
4. Identify and design the general structure of the separation system.
5. Identify and design the heat-exchanger network or process energy recovery system.

In designing a new process, Steps 1 through 5 are followed in that order. Alternatively, by looking at an existing process, and working backward from Step 5, it is possible to eliminate or greatly simplify the PFD. Hence, much about the structure of the underlying process can be determined.

This five-step design algorithm will now be applied to a chemical process. Each of the steps is discussed in some detail, and the general philosophy about the decision-making process will be covered. However, because Steps 4 and 5 require extensive discussion, these will be covered in separate chapters (Chapter 12 for separations, and Chapter 15 for energy recovery).

2.2 STEP 1—BATCH VERSUS CONTINUOUS PROCESS

It should be pointed out that there is a difference between a batch process and a batch (unit) operation. Indeed, there are very few, if any, processes that use only continuous operations. For example, most chemical processes described as continuous receive their raw material feeds and ship their products to and from the plant in rail cars, tanker trucks, or barges. The unloading and loading of these materials are done in a batch manner. Indeed, the demarcation between continuous and batch processes is further complicated by situations when plants operate continuously but feed or receive material from other process units within the plant that operate in a batch mode. Such processes are often referred to as semi-batch. A **batch process** is one in which a finite quantity (batch) of product is made during a period of a few hours or days. The batch process most often consists of metering feed(s) into a vessel followed by a series of unit operations (mixing, heating, reaction, distillation, etc.) taking place at discrete scheduled intervals. This is then followed by the removal and storage of the products, by-products, and waste streams. The equipment is then cleaned and made ready for the next process. Production of up to 100 different products from the same facility has been reported [3]. This type of operation is in contrast to **continuous processes**, in which feed is sent continuously to a series of equipment, with each piece usually performing a single unit operation. Products, by-products, and waste streams leave the process continuously and are sent to storage or for further processing.

There are a number of considerations to weigh when deciding between batch and continuous processes, and some of the more important of these are listed in Table 2.1. As this table indicates, there are many things to consider when making the decision regarding batch versus continuous operation. Probably the most important of these are size and flexibility. If it is desired to produce relatively small quantities, less than approximately 500 tonne/y [1], of a variety of different products using a variety of different feed materials, then batch processing is probably the correct choice. For large quantities, greater than 5000 tonne/y of product [1], using a single or only a few raw materials, then a continuous process is probably the best choice. There are

Table 2.1 Some Factors to Consider When Deciding between Batch and Continuous Processes

Factor	Advantages/Disadvantages for Batch Processes	Advantages/Disadvantages for Continuous Processes
Size	Smaller throughput favors batch operations. As throughput increases, the required size of the process equipment increases, and the technical difficulties of moving large amounts of chemicals from equipment to equipment rapidly increase.	Economies of scale favor continuous processes for large throughput.
Batch Accountability/ Product Quality	When the product quality of each batch of material must be verified and certified, batch operations are preferred. This is especially true for pharmaceutical and food products. The manufacture of these products is strictly monitored by the Food and Drug Administration (FDA). If reworking (reprocessing) of off-specification product is usually not permitted, small batches are favored.	Continuous or periodic testing of product quality is carried out, but some potentially large quantities of off-specification product can be produced. If off-specification material may be blended or stored in dump/slop tanks and reworked through the process when the schedule permits, continuous processes are favored.
Operational Flexibility	Often the same equipment can be used for multiple operations—for example, a stirred tank can be used as a mixer, then a reactor, and then as a stage of a mixer-settler for liquid-liquid extraction.	Operational flexibility can be built in to continuous processes but often leads to inefficient use of capital. Equipment not required for one process but needed for another may sit idle for months. Often continuous processes are designed to produce a fixed suite of products from a well-defined feed material. If market forces change the feed/product availability or demand, then the plant will often be retrofitted to accommodate the change.
Standardized Equipment—Multiple Products	Often batch processes can be easily modified to produce several different products using essentially the same equipment. Examples of batch plants that can produce 100 different products are known [3]. For such processes the optimal control and sequencing of operations are critical to the success of such a plant.	The product suite or slate produced from continuous processes is usually fixed. Equipment tends to be designed and optimized for a single or small number of operating conditions.

(*continued*)

Table 2.1 Some Factors to Consider When Deciding between Batch and Continuous Processes (*Continued*)

Factor	Advantages/Disadvantages for Batch Processes	Advantages/Disadvantages for Continuous Processes
Processing Efficiency	Operation of batch processes requires strict scheduling and control. Because different products are scheduled back-to-back, changes in schedules have a ripple effect and may cause serious problems with product availability for customers. If the same equipment is used to produce many different products, then this equipment will not be optimized for any one product. Energy integration is usually not possible, so utility usage tends to be higher than for continuous processes. Separation and reuse of raw materials are more difficult than for continuous processes.	Generally, as throughput increases, continuous processes become more efficient. For example, fugitive energy losses are reduced, and rotating equipment (pumps, compressors, etc.) operates with higher efficiency. Recycle of unused reactants and the integration of energy within the process or plant are standard practices and relatively easy to achieve.
Maintenance and Operating Labor	There are higher operating labor costs in standard batch plants due to equipment cleaning and preparation time. These costs have been shown to be reduced for the so-called pipeless batch plants [4].	For the same process, operating labor will be lower for continuous processes.
Feedstock Availability	Batch operations are favored when feedstock availability is limited, for example, seasonally. Canneries and wineries are examples of batch processing facilities that often operate for only part of the year.	Continuous plants tend to be large and need to operate throughout the year to be profitable. The only way that seasonal variations in feeds can be accommodated is through the use of large storage facilities that are very expensive.
Product Demand	Seasonal demand for products such as fertilizers, gas-line antifreeze, deicing chips for roads and pavements, and so on, can be easily accommodated. Because batch plants are flexible, other products can be made during the off-season.	It is difficult to make other products during the off-season. However, similar but different products—for example, a family of solvents— can be produced using the same processes through a series of campaigns at different times during the year. Each campaign may last several months.

Rate of Reaction to Produce Products	Batch operations favor processes that have very slow reaction rates and subsequently require long residence times. Examples include fermentation, aerobic and anaerobic wastewater treatment, and many other biological reactions.	Very slow reactions require very large equipment. The flow through this equipment will be slow, and dispersion can be a problem if very high conversion is desired and plug flow is required.
Equipment Fouling	When there is significant equipment fouling, batch operations are favored because cleaning of equipment is always a standard operating procedure in a batch process and can be accommodated easily in the scheduling of the process.	Significant fouling in continuous operations is a serious problem and is difficult to handle. Operating identical units in parallel, one on-line and the other off-line for cleaning, can solve this problem. However, capital investment is higher, additional labor is required, and safety problems are more likely.
Safety	Generally, worker exposure to chemicals and operator error will be higher (per pound of product) than for continuous processes. Operator training in chemical exposure and equipment operation is critical.	Large chemical plants operating continuously have excellent safety records [6], and safety procedures are well established. Operator training is still of great importance, but many of the risks associated with operating equipment containing chemicals are eliminated.
Controllability	Controllability of batch processes using the same equipment for different unit operations and sometimes to produce different products may be difficult. The efficient scheduling of equipment becomes very important. The control used for this scheduling is complicated [3].	Generally, continuous processes are easier to control. Also, more work and research have been done for these processes. However, for complicated and highly integrated (energy and/or raw materials) plants, the control becomes complex, and operational flexibility is greatly reduced.

many trade-offs between the two types of processes. However, like most things, it boils down to cost. For a batch process compared to the equivalent continuous process, the capital investment is usually much lower because the same equipment can be used for multiple unit operations and can be reconfigured easily for a wide variety of feeds and products. On the other hand, operating labor costs and utility costs tend to be much higher. Recent developments in batch processing have led to the concept of the "pipeless batch process" [4]. In this type of operation, equipment is automatically moved to different workstations at which different processes are performed. For example, a reactor may be filled with raw materials and mixed at station 1, moved to station 2 for heating and reaction, to station 3 for product separation, and finally to station 4 for product removal. The workstations contain a variety of equipment to perform functions such as mixing, weighing, heating/cooling, filtration, and so on. This modular approach to the sequencing of batch operations greatly improves productivity and eases the scheduling of different events in the overall process.

Finally, it is important to recognize the role of pilot plants in the development of processes. It has been long understood that what works well in the laboratory often does not work as well on the large scale. Of course, much of the important preliminary work associated with catalyst development and phase equilibrium is most efficiently and inexpensively completed in the laboratory. However, problems associated with trace quantities of unwanted side products, difficult material handling problems, and multiple reaction steps are not easily scaled up from laboratory-scale experiments. In such cases, specific unit operations or the entire process may be "piloted" to gain better insight into the proposed full-scale operation. Often, this pilot plant work is carried out in batch equipment in order to reduce the inventory of raw materials. Sometimes, the pilot plant serves the dual purpose of testing the process at an intermediate scale and producing enough material for customers and other interested parties to test. The role and importance of pilot plants are covered in detail by Lowenstein [5].

2.3 STEP 2—THE INPUT/OUTPUT STRUCTURE OF THE PROCESS

Although all processes are different, there are common features of each. The purpose of this section is to investigate the input/output structure of the process. The inputs represent feed streams and the outputs are product streams, which may be desired products, by-products, or waste streams.

2.3.1 Process Concept Diagram

The first step in evaluating a process route is to construct a process concept diagram. Such a diagram uses the stoichiometry of the main reaction pathway to identify the feed and product chemicals. The first step to construct such a diagram is to identify the chemical reaction or reactions taking place within the process. The balanced chemical reaction(s) form the basis for the overall process concept diagram. Figure 2.1 shows this diagram for the toluene hydrodealkylation process discussed in Chapter 1. It should be noted that only chemicals taking place in the reaction are identified on this diagram. The steps used to create this diagram are as follows:

1. A single "cloud" is drawn to represent the concept of the process. Within this cloud the stoichiometry for all reactions that take place in the process is written. The normal convention of the reactants on the left and products on the right is used.
2. The reactant chemicals are drawn as streams entering from the left. The number of streams corresponds to the number of reactants (two). Each stream is labeled with the name of the reactant (toluene and hydrogen).

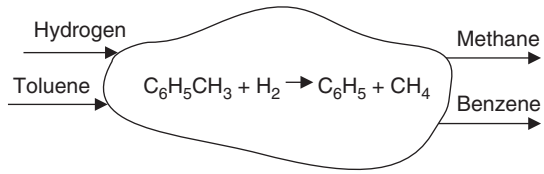

Figure 2.1 Input/Output Structure of the Process Concept Diagram for the Toluene Hydrodealkylation Process

3. Product chemicals are drawn as streams leaving to the right. The number of streams corresponds to the number of products (two). Each stream is labeled with the name of the product (benzene and methane).
4. Seldom does a single reaction occur, and unwanted side reactions must be considered. All reactions that take place and the reaction stoichiometry must be included. The unwanted products are treated as by-products and must leave along with the product streams shown on the right of the diagram.

2.3.2 The Input/Output Structure of the Process Flow Diagram

If the process concept diagram represents the most basic or rudimentary representation of a process, then the process flow diagram (PFD) represents the other extreme. However, the same input/output structure is seen in both diagrams. The PFD, by convention, shows the process feed stream(s) entering from the left and the process product stream(s) leaving to the right.

There are other auxiliary streams shown on the PFD, such as utility streams that are necessary for the process to operate but that are not part of the basic input/output structure. Ambiguities between process streams and utility streams may be eliminated by starting the process analysis with an overall input/output concept diagram.

Figure 2.2 shows the basic input/output structure for the PFD (see Figure 1.3). The input and output streams for the toluene HDA PFD are shown in bold. Both Figures 2.1 and 2.2 have the same overall input/output structure. The input streams labeled toluene and hydrogen shown on the left in Figure 2.1 appear in the streams on the left of the PFD in Figure 2.2. In Figure 2.2, these streams contain the reactant chemicals plus other chemicals that are present in the raw feed materials. These streams are identified as Streams 1 and 3, respectively. Likewise, the output streams, which contain benzene and methane, must appear on the right on the PFD. The benzene leaving the process, Stream 15, is clearly labeled, but there is no clear identification for the methane. However, by referring to Table 1.5 and looking at the entry for Stream 16, it can be seen that this stream contains a considerable amount of methane. From the stoichiometry of the reaction, the amount of methane and benzene produced in the process should be equal (on a mole basis). This is easily checked from the data for Streams 1, 3, 15, and 16 (Table 1.5) as follows:

$$\begin{aligned}\text{Benzene produced in process} &= \text{Benzene leaving} - \text{Benzene entering}\\ &= 105.2\ (\text{Stream15}) + 2.85\ (\text{Stream16}) - 0\\ &= 108.05\,\text{kmol/h}\end{aligned}$$

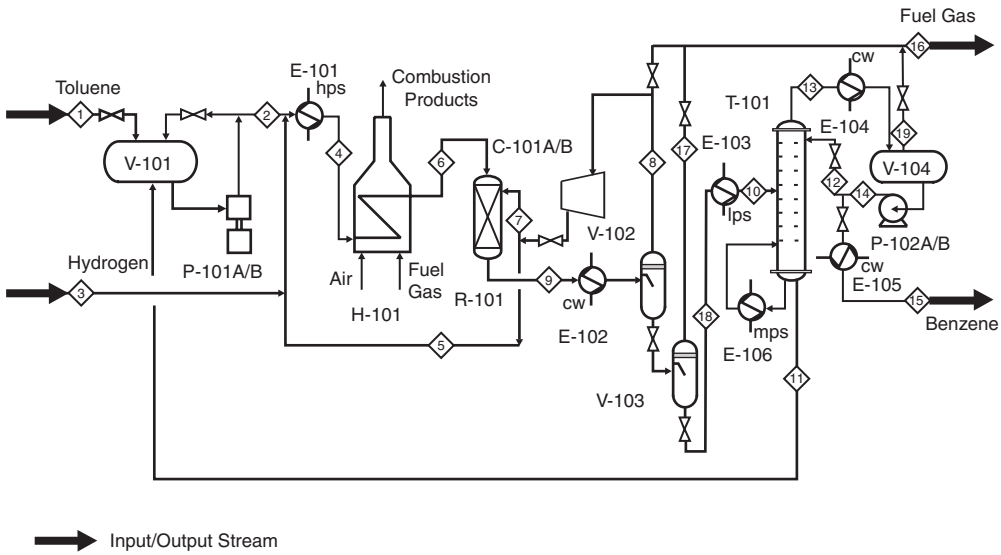

Figure 2.2 Input and Output Streams on Toluene Hydrodealkylation PFD

$$\begin{aligned}\text{Methane produced in process} &= \text{Methane leaving} - \text{Methane entering}\\ &= 123.05\ (\text{Stream 16}) - 15.0\ (\text{Stream 3})\\ &= 108.05\,\text{kmol/h}\end{aligned}$$

At times, it will be necessary to use the process conditions or the flow table associated with the PFD to determine where a chemical is to be found.

There are several important factors to consider in analyzing the overall input/output structure of a PFD. Some of these factors are listed below.

1. Chemicals entering the PFD from the left that are not consumed in the chemical reactor are either required to operate a piece of equipment or are inert material that simply passes through the process. Examples of chemicals required but not consumed include catalyst makeup, solvent makeup, and inhibitors. In addition, feed materials that are not pure may contain inert chemicals. Alternatively, chemicals may be added in order to control reaction rates, to keep the reactor feed outside of the explosive limits, or to act as a heat sink or heat source to control temperatures.
2. Any chemical leaving a process must either have entered in one of the feed streams or have been produced by a chemical reaction within the process.
3. Utility streams are treated differently from process streams. Utility streams, such as cooling water, steam, fuel, and electricity, rarely directly contact the process streams. They usually provide or remove thermal energy or work.

Figure 2.3 identifies, with bold lines, the utility streams in the benzene process. It can be seen that two streams—fuel gas and air—enter the fired heater. These are burned to provide heat to the process, but never come in direct contact (that is, mix) with the process streams. Other streams such as cooling water and steam are also highlighted in Figure 2.3. All these streams are utility

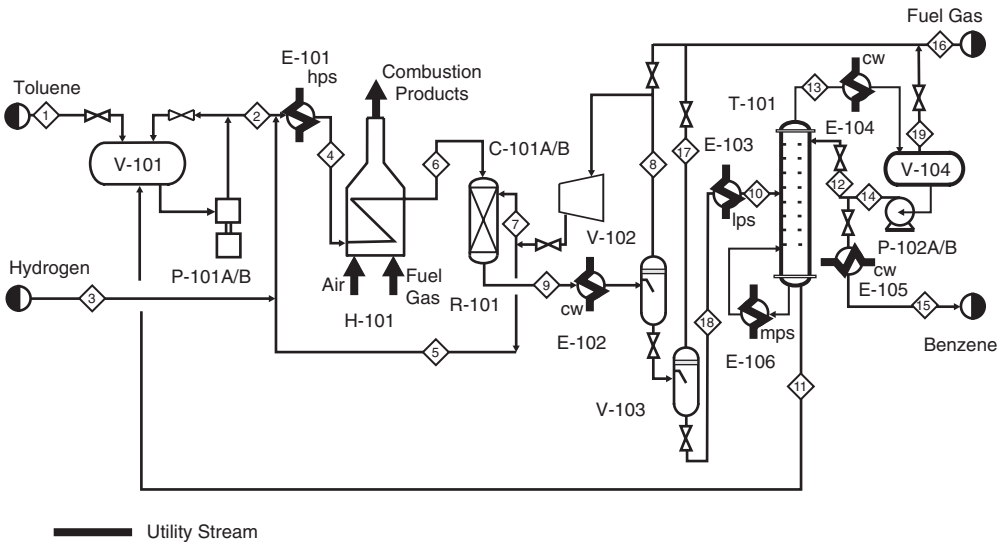

Figure 2.3 Identification of Utility Streams on the Toluene Hydrodealkylation PFD

streams and are not extended to the left or right boundaries of the diagram, as were the process streams. Other utility streams are also provided but are not shown in the PFD. The most important of these is electrical power, which is most often used to run rotating equipment such as pumps and compressors. Other utilities, such as plant air, instrument air, nitrogen for blanketing of tanks, process water, and so on, are also consumed.

2.3.3 The Input/Output Structure and Other Features of the Generic Block Flow Process Diagram

The generic block flow diagram is intermediate between the process concept diagram and the PFD. This diagram illustrates features, in addition to the basic input/output structure, that are common to all chemical processes. Moreover, in discussing the elements of new processes it is convenient to refer to this diagram because it contains the logical building blocks for all processes. Figure 2.4(a) provides a generic block flow process diagram that shows a chemical process broken down into six basic areas or blocks. Each block provides a function necessary for the operation of the process. These six blocks are as follows:

1. Reactor feed preparation
2. Reactor
3. Separator feed preparation
4. Separator
5. Recycle
6. Environmental control

An explanation of the function of each block in Figure 2.4(a) is given below.

1. **Reactor Feed Preparation Block:** In most cases, the feed chemicals entering a process come from storage. These chemicals are most often not at a suitable concentration, temperature,

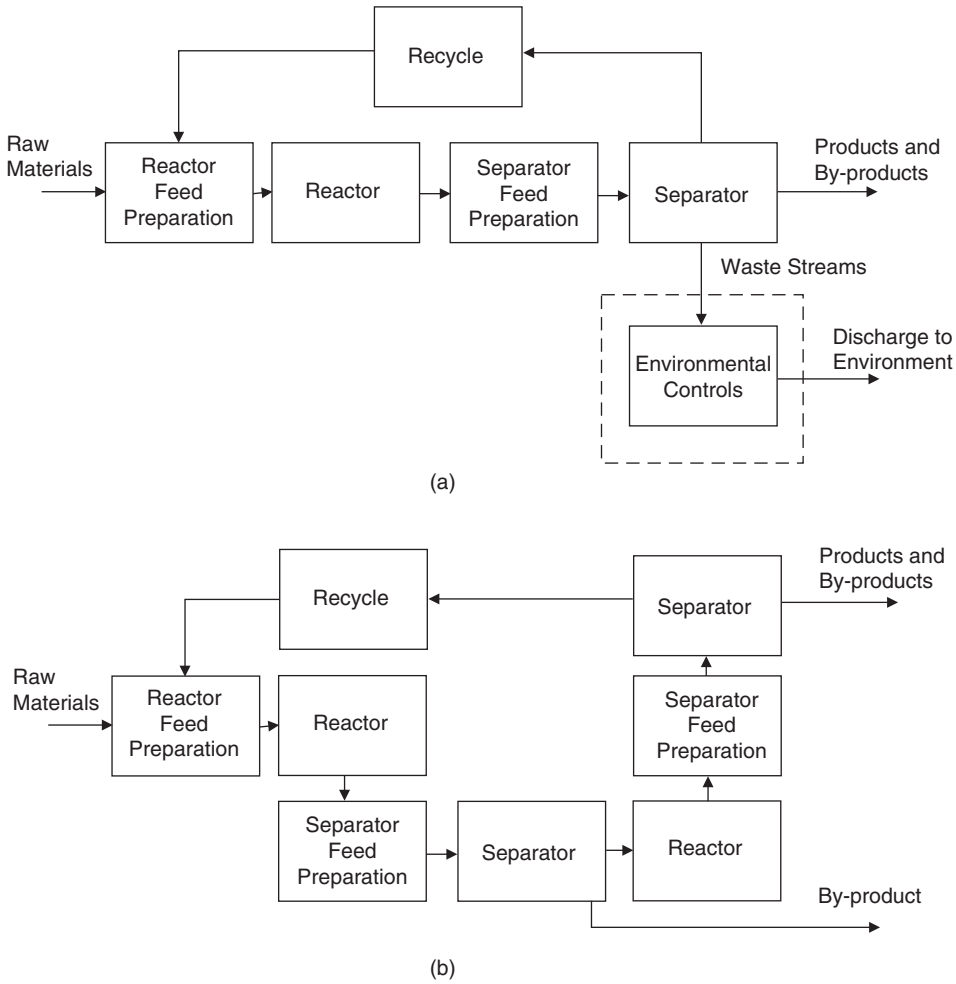

Figure 2.4 (a) The Six Elements of the Generic Block Flow Process Diagram; (b) A Process Requiring Multiple Process Blocks

and pressure for optimal performance in the reactor. The purpose of the reactor feed preparation section is to change the conditions of these process feed streams as required in the reactor.

2. **Reactor Block:** All chemical reactions take place in this block. The streams leaving this block contain the desired product(s), any unused reactants, and a variety of undesired by-products produced by competing reactions.
3. **Separator Feed Preparation Block:** The output stream from the reactor, in general, is not at a condition suitable for the effective separation of products, by-products, waste streams, and unused feed materials. The units contained in the separator feed preparation block alter the temperature and pressure of the reactor output stream to provide the conditions required for the effective separation of these chemicals.
4. **Separator Block:** The separation of products, by-products, waste streams, and unused feed materials is accomplished via a wide variety of physical processes. The most common

of these techniques are typically taught in unit operations and/or separations classes—for example, distillation, absorption, and extraction.

5. **Recycle Block:** The recycle block represents the return of unreacted feed chemicals, separated from the reactor effluent, back to the reactor for further reaction. Because the feed chemicals are not free, it most often makes economic sense to separate the unreacted reactants and recycle them back to the reactor feed preparation block. Normally, the only equipment in this block is a pump or compressor and perhaps a heat exchanger.
6. **Environmental Control Block:** Virtually all chemical processes produce waste streams. These include gases, liquids, and solids that must be treated prior to being discharged into the atmosphere, sequestered in landfills, and so on. These waste streams may contain unreacted materials, chemicals produced by side reactions, fugitive emissions, and impurities coming in with the feed chemicals and the reaction products of these chemicals. Not all of the unwanted emissions come directly from the process streams. An example of an indirect source of pollution results when the energy needs of the plant are met by burning high sulfur oil. The products of this combustion include the pollutant sulfur dioxide, which must be removed before the gaseous combustion products can be vented to the atmosphere. The purpose of the environmental control block is to reduce significantly the waste emissions from a process and to render all nonproduct streams harmless to the environment.

It can be seen that a dashed line has been drawn around the block containing the environmental control operations. This identifies the unique role of environmental control operations in a chemical plant complex. A single environmental control unit may treat the waste from several processes. For example, the wastewater treatment facility for an oil refinery might treat the wastewater from as many as 20 separate processes. In addition, the refinery may contain a single stack and incinerator to deal with gaseous wastes from these processes. Often, this common environmental control equipment is not shown in the PFD for an individual process, but is shown on a separate PFD as part of the "off-site" section of the plant. Just because the environmental units do not appear on the PFD does not indicate that they do not exist or that they are unimportant.

Each of the process blocks may contain several unit operations. Moreover, several process blocks may be required in a given process. An example of multiple process blocks in a single process is shown in Figure 2.4(b). In this process, an intermediate product is produced in the first reactor and is subsequently separated and sent to storage. The remainder of the reaction mixture is sent to a second stage reactor in which product is formed. This product is subsequently separated and sent to storage, and unused reactant is also separated and recycled to the front end of the process. Based upon the reason for including the unit, each unit operation found on a PFD can be placed into one of these blocks. Although each process may not include all the blocks, all processes will have some of these blocks.

In Example 2.6, at the end of this chapter, different configurations will be investigated for a given process. It will be seen that these configurations are most conveniently represented using the building blocks of the generic block flow diagram.

2.3.4 Other Considerations for the Input/Output Structure of the Process Flowsheet

The effects of feed impurities and additional flows that are required to carry out specific unit operations may have a significant impact on the structure of the PFD. These issues are covered in the following section.

Feed Purity and Trace Components. In general, the feed streams entering a process do not contain pure chemicals. The option always exists to purify further the feed to the process. The question of whether this purification step should be performed can be only answered using a detailed economic analysis. However, some commonsense heuristics may be used to choose a good base case or starting point. The following heuristics are modified from Douglas [1]:

- If the impurities are not present in large quantities (say, <10%–20%) and these impurities do not react to form by-products, then do not separate them prior to feeding to the process. For example, the hydrogen fed to the toluene HDA process contains a small amount of methane (5 mol%—see Stream 3 in Table 1.5). Because the methane does not react (it is inert) and it is present as a small quantity, it is probably not worth considering separating it from the hydrogen.
- If the separation of the impurities is difficult (for example, an impurity forms an azeotrope with the feed or the feed is a gas at the feed conditions), then do not separate them prior to feeding to the process. For example, again consider the methane in Stream 3. The separation of methane and hydrogen is relatively expensive (see Example 2.3) because it involves low temperature and/or high pressure. This fact, coupled with the reasons given above, means that separation of the feed would not normally be attempted.
- If the impurities foul or poison the catalyst, then purify the feed. For example, one of the most common catalyst poisons is sulfur. This is especially true for catalysts containing Group VIII metals such as iron, cobalt, nickel, palladium, and platinum [7]. In the steam reformation of natural gas (methane) to produce hydrogen, the catalyst is rapidly poisoned by the small amounts of sulfur in the feed. A guard bed of activated carbon (or zinc oxide) is placed upstream of the reactor to reduce the sulfur level in the natural gas to the low ppm level, which reduces the catalyst poisoning to an acceptable level.
- If the impurity reacts to form difficult-to-separate or hazardous products, then purify the feed. For example, in the manufacture of isocyanates for use in the production of polyurethanes, the most common synthesis path involves the reaction of phosgene with the appropriate amine [8]. Because phosgene is a highly toxic chemical, all phosgene is manufactured on-site via the reaction of chlorine and carbon monoxide:

$$CO + Cl_2 \rightarrow \underset{phosgene}{COCl_2}$$

  If carbon monoxide is not readily available (by pipeline), then it must be manufactured via the steam reformation of natural gas. The following equation shows the overall main reaction (carbon dioxide may also be formed in the process, but it is not considered here):

$$CH_4 + H_2O \rightarrow CO + 3H_2$$

  The question to ask is, at what purity must the carbon monoxide be fed to the phosgene unit? The answer depends on what happens to the impurities in the CO. The main impurity is hydrogen. The hydrogen reacts with the chlorine to form hydrogen chloride, which is difficult to remove from the phosgene, is highly corrosive, and is detrimental to the isocyanate product. With this information, it makes more sense to remove the hydrogen to the desired level in the carbon monoxide stream rather than send it through with the CO and cause more separation problems in the phosgene unit and further downstream. Acceptable hydrogen levels in carbon monoxide feeds to phosgene units are less than 1%.
- If the impurity is present in large quantities, then purify the feed. This heuristic is fairly obvious because significant additional work and heating/cooling duties are required to process the large amount of impurity. Nevertheless, if the separation is difficult and the impurity acts

as an inert, then separation may still not be warranted. An obvious example is the use of air, rather than pure oxygen, as a reactant. Because nitrogen often acts as an inert compound, the extra cost of purifying the air is not justified compared with the lesser expense of processing the nitrogen through the process. An added advantage of using air, as opposed to pure oxygen, is the heat-absorbing capacity of nitrogen, which helps moderate the temperature rise of many highly exothermic oxidation reactions.

Addition of Feeds Required to Stabilize Products or Enable Separations. Generally, product specifications are given as a series of characteristics that the product stream must meet or exceed. Clearly, the purity of the main chemical in the product is the major concern. However, other specifications such as color, density or specific gravity, turbidity, maximum amount of certain trace chemicals, and so on, may also be specified. Often many of these specifications can be met in a single piece or train of separation equipment. However, if the product stream is, for example, reactive or unstable, then additional stabilizing chemicals may need to be added to the product before it goes to storage. These stabilizing chemicals are additional feed streams to the process. The same argument can be made for other chemicals such as solvents or catalysts that are effectively consumed in the process. If a solvent such as water or an organic chemical is required to make a separation take place—for example, absorption of a solvent-soluble chemical from a gas stream—then this solvent is an additional feed to the process (see Appendix B.5—the production of maleic anhydride via the partial oxidation of propylene). Accounting for these chemicals both in feed costs and in the overall material balance (in the product streams) is very important.

Inert Feed Material to Control Exothermic Reactions. In some cases, it may be necessary to add additional inert feed streams to the process in order to control the reactions taking place. Common examples of this are partial oxidation reactions of hydrocarbons. For example, consider the partial oxidation of propylene to give acrylic acid, an important chemical in the production of acrylic polymers. The feeds consist of nearly pure propylene, air, and steam. The basic reactions that take place are as follows:

$$C_3H_6 + \frac{3}{2}O_2 \rightarrow C_3H_4O_2 + H_2O \qquad \text{Reaction 1}$$

$$C_3H_6 + \frac{5}{2}O_2 \rightarrow C_2H_4O_2 + H_2O + CO_2 \qquad \text{Reaction 2}$$

$$C_3H_6 + \frac{9}{2}O_2 \rightarrow 3H_2O + 3CO_2 \qquad \text{Reaction 3}$$

All these reactions are highly exothermic, not limited by equilibrium, and potentially explosive. In order to eliminate or reduce the potential for explosion, steam is fed to the reactor to dilute the feed and provide thermal ballast to absorb the heat of reaction and make control easier. In some processes, enough steam (or other inert stream) is added to move the reaction mixture out of the flammability limits, thus eliminating the potential for explosion. The steam (or other inert stream) is considered a feed to the process, must be separated, and leaves as a product, by-product, or waste stream.

Addition of Inert Feed Material to Control Equilibrium Reactions. Sometimes it is necessary to add an inert material to shift the equilibrium of the desired reaction. Consider the production of styrene via the catalytic dehydrogenation of ethyl benzene:

$$\underset{\text{ethyl benzene}}{C_6H_5CH_2CH_3} \rightleftharpoons \underset{\text{styrene}}{C_6H_5CH{=}CH_2} + H_2$$

This reaction takes place at high temperature (600°C–750°C) and low pressure (<1 bar) and is limited by equilibrium. The ethyl benzene is co-fed to the reactor with superheated steam. The steam acts as an inert in the reaction and both provides the thermal energy required to preheat the ethyl benzene and dilutes the feed. As the steam-to-ethyl benzene ratio increases, the equilibrium shifts to the right (Le Chatelier's principle) and the single-pass conversion increases. The optimum steam-to-ethyl benzene feed ratio is based on the overall process economics.

2.3.5 What Information Can Be Determined Using the Input/Output Diagram for a Process?

The following basic information, obtained from the input/output diagram, is limited but nevertheless very important:

- Basic economic analysis on profit margin
- What chemical components must enter with the feed and leave as products
- All the reactions, both desired and undesired, that take place

The potential profitability of a proposed process can be evaluated and a decision whether to pursue the process can be made. As an example, consider the profit margin for the toluene HDA process given in Figure 2.1.

The profit margin will be formally introduced in Chapter 10, but it is defined as the difference between the value of the products and the cost of the raw materials. To keep things simple the stoichiometry of the reaction is used as the basis. If the profit margin is a negative number, then there is no potential to make money. The profit margin for the HDA process is given in Example 2.1.

Example 2.1

Evaluate the profit margin for the HDA process.

From Tables 8.3 and 8.4, the following prices for raw materials and products are found:
Benzene = \$1.196/kg
Toluene = \$1.019/kg
Natural gas (methane, MW = 16) = \$0.1119/std m^3 = \$0.165/kg
Hydrogen = \$0.381/kg (based on the same equivalent energy cost as natural gas)

Using 1 kmol of toluene feed as a basis

Cost of Raw Materials

92 kg of Toluene = (92 kg)(\$1.019/kg) = \$93.75
2 kg of Hydrogen = (2 kg)(\$0.381/kg) = \$0.76

Value of Products

78 kg of Benzene = (78 kg)(\$1.196/kg) = \$93.29
16 kg of Methane = (16 kg)(\$0.165/kg) = \$2.64

Profit Margin

Profit Margin = (93.29 + 2.64) – (93.75 + 0.76) = \$1.42 or \$0.0154/kg toluene

Based on this result, it is concluded that further investigation of this process may be warranted.

The results in Example 2.1 show that the profit margin for benzene using the HDA process are positive but small. It is unlikely that when the costs of equipment, utilities, and all other operating costs are correctly accounted for that production of benzene via the HDA process would be profitable. Nevertheless, benzene has been produced for the last 50 years and is a viable starting material for a host of petrochemical products. How is this possible? It must be concluded that benzene can be produced via at least one other route, which is less sensitive to changes in the price of toluene, benzene, and natural gas. One such commercial process is the disproportionation or transalkylation of toluene to produce benzene and a mixture of para-, ortho-, and meta-xylene via the following reaction:

$$\underset{toluene}{2C_7H_8} \rightarrow \underset{benzene}{C_6H_6} + \underset{xylene}{C_8H_{10}}$$

The profit margin for this process is given in Example 2.2.

Example 2.2

Evaluate the profit margin for the toluene disproportionation process.
From Table 8.4:
Mixed Xylenes = \$1.06/kg
Using 2 kmols of toluene feed as a basis

Cost of Raw Materials

184 kg of Toluene = (184 kg)(\$1.019/kg) = \$187.50

Value of Products

78 kg of Benzene = (78 kg)(\$1.196/kg) = \$93.29
106 kg of Xylene = (106 kg)(\$1.06/kg) = \$112.36

Margin

Profit Margin = 93.29 + 112.36 − 187.50 = \$18.15 or \$0.099/kg toluene feed

From the results of Example 2.2, the profit margin for the production of benzene via the disproportionation of toluene is greater than the toluene HDA process. In addition, a closer look at the cost of purified xylenes (from Table 8.4) shows that these purified xylenes are considerably more valuable (ranging in value from \$1.235 to \$2.91/kg) than the mixed xylene stream (\$1.06/kg). Therefore, the addition of a xylene purification section to the disproportionation process might well yield a significantly more profitable process. Historically, the prices of toluene and benzene fluctuate in phase with each other. In general, toluene disproportionation has been the preferred process for benzene production over the last two decades.

In carrying out Examples 2.1 and 2.2, a single-point price for each chemical was used. In general in order to determine a more accurate margin for a process, cost data for the feed and product chemicals over a period of several years should be sought in order to get average values and then these values should be used to evaluate the margin. Another important point to note is that there are often two or more different chemical paths to produce a given product. These paths may all be technically feasible; that is, catalysts for the reactions and separation processes to isolate and purify the products probably exist. However, it is the costs of the raw materials that usually play the major role when deciding which process to choose.

2.4 STEP 3—THE RECYCLE STRUCTURE OF THE PROCESS

The remaining three steps in building the process flow diagram basically involve the recovery of materials and energy from the process. It may be instructive to break down the operating costs for a typical chemical process. This analysis for the toluene process is given in Chapter 8, Example 8.10. From the results of Example 8.10, it can be seen that raw material costs (toluene and hydrogen) account for (87.398)/(114.6) × 100 = 76% of the total manufacturing costs. This value is typical for chemical processes. Peters and Timmerhaus [9] suggest that raw materials make up between 10% and 50% of the total operating costs for processing plants; however, due to increasing conservation and waste minimization techniques this estimate may be low, and an upper limit of 80% is more realistic. Because these raw materials are so valuable, it is imperative that unused reactants are separated and recycled. Indeed, high efficiency for raw material usage is a requirement of the vast majority of chemical processes. This is why the generic block flow process diagram (Figure 2.4) shows a recycle stream. However, the extent of recycling of unused reactants depends largely on the ease with which these unreacted raw materials can be separated (and purified) from the products that are formed within the reactor.

2.4.1 Efficiency of Raw Material Usage

It is important to understand the difference between single-pass conversion in the reactor, the overall conversion in the process, and the yield.

$$\text{Single-pass conversion} = \frac{\text{Reactant consumed in reaction}}{\text{Reactant fed to the reactor}} \tag{2.1}$$

$$\text{Overall conversion} = \frac{\text{Reactant consumed in process}}{\text{Reactant fed to the reactor}} \tag{2.2}$$

$$\text{Yield} = \frac{\text{Moles of reactant to produce desired product}}{\text{Moles of limiting reactant reacted}} \tag{2.3}$$

For the HDA process introduced in Chapter 1, the following values are obtained for the most costly reactant (toluene) from Table 1.5:

$$\text{Single-pass conversion} = \frac{(144.0 - 36.0)}{144.0} = 0.75 \text{ or } 75\%$$

$$\text{Overall conversion} = \frac{(108.7 - 0.4 - 0.31)}{108.7} = 0.993 \text{ or } 99.3\%$$

$$\text{Yield} = \frac{(105.2 + 2.85)}{(108.7 - 0.4 - 0.31)} = 0.9995 \text{ or } 99.95\%$$

The single-pass conversion indicates how much of the toluene that enters the reactor is converted to benzene. The lower the single-pass conversion, the greater the recycle must be, assuming that the unreacted toluene can be separated and recycled. In terms of the overall economics of the process, the single-pass conversion will affect equipment size and utility flows, because both of these are directly affected by the amount of recycle. However, the raw material costs are not changed significantly, assuming that the unreacted toluene is separated and recycled.

The overall conversion indicates what fraction of the toluene in the feed to the process (Stream 1) is converted to products. For the hydrodealkylation process, it is seen that this fraction is high (99.3%). This high overall conversion is typical for chemical processes and shows that unreacted raw materials are not being lost from the process.

Finally the yield indicates what fraction of the reacted toluene ends up in the desired product: benzene. For this case, the yield is unity (within round-off error), and this is to be expected because no competing or side reactions were considered. In reality, there is at least one other significant reaction that can take place, and this may reduce the yield of toluene. This case is considered in Problem 2.1 at the end of the chapter. Nevertheless, yields for this process are generally very high. For example, Lummus [10] quotes yields from 98% to 99% for their DETOL hydrodealkylation process.

By looking at the conversion of the other reactant, hydrogen, it can be seen from the data in Table 1.5 that

$$\text{Single-pass conversion} = \frac{(735.4 - 652.6)}{735.4} = 0.113 \text{ or } 11.3\%$$

$$\text{Overall conversion} = \frac{(286.0 - 178.0)}{286.0} = 0.378 \text{ or } 37.8\%$$

Clearly these conversions are much lower than for toluene. The single-pass conversion is kept low because a high hydrogen-to-hydrocarbon ratio is desired everywhere in the reactor so as to avoid or reduce coking of the catalyst. However, the low overall conversion of hydrogen indicates poor raw material usage. Therefore, the questions to ask are "Why is the material usage for toluene so much better than for hydrogen?" and "How can the hydrogen usage be improved?" These questions can be answered by looking at the ease of separation of hydrogen and toluene from their respective streams and leads us to investigate the recycle structure of the process.

2.4.2 Identification and Definition of the Recycle Structure of the Process

There are basically three ways that unreacted raw materials can be recycled in continuous processes.

1. Separate and purify unreacted feed material from products and then recycle.
2. Recycle feed and product together and use a purge stream.
3. Recycle feed and product together and do not use a purge stream.

Separate and Purify. Through the ingenuity of chemical engineers and chemists, technically feasible separation paths exist for mixtures of nearly all commercially desired chemicals. Therefore, the decision on whether to separate the unreacted raw materials must be made purely from economic considerations. In general, the ease with which a given separation can be made is dependent on two principles.

- First, for the separation process (unit operation) being considered, what conditions (temperature and pressure) are necessary to operate the process?
- Second, for the chemical species requiring separation, are the differences in physical or chemical properties for the species, on which the separation is based, large or small?

Examples that illustrate these principles are given below.

For the HDA process, the reactor effluent, Stream 9, is cooled and separated in a two-stage flash operation. The liquid, Stream 18, contains essentially benzene and toluene. The combined vapor stream, Streams 8 and 17, contains essentially methane and hydrogen. In Example 2.3, methods to separate the hydrogen in these two streams are considered and are used to screen potential changes in the recycle structure of the HDA process.

Example 2.3

For the separation of methane and hydrogen, first look at distillation:

Normal boiling point of methane = –161°C
Normal boiling point of hydrogen = –252°C

Separation should be easy using distillation due to the large difference in boiling points of the two components. However, in order to obtain a liquid phase, a combination of high pressure and very low temperature must be used. This will be very costly and suggests that distillation is not the best operation for this separation.

Absorption

It might be possible to absorb or scrub the methane from Streams 8 and 17 into a hydrocarbon liquid. In order to determine which liquids, if any, are suitable for this process, the solubility parameters for both methane and hydrogen in the different liquids must be determined. This information is available in Walas [11]. Because of the low boiling point of methane, a low temperature and high pressure would be required for effective absorption.

Pressure-Swing Adsorption

The affinity of a molecule to adhere (either chemically or physically) to a solid material is the basis of adsorption. In pressure-swing adsorption, the preferential adsorption of one species from the gas phase occurs at a given pressure, and the desorption of the adsorbed species is facilitated by reducing the pressure and allowing the solid to "de-gas." Two (or more) beds operate in parallel, with one bed adsorbing and the other desorbing. The separation and purification of hydrogen contained in gaseous hydrocarbon streams could be carried out using pressure-swing adsorption. In this case, the methane would be preferentially adsorbed onto the surface of a sorbent, and the stream leaving the unit would contain a higher proportion of hydrogen than the feed. This separation could be applied to the HDA process.

Membrane Separation

Commercial membrane processes are available to purify hydrogen from hydrocarbon streams. This separation is facilitated because hydrogen passes more readily through certain membranes than does methane. This process occurs at moderate pressures, consistent with the operation of the HDA process. However, the hydrogen is recovered at a fairly low pressure and would have to be recompressed prior to recycling. This separation could be applied to the HDA process.

From Example 2.3, it can be seen that pressure-swing adsorption and membrane separation of the gas stream should be considered as viable process alternatives, but for the preliminary PFD for this process, no separation of hydrogen was attempted. In Example 2.4, the separation of toluene from a mixture of benzene and toluene is considered.

Example 2.4

What process should be used in the separation of toluene and benzene?

Distillation

Normal boiling point of benzene = 80.1°C
Normal boiling point of toluene = 110.6 °C

Separation should be easy using distillation, and neither excessive temperatures nor pressures will be needed. This is a viable operation for the separation of benzene and toluene in the HDA process.

Economic considerations often make distillation the separation method of choice. The separation of benzene and toluene is routinely practiced through distillation and this is the preferred method in the preliminary PFD for this process.

Recycle Feed and Product Together with a Purge Stream. If separation of unreacted feed and products is not accomplished easily, then recycling both feed and product should be considered. In the HDA process, the methane product will act as an inert because it will not react with toluene. In addition, this process is not limited by equilibrium considerations; therefore, the reaction of methane and benzene to give toluene and hydrogen (the undesired path for this reaction), under the conditions used in this process, is not significant. It should be noted that for the case when a product is recycled with an unused reactant and the product does not react further, then a purge stream must be used to avoid the accumulation of product in the process. For the HDA process, the purge is the fuel gas containing the methane product and unused hydrogen, Stream 16, leaving the process. The recycle structure for the hydrogen and methane in the HDA process is illustrated in Figure 2.5.

Recycle Feed and Product Together without a Purge Stream. This recycle scheme is feasible only when the product can react further in the reactor and therefore there is no need to purge it from the process. If the product does not react and it does not leave the system with the other products, then it would accumulate in the process, and steady-state operations could not be achieved. In the previous case, with hydrogen and methane, it was seen that the methane did not react further and that it was necessary to purge some of the methane and hydrogen in Stream 16 in order to prevent accumulation of methane in the system.

An example where this strategy could be considered is again given in the toluene HDA process. Up to this point, only the main reaction between toluene and hydrogen has been considered:

$$\underset{\text{toluene}}{C_7H_8} + H_2 \rightarrow \underset{\text{benzene}}{C_6H_6} + CH_4$$

However, even when using a catalyst that is very specific to the production of benzene, some amount of side reaction will occur. For this process, the yield of toluene for commercial processes is on the order of 98% to 99%. Although this is high, it is still lower than the 100% that was originally assumed. A very small amount of toluene may react with the hydrogen to form

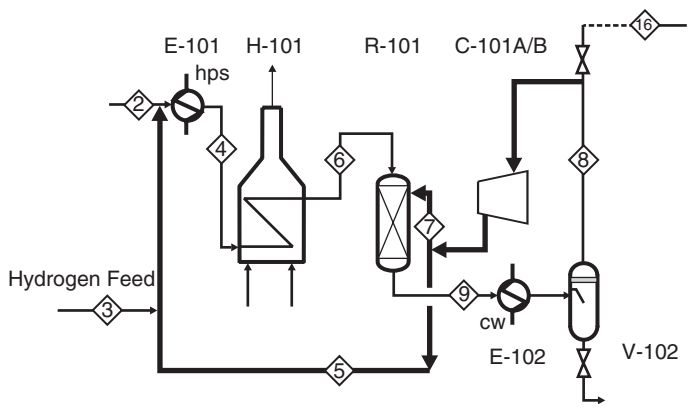

Figure 2.5 Recycle Structure of Hydrogen Stream in Toluene Hydrodealkylation Process. Methane Is Purged from the System via Stream 16.

small-molecule, saturated hydrocarbons, such as ethane, propane, and butane. More important, a proportion of the benzene reacts to give a two ring aromatic, diphenyl:

$$\underset{\text{benzene}}{2C_6H_6} \rightleftharpoons \underset{\text{diphenyl}}{C_{12}H_{10}} + H_4$$

The primary separation between the benzene and toluene in T-101 (see Figure 2.1) will remain essentially unchanged, because the light ends (hydrogen, methane, and trace amounts of C2–C4 hydrocarbons) will leave in the flash separators (V-102 and V-103) or from the overhead reflux drum (V-104). However, the bottoms product from T-101 will now contain toluene and essentially all the diphenyl produced in the reactor, because it has a much higher boiling point than toluene. It is known that the benzene/diphenyl reaction is equilibrium limited at the conditions used in the reactor. Therefore, if the diphenyl is recycled with the toluene, it will simply build up in the recycle loop until it reaches its equilibrium value. At steady state, the amount of diphenyl entering the reactor in Stream 6 will equal the diphenyl in the reactor effluent, Stream 9. Because diphenyl reacts back to benzene, it can be recycled without purging it from the system. The changes to the structure of the process that would be required if diphenyl were produced are considered in Example 2.5.

Example 2.5

Consider the following two process alternatives for the toluene HDA process when the side reaction of benzene to form diphenyl occurs.

Clearly for Alternative B, shown in Figure E2.5(b), an additional separator is required, shown here as a second distillation column T-102, along with the associated equipment (not shown) and extra utilities to carry out the separation. For Alternative A, shown in Figure E2.5(a), the cost of additional equipment is avoided, but the recycle stream (Stream 11) will be larger because it now contains toluene and diphenyl, and the utilities and equipment through which this stream passes (H-101, E-101, R-101, E-102, V-102, V-103, T-101, E-106) will all be greater. Which is the economically preferable alternative?

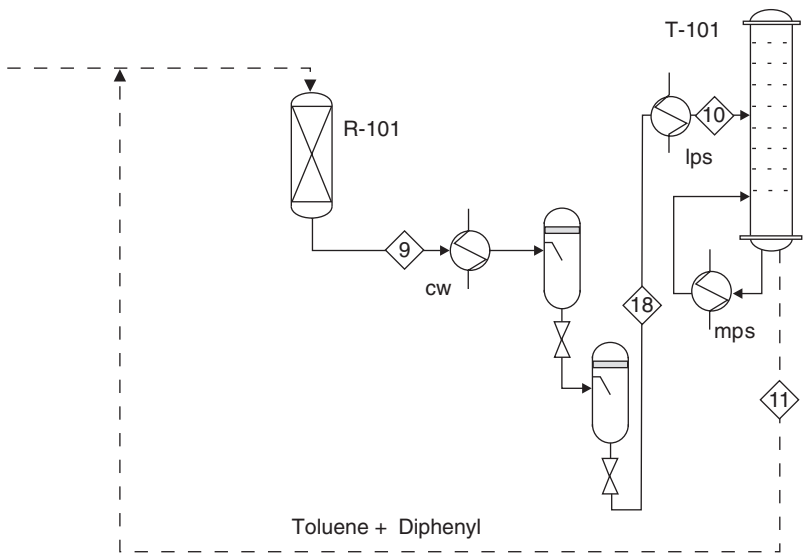

Figure E2.5(a) PFD for Alternative A in Example 2.5—Recycle of Diphenyl without Separation (E-101 and H-101 Not Shown)

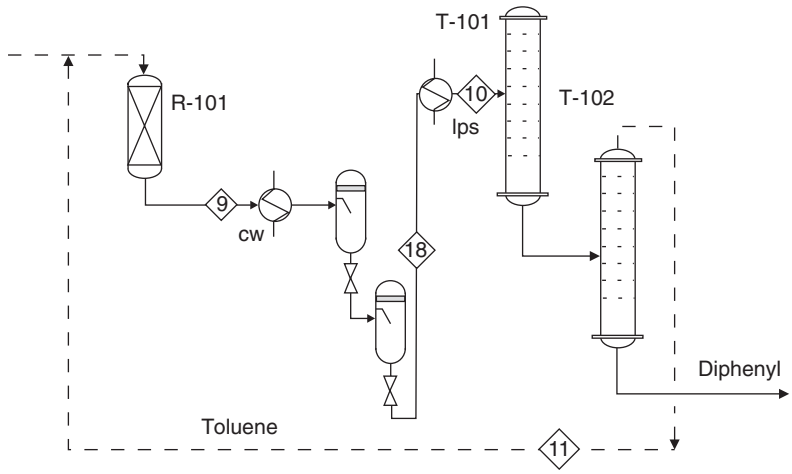

Figure E2.5(b) PFD for Alternative B in Example 2.5—Recycle of Diphenyl with Separation (E-101 and H-101 Not Shown)

The answer depends upon the value of the equilibrium constant for the benzene-diphenyl reaction. If the equilibrium conversion of benzene is high, then there will be a large amount of diphenyl in the recycle and the costs to recycle this material will be high, and vice versa. The equilibrium constant for this reaction is given as

$$\ln K_{eq} = 1.788 - \frac{4135.2}{T(K)}$$

The exit conditions of the reactor can be estimated by assuming that the benzene-diphenyl reaction has reached equilibrium, a conservative assumption. Using this assumption and data from Table 1.5 for Stream 9, if x kmol/h of diphenyl is present in the reactor effluent, then

$$K_{eq} = \frac{[C_{10}H_{12}][H_2]}{[C_6H_6]^2} \Rightarrow \exp\left[1.788 - \frac{4135.2}{(654 + 273)}\right] = \frac{(x)(652.6+x)}{(116-2x)^2}$$

Solving for the only unknown gives $x = 1.36$ kmol/h. Thus, the toluene recycle, Stream 11, will be increased from 35.7 to 37.06 kmol/h, an increase of 4%, while the increases in Streams 4 and 6 will be approximately 0.1%. Based on this result, Alternative A will probably be less expensive than Alternative B.

2.4.3 Other Issues Affecting the Recycle Structure That Lead to Process Alternatives

There are many other issues that affect the recycle structure of the PFD. The use of excess reactant, the recycling of inert materials, and the control of an equilibrium reaction are some examples that are addressed in this section.

How Many Potential Recycle Streams Are There? Consider first the reacting species that are of value. These are essentially all reactants except air and maybe water. Each reacting species that does not have a single-pass conversion >99% should be considered as a potential recycle stream. The value of 99% is an arbitrarily high number, and it could be anywhere from 90% to >99%,

depending on the cost of raw materials, the cost to separate and recycle unused raw materials, and the cost of disposing of any waste streams containing these chemicals.

How Does Excess Reactant Affect the Recycle Structure? When designing the separation of recycled raw materials, it is important to remember which reactant, if any, should be in excess and how much this excess should be. For the toluene HDA process, the hydrogen is required to be in excess in order to suppress coking reactions that foul the catalyst. The result is that the hydrogen:toluene ratio at the inlet of the reactor (from Table 1.5) is 735.4/144, or slightly greater than 5/1. This means that the hydrogen recycle loop must be large, and a large recycle compressor is required. If it were not for the fact that this ratio needs to be high, the hydrogen recycle stream, and hence the recycle compressor, could be eliminated.

How Many Reactors Are Required? The reasons for multiple reactors are as follows:

- **Approach to Equilibrium:** The classic example is the synthesis of ammonia from hydrogen and nitrogen. As ammonia is produced in a packed-bed reactor, the heat of reaction heats the products and moves the reaction closer to equilibrium. By adding additional reactants between staged packed beds arranged in series, the concentration of the reactants is increased, and the temperature is decreased. Both these factors move the reaction away from equilibrium and allow the reaction to proceed further to produce the desired product, ammonia.
- **Temperature Control:** If the reaction is mildly exothermic or endothermic, then internal heat transfer may not be warranted, and temperature control for gas-phase reactions can be achieved by adding a "cold (or hot) shot" between staged adiabatic packed beds of catalyst. This is similar to the ammonia converter described earlier. More information on the design of exothermic and endothermic reactions is given in Chapter 22.
- **Concentration Control:** If one reactant tends to form by-products, then it may be advantageous to keep this reactant at a low concentration. Multiple side feeds to a series of staged beds or reactors may be considered. See Chapter 22 for more details.
- **Optimization of Conditions for Multiple Reactions:** When several series reactions ($A \rightarrow R \rightarrow S \rightarrow T$) must take place to produce the desired product (T) and these reactions require different catalysts and/or different operating conditions, then operating a series of staged reactors at different conditions may be warranted.

Do Unreacted Raw Material Streams Need to Be Purified Prior to Recycling? The next issue is whether the components need to be separated prior to recycle. For example, if distillation is used to separate products from unused reactants, and if two of the reactants lie next to each other in a list of relative volatility, then no separation of these products is necessary. They can be simply recycled as a mixed stream.

Is Recycling of an Inert Warranted? The components in the feed streams that do not react, that is, are inert, are considered next. Depending on the process, it may be worth recycling these streams. For example, consider the water feed to the absorber, Stream 8, in the acetone production process (Appendix B, Figure B.10.1). This water stream is used to absorb trace amounts of isopropyl alcohol and acetone from the hydrogen vent, Stream 5. After purification, the water leaves the process as a wastewater stream, Stream 15. This water has been purified in column T-1103 and contains only trace amounts of organics. An alternative process configuration would be to recycle this water back to the absorber. This type of pollution prevention strategy is discussed further in Chapter 27.

Can Recycling an Unwanted Product or an Inert Shift the Reaction Equilibrium to Produce Less of an Unwanted Product? Another example of recycling an inert or unwanted product is to use that material to change the conversion and selectivity of an equilibrium reaction. For example, consider the production of synthesis gas (H_2 and CO) via the partial oxidation (gasification) of coal:

$$C_mH_n + \left(\frac{m}{2} + \frac{n}{4}\right)O_2 \rightarrow mCO + \frac{n}{2}H_2O \qquad \text{Partial oxidation}$$

$$C_mH_n + \left(m + \frac{n}{4}\right)O_2 \rightarrow mCO_2 + \frac{n}{2}H_2O \qquad \text{Complete oxidation}$$

$$CO + H_2O \rightleftharpoons CO_2 + H_2 \qquad \text{Water-gas shift}$$

Coal, shown here simply as a mixture of carbon and hydrogen, is reacted with a substoichiometric amount of pure oxygen in a gasifier, and steam is added to moderate the temperature. The resulting mixture of product gases forms the basis of the synthesis gas. The carbon dioxide is an unwanted by-product of the reaction and must be removed from the product stream, usually by a physical or chemi-physical absorption process. A viable process alternative is recycling a portion of the separated carbon dioxide stream back to the reactor. This has the effect of pushing the equilibrium of the water-gas shift reaction to the left, thus favoring the production of carbon monoxide.

Is Recycling of an Unwanted Product or an Inert Warranted for the Control of Reactor Operation? As mentioned previously, for highly exothermic reactions such as the partial oxidation of organic molecules, it is sometimes necessary to add an inert material to the reactor feed to moderate the temperature rise in the reactor and/or to move the reacting components outside of the explosive (flammability) limits. The most often used material for this purpose is steam, but any inert material that is available may be considered. For example, in the coal gasification example given earlier, steam is used to moderate the temperature rise in the reactor. For the case of recycling carbon dioxide to affect the water-gas shift reaction, there is another potential benefit. The recycling of carbon dioxide reduces the amount of steam needed in the feed to the reactor, because the carbon dioxide can absorb heat and reduce the temperature rise in the reactor.

What Phase Is the Recycle Stream? The phase of the stream to be recycled plays an important role in determining the separation and recycle structure of the process. For liquids, there are concerns about azeotropes that complicate the separations scheme. For gases, there are concerns about whether high pressures and/or low temperatures must be used to enable the desired separation to take place. In either case gas compression is required, and, generally, this is an expensive operation. For example, the use of membrane separators or pressure-swing adsorption requires that the gas be fed at an elevated pressure to these units. If separation of a gas (vapor) is to be achieved using distillation, then a portion of the gas must be condensed, which usually requires cooling the gas significantly below ambient temperatures. This cooling process generally requires the use of compressors in the refrigeration cycle and the lower the desired temperature, the more expensive is the refrigeration. Some typical refrigerants and their temperature ranges are given in Table 2.2. Because separations of gases require expensive, low-temperature refrigeration, they are avoided unless absolutely necessary.

Table 2.2 Common Refrigerants and Their Ranges of Cooling (Data from References [12] and [13])

Refrigerant	Typical Operating Temperature Range (°C)	Vapor Pressure at 45°C (bar)	Critical Pressure (bar)	Critical Temperature (°C)
Methane	–129 to –184	749	46.0	–82.5
Ethane	–59 to –115	1453	48.8	32.3
Ethylene	–59 to –115	2164	50.3	9.3
Propane	4 to –46	15.3	42.5	96.7
Propylene	4 to –46	18.45	46.1	91.6
N-Butane	16 to –12	4.35	38.0	152.0
Ammonia	27 to –32	17.8	112.8	132.5
Carbon Dioxide	4 to –50	787	73.8	31.1
Methylene Chloride	4 to –12	1.21	60.8	236.9
Methyl Chloride	4 to –62	9.84	66.8	143.1
R-134a (1,1,1,2-tetrafluoro-ethane)	4 to –50	11.6	40.6	101.0
R-152a (1,1-difluoro-ethane)	4 to –50	10.4	45.0	113.5

Only refrigerants with critical temperatures above the typical cooling water condenser temperature of 45°C can be used in single-stage, noncascaded refrigeration systems. Therefore, such systems are usually limited to the range of –45°C to –60°C (for example using propylene, propane, or methyl chloride). For lower temperatures, refrigeration systems with two different refrigerants are required, with the lower-temperature refrigerant rejecting heat to the higher-temperature refrigerant, which in turn rejects heat to the cooling water. Costs of refrigeration are given in Chapter 8, and these costs increase drastically as the temperature decreases. For this reason, separations of gases requiring very low temperatures are avoided unless absolutely necessary.

As a review of the concepts covered in this chapter, Example 2.6 is presented to illustrate the approach to formulating a preliminary process flow diagram.

Example 2.6

Illustrative Example Showing the Input/Output and Recycle Structure Decisions Leading to the Generation of Flowsheet Alternatives for a Process

Consider the conversion of a mixed feed stream of methanol (88 mol%), ethanol (11 mol%), and water (1 mol%) via the following dehydration reactions:

$$\underset{\text{methanol}}{2CH_3OH} \rightleftharpoons \underset{\text{dimethyl ether (desired product)}}{(CH_3)_2O} + H_2O \qquad {}^{\circ}H_{reac} = -11{,}770 \text{ kJ/kmol}$$

$$\underset{\text{ethanol}}{2C_2H_5OH} \rightleftharpoons \underset{\text{diethyl ether (valuable by-product)}}{(C_2H_5)_2O} + H_2O \qquad {}^{\circ}H_{reac} = -11{,}670 \text{ kJ/kmol}$$

$$\underset{\text{ethanol}}{C_2H_5OH} \rightarrow \underset{\text{ethylene (less valuable by-product)}}{C_2H_4} + H_2O \qquad \Delta H_{reac} = -1570 \text{ kJ/kmol}$$

The reactions take place in the gas phase, over an alumina catalyst [14, 15], and are mildly exothermic but do not require additional diluents to control reaction temperature. The stream leaving the reactor (reactor effluent) contains the following components, listed in order of decreasing volatility (increasing boiling point):

1. Ethylene (C_2H_4)
2. Dimethyl Ether (DME)
3. Diethyl Ether (DEE)
4. Methanol (MeOH)
5. Ethanol (EtOH)
6. Water (H_2O)

Moreover, because these are all polar compounds, with varying degrees of hydrogen bonding, it is not surprising that these compounds are highly nonideal and form a variety of azeotropes with each other. These azeotropes are as follows:

- DME – H_2O (but no azeotrope with significant presence of alcohol)
- DME – EtOH
- DEE – EtOH
- DEE – H_2O
- EtOH – H_2O

For this problem, it is assumed that the mixed alcohol stream is available at a relatively low price from a local source ($0.75/kg). However, pure methanol ($0.672/kg) and/or ethanol ($1.138/kg) streams may be purchased if necessary. The selling prices for DME, DEE, and ethylene are $0.841/kg, $1.75/kg, and $1.488/kg, respectively. Preliminary market surveys indicate that up to 15,000 tonne/y of DEE and up to 10,000 tonne/y of ethylene can be sold.

For a proposed process to produce 50,000 tonne/y of DME, determine the viable process alternatives.

Step 1: Batch versus Continuous

For a plant of this magnitude, a continuous process would probably be chosen. However, this issue will be reviewed after considering some process alternatives and it will be seen that a hybrid batch/continuous process should also be considered.

Step 2: Define the Input/Output Structure of the Process

The basic input/output diagram of the process is shown in the process concept diagram of Figure E2.6(a). First, consider a material balance for the process and estimate the profit margin:

$$\text{Desired DME production} = 50{,}000{,}000\ \text{kg/y} = \frac{50\times10^6}{46} = 1.087\times10^6\ \text{kmol/y}$$

$$\text{Required MeOH feed} = (2)(1.087\times10^6) = 2.174\times10^6\ \text{kmol/y}$$

$$\text{EtOH feed entering with methanol} = \frac{2.174\times10^6}{88}(11) = 0.2718\times10^6\ \text{kmol/y}$$

$$\text{Maximum DEE production} = \frac{0.2718\times10^6}{2} = 0.1309\times10^6\ \text{kmol/y or } 9.69\times10^3\ \text{tonne/y}$$

$$\text{Maximum ethylene production} = 0.2718\times10^6\ \text{kmol/y or } 7.61\times10^3\ \text{tonne/y}$$

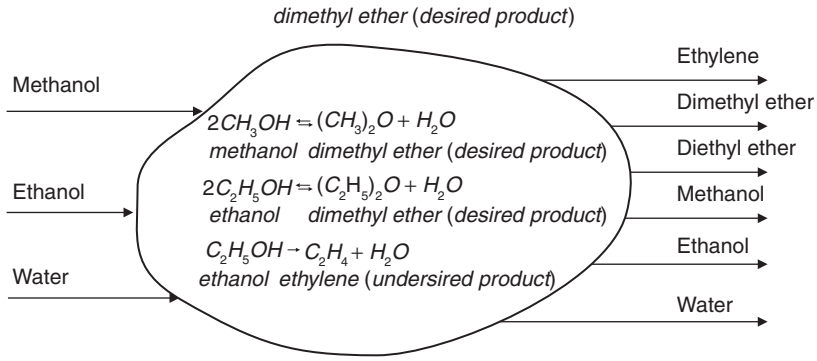

Figure E2.6(a) Process Concept Diagram for the Mixed Ethers Process of Example 2.6

$$\text{Cost of feed} = \left((2.174 \times 10^6)(30) + (0.2718 \times 10^6)(46) + \frac{(2.174 \times 10^6)}{88}(18) \right)(0.75) = \$58.62 \times 10^6$$

$$\text{Value of DME} = (50 \times 10^6)(0.841) = \$42.05 \times 10^6 / \text{y}$$

$$\text{Value of DEE (maximum production)} = (0.1309 \times 10^6)(74)(1.75) = \$16.95 \times 10^6 / \text{y}$$

$$\text{Value of ethylene (maximum production)} = (0.2718 \times 10^6)(28)(1.488) = \$11.32 \times 10^6 / \text{y}$$

Margin will vary between (42.05 + 16.95 − 58.62) = \$0.38 million and (42.05 + 11.32 − 58.62) = −\$5.24 million per year.

Important Points

From this margin analysis, it is clear that the amount of DEE produced should be optimized, because making ethylene is far less profitable. In addition, the maximum amount of DEE that the market can support is not currently being produced. Therefore, supplementing the feed with ethanol should be considered.

Because the main feed stream contains both reactants and an impurity (water), separation or purification of the feed prior to processing should be considered.

In order to minimize the production of by-products (ethylene), the selectivity of the DEE reaction should be optimized.

Alternative 1

In this option, shown in Figure E2.6(b), the mixed alcohol feed is not separated, but feed is supplemented with ethanol. One reactor is used for both reactions. The disadvantages of this case are that the separations are complicated and the reactor for both DME and DEE production cannot be optimized easily.

Alternative 2

In this option, shown in Figure E2.6(c), feed is supplemented with ethanol and is separated into separate methanol and ethanol streams. Two reaction trains are used: one for DME and the other for DEE production. This allows the production of DME and DEE to be optimized separately and eliminates problems associated with the DME-ethanol azeotrope. However, there are two reactors and at least one more separation (column).

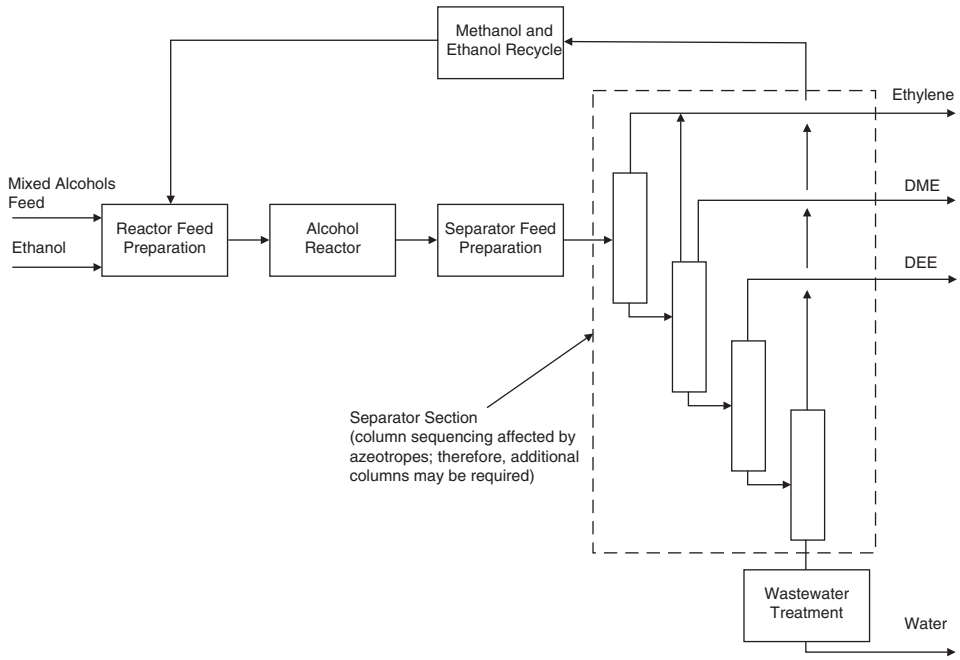

Figure E2.6(b) Structure of Process for Alternative 1 in Example 2.6

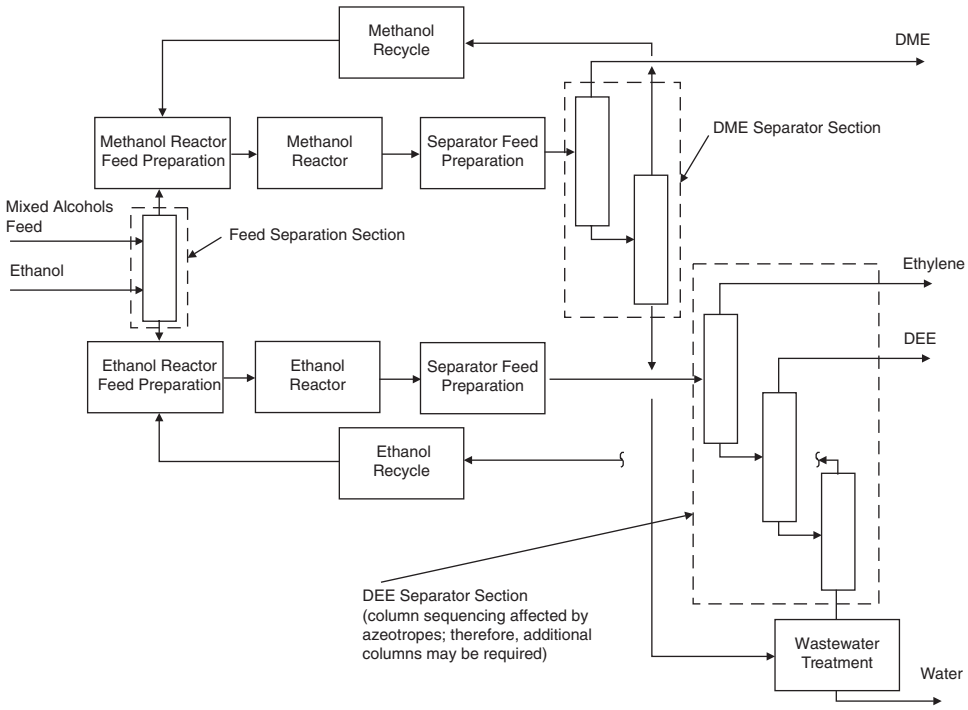

Figure E2.6(c) Structure of Process for Alternative 2 in Example 2.6

Alternative 3

This option is a hybrid between batch and continuous processes. The methanol is continuously separated from ethanol in the first column. However, the same equipment is used to produce both DME and DEE but at different times. The equipment is run in two "campaigns" per year. In the first campaign (Figure E2.6[d]), DME is produced and ethanol is stored for use in the second campaign.

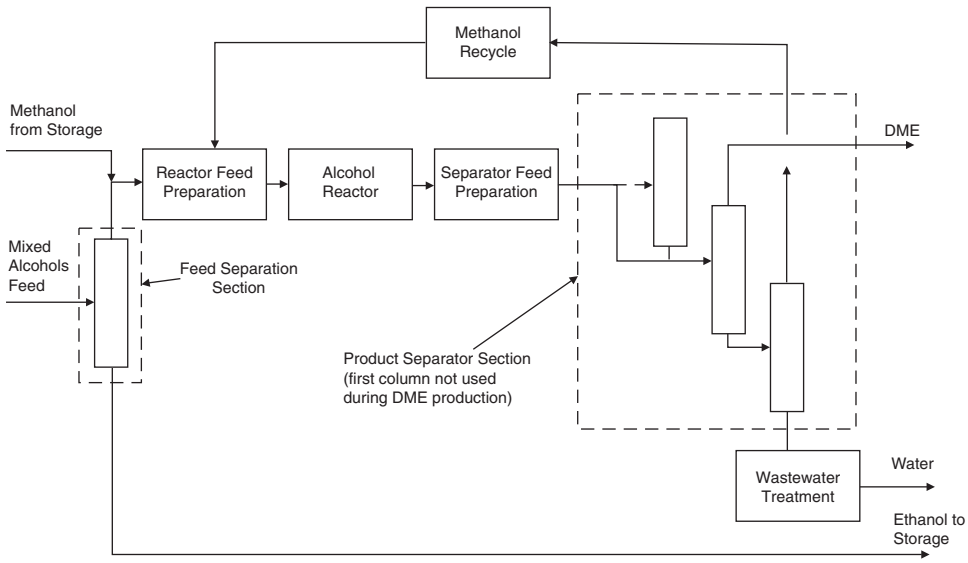

Figure E2.6(d) Structure of Process for Alternative 3—DME Campaign in Example 2.6

In the second campaign, shown in Figure E2.6(e), methanol is sent to storage, and ethanol is taken from storage to produce DEE and ethylene using the same equipment that was used to produce DME. For this part of the campaign, the first column is used to remove the ethylene.

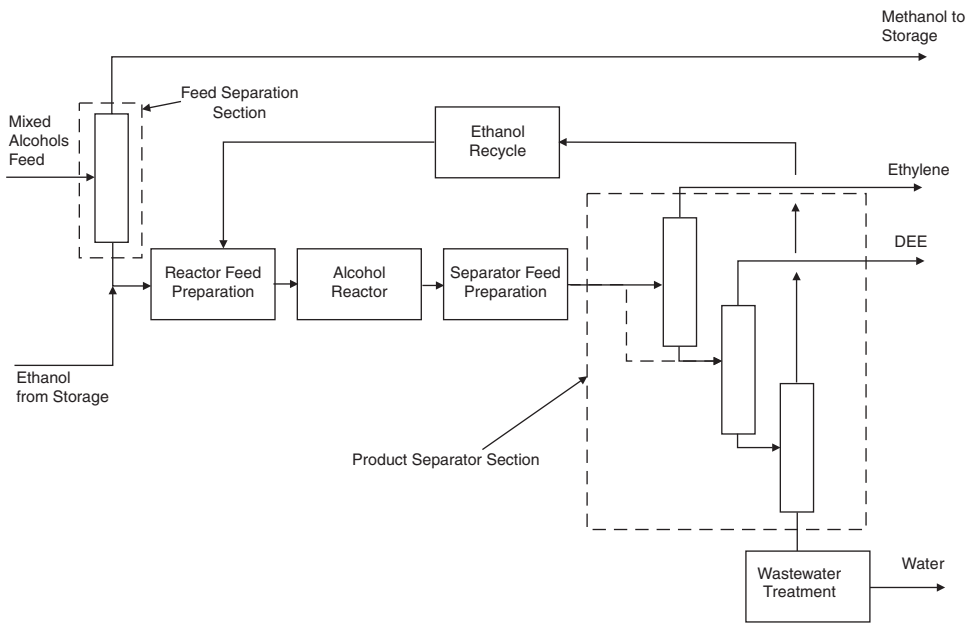

Figure E2.6(e) Structure of Process for Alternative 3—DEE Campaign in Example 2.6

For this option, there is significantly less equipment to buy. However, the design and optimization of the process are more complicated because the equipment must be designed to perform two separate and quite different functions.

2.5 STEP 4—GENERAL STRUCTURE OF THE SEPARATION SYSTEM

As pointed out previously, the structure of the separation sequence is covered in detail in Chapter 12. In that chapter, considerable emphasis is placed on the sequencing of distillation columns, and some of the problems associated with azeotropic systems are covered.

2.6 STEP 5—HEAT-EXCHANGER NETWORK OR PROCESS ENERGY RECOVERY SYSTEM

The main objective of process energy recovery is to optimize the energy that a process exchanges with the utilities. At the expense of capital investment, the utility usage can be decreased by exchanging energy between process streams. The amount of energy integration is a function of the relative costs of the utilities. In addition, the process becomes more complex and more difficult to control. This loss in flexibility must be weighed against the savings in operating costs. These and other issues are covered in more detail in Chapter 15.

2.7 INFORMATION REQUIRED AND SOURCES

In formulating a process flow diagram, one of the most important tasks is the collection and synthesis of data. These data are available in a wide variety of publications. As a guide, a summary of useful resources is presented in Table 2.3. The data in this table are partitioned into information pertaining to new and existing processes and data on new and existing chemical pathways.

2.8 SUMMARY

In this chapter, the development of a process flow diagram has been investigated. The first step in synthesizing a PFD was to establish and examine all possible chemical routes that form the desired product(s). The next step was to establish whether the process should operate in a batch or continuous manner. Guidelines to make this decision were presented in Table 2.1. The next step was to establish the input/output structure of the process. A process concept diagram was introduced that only required the identification of the raw materials, products, and stoichiometry of all the reactions that take place. At the process level, it was shown that all processes possess the same basic structure given in the generic block flow diagram.

Table 2.3 Summary of Resources for Obtaining Information on Chemical Processes

Resource	Information Available
	Existing Processes
Shreve's Chemical Process Industries [16]	Gives a good review of basic processes to produce a wide variety of chemicals. Both organic and inorganic chemicals are covered.
Refinery Processes Handbook [17]	Published every other year in *Hydrocarbon Processing*. Gives basic block flow diagrams and operating cost and capital investment data for a wide range of refinery operations.
Gas Processes Handbook [18]	Published every other year in *Hydrocarbon Processing*. Gives basic block flow diagrams and operating cost and capital investment data for a wide range of gas processing operations.
Petrochemical Processes Handbook [19]	Published every other year *in Hydrocarbon Processing*. Gives basic block flow diagrams and operating cost and capital investment data for a wide range of gas petrochemical operations.
Kirk-Othmer Encyclopedia of Chemical Technology [20]	Comprehensive 25-volume encyclopedia has background information and PFDs for a wide variety of organic and inorganic chemical processes.
Encyclopedia of Chemical Processing and Design [21]	Comprehensive 20-volume encyclopedia contains background information on a variety of chemical processes. Many solutions to previous AIChE student contest problems are published as case studies.
	Reaction and Kinetics
Chemical Reactor Design for Process Plants [22]	Vol. 2 has several excellent case studies for processes, including reaction kinetics and reactor designs.
Industrial and Engineering Chemistry Research	This journal is published monthly by the American Chemical Society and contains numerous research articles containing information about processes and reaction kinetics.
Journal of Catalysis—Academic Press *Applied Catalysis*—Elsevier *Catalysis Today*—Elsevier	These (and other) journals concentrate on research conducted into the field of heterogeneous catalysis. Kinetic expressions and activity data are given for many processes of industrial importance.
Patents	The patent literature contains a wealth of information about new processes. Typically, single-pass conversions and catalyst activities are given. However, reaction kinetics are generally not provided and may not be derived easily from patent data. An excellent on-line patent search engine is at http://www.delphion.com.
SRI Reports	Excellent source of background information on all aspects of processes. Unfortunately, this information is available only to industrial clients of this service.

The recycle structure of the PFD was introduced, and the three basic methods of recycle were discussed. Reasons and examples were provided to illustrate why inert material or products are sometimes recycled with unreacted raw materials. Difficulties in separating streams of products and reactants were given, and these were shown to influence the recycle structure and type of separation used.

The separation of products and unreacted raw materials and the integration of energy were covered briefly and are covered in greater depth in Chapters 12 and 15, respectively. An example showing how process alternatives are generated using the methods outlined in this chapter was provided, and several process alternatives were illustrated for this example using generic block flow diagrams. Finally, a list of resources was presented to help guide the reader to obtain basic data on chemical reactions and processes.

WHAT YOU SHOULD HAVE LEARNED

- The first choice is whether to use batch or continuous operation.
- Continuous chemical processes have a general structure:
  - Input-output
  - Recycle
  - Separation
- The input-output structure of a continuous chemical process consists of
  - Reactor feed preparation
  - Reactor
  - Separation feed preparation
  - Separation
  - Recycle
  - Environmental control

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SHORT ANSWER QUESTIONS

1. What are the five elements of the hierarchy of process design?
2. What are the three types of recycle structures possible in a chemical process? Explain when each is used.
3. Give three criteria for choosing a batch process as opposed to a continuous process.
4. When would one purposely add an inert material to a feed stream? Illustrate this strategy with an example, and explain the advantages (and disadvantages) of doing this.
5. In general, when would one purify a material prior to feeding it to a process unit? Give at least one example for each case you state.

PROBLEMS

6. In modern integrated gasification combined cycle (IGCC) coal-fed power plants, oxygen is produced via cryogenic separation of air and is fed to the IGCC plant along with coal. The separation of oxygen from air is expensive; what reason(s) can you give for doing this?

7. The production of ethylbenzene is described in Appendix B, Project B.2. From the PFD (Figure B.2.1) and accompanying stream table (Table B.2.1), determine the following:
   a. The single-pass conversion of benzene
   b. The single-pass conversion of ethylene
   c. Overall conversion of benzene
   d. Overall conversion of ethylene

   Suggest two strategies to increase the overall conversion of ethylene and discuss their merits.
8. Consider the following statement: "If a reactant (*G*) in a process is a gas at the feed conditions, subsequent separation from the reactor effluent is difficult, hence unused *G* cannot be recycled." Do you agree with this statement? Give your reasoning why you agree or disagree.
9. Most pharmaceutical products are manufactured using batch processes. Give at least three reasons why this is so.
10. The formation of styrene via the dehydrogenation of ethylbenzene is a highly endothermic reaction. In addition, ethylbenzene may decompose to benzene and toluene and also may react with hydrogen to form toluene and methane:

$$\underset{\text{ethylbenzene}}{C_6H_5C_2H_5} \overset{1}{\underset{2}{\rightleftharpoons}} \underset{\text{styrene}}{C_6H_5C_2H_3} + \underset{\text{hydrogen}}{H_2} \tag{B.2.1}$$

$$\underset{\text{ethylbenzene}}{C_6H_5C_2H_5} \overset{3}{\rightarrow} \underset{\text{benzene}}{C_6H_6} + \underset{\text{ethylene}}{C_2H_4} \tag{B.2.2}$$

$$\underset{\text{ethylbenzene}}{C_6H_5C_2H_5} + \underset{\text{hydrogen}}{H_2} \overset{4}{\circ} \underset{\text{toluene}}{C_6H_6CH_3} + \underset{\text{methane}}{CH_4} \tag{B.2.3}$$

   This process is presented in Appendix B as Project B.3 From the information given in Appendix B, determine the following:
   a. The single-pass conversion of ethylbenzene
   b. The overall conversion of ethylbenzene
   c. The yield of styrene

   Suggest one strategy to increase the yield of styrene, and sketch any changes to the PFD that this strategy would require.
11. There are two technically viable routes to the production of a hydrocarbon solvent, *S*, starting with feed material *A*. Route 1 uses a disproportionation reaction, in which feed material *A* is converted to the desired solvent *S* and another solvent *R*, both of which are marketable products. Route 2 starts with the same chemical *A* but uses a hydrodealkylation reaction to produce the desired solvent. The reaction schemes for each process are shown below.

$$\text{Route 1} \qquad 2A \rightarrow S + R$$

$$\text{Route 2} \qquad A + H_2 \circ S + CH_4$$

   Assuming that pure *A* is fed to the process, the solvents *S* and *R* are separable by simple distillation, and both are much less volatile than either methane or hydrogen, sketch PFDs for Routes 1 and 2. Which process do you think will be more profitable? Explain your reasoning and assumptions.

12. When considering the evolution of a process flowsheet, it was noted that there are three forms of recycle structure for unused reactants, given as a–c below. For each case, carefully explain under what conditions you would consider or implement each strategy.
    a. Separate, purify, and recycle
    b. Recycle without separation and use a purge
    c. Recycle without separation and do not use a purge
13. Acetaldehyde is a colorless liquid with a pungent, fruity odor. It is primarily used as a chemical intermediate, principally for the production of acetic acid, pyridine and pyridine bases, peracetic acid, pentaeythritol, butylene glycol, and chloral. Acetaldehyde is a volatile and flammable liquid that is miscible in water, alcohol, ether, benzene, gasoline, and other common organic solvents. In this problem, the synthesis of acetaldehyde via the dehydrogenation of ethanol is to be considered. The following reactions occur during the dehydrogenation of ethanol:

$$CH_3CH_2OH \rightarrow \underset{\text{acetaldehyde}}{CH_3CHO} + H_2 \quad (1)$$

$$2CH_3CH_2OH \rightarrow \underset{\text{ethyl acetate}}{CH_3COOC_2H_5} + 2H_2 \quad (2)$$

$$2CH_3CH_2OH \rightarrow \underset{\text{butanol}}{CH_3(CH_2)_3OH} + H_2O \quad (3)$$

$$CH_3CH_2OH + H_2O \rightleftharpoons \underset{\text{acetic acid}}{CH_3COOH} + 2H_2 \quad (4)$$

    The single-pass conversion of ethanol is typically 60%. The yields for each reaction are approximately:
    1. Acetaldehyde 92%
    2. Ethyl acetate 4%
    3. Butanol 2%
    4. Acetic acid 2%

    a. For this process, generate a process concept diagram showing all the input and output chemicals.
    b. Develop two alternative preliminary process flow diagrams for this process.
14. Consider the following process in which liquid feed material *A* (normal BP of 110°C) is reacted with gaseous feed material *G* to produce main product *C* and by-products *R* and *S* via the following reactions:

$$A + G \rightleftharpoons C + S$$

$$G + C \rightleftharpoons R$$

    Both feeds enter the process at ambient temperature and pressure. Both reactions occur in the gas phase at moderate temperature and pressure (250°C and 10 bar). The normal boiling points of *G, S,* and *C* are less than –120°C. By-product *R* has a normal boiling point of 75°C and is highly soluble in water. Product *C* is very soluble in water but *G* and *S* are insoluble. The single-pass conversion through the reactor is low for feed *A*, and the ratio of *G* to *A* in the feed to the reactor

should be maintained in excess of 4 to minimize the chance of other unwanted side reactions. Using this information, and assuming that both *A* and *G* are expensive, do the following:

a. Draw a preliminary process flow diagram identifying the main unit operations (reactors, compressors, pumps, heat exchangers, and separators), and identify the recycle structure of the process.
b. Justify the methods used to recycle *A* and *G*.
c. What unit operations do you suggest for your separators? Justify your choices.
d. How would your PFD change if the price of feed material *G* were very low?

15. How is Scotch whisky made?

The following descriptions of malt and grain whisky manufacturing are given here courtesy of the University of Edinburgh at http://www.dcs.ed.ac.uk/home/jhb/ whisky/swa/chap3 .html. For each of the two processes, sketch a process flow diagram.

There are two kinds of Scotch whisky: malt whisky, which is made by the pot still process, and grain whisky, which is made by the patent still (or Coffey still) process. Malt whisky is made from malted barley only, whereas grain whisky is made from malted barley together with unmalted barley and other cereals.

Malt Whisky

The pot still process by which malt whisky is made may be divided into four main stages: malting, mashing, fermentation, and distillation.

(1) Malting

The barley is first screened to remove any foreign matter and then soaked for two or three days in tanks of water known as steeps. After this it is spread out on a concrete floor known as the malting floor and allowed to germinate. Germination may take from 8 to 12 days depending on the season of the year, the quality of the barley used, and other factors. During germination the barley secretes the enzyme diastase, which makes the starch in the barley soluble, thus preparing it for conversion into sugar. Throughout this period the barley must be turned at regular intervals to control the temperature and rate of germination.

At the appropriate moment germination is stopped by drying the malted barley or green malt in the malt kiln. More usually nowadays malting is carried out in Saladin boxes or in drum maltings, in both of which the process is controlled mechanically. Instead of germinating on the distillery floor, the grain is contained in large rectangular boxes (Saladin) or in large cylindrical drums. Temperature is controlled by blowing air at selected temperatures upward through the germinating grain, which is turned mechanically. A recent development caused by the rapid expansion of the Scotch whisky industry is for distilleries to obtain their malt from centralized maltings that supply a number of distilleries, thereby enabling the malting process to be carried out more economically.

(2) Mashing

The dried malt is ground in a mill, and the grist, as it is now called, is mixed with hot water in a large circular vessel called a mash tun. The soluble starch is thus converted into a sugary liquid known as wort. This is drawn off from the mash tun, and the solids remaining are removed for use as cattle feed.

(3) Fermentation

After cooling, the wort is passed into large vessels holding anything from 9000 to 45,000 liters of liquid, where it is fermented by the addition of yeast. The living yeast attacks the sugar in the wort and converts it into crude alcohol. Fermentation takes about 48 hours and produces a liquid known as wash, containing alcohol of low strength, some unfermentable matter, and certain by-products of fermentation.

(4) Distillation

Malt whisky is distilled twice in large copper pot stills. The liquid wash is heated to a point at which the alcohol becomes vapor. This rises up the still and is passed into the cooling plant, where it is condensed into liquid state. The cooling plant may take the form of a coiled copper tube or worm that is kept in continuously running cold water, or it may be another type of condenser.

The first distillation separates the alcohol from the fermented liquid and eliminates the residue of the yeast and unfermentable matter. This distillate, known as low wines, is then passed into another still, where it is distilled a second time. The first runnings from this second distillation are not considered potable, and it is only when the spirit reaches an acceptable standard that it is collected in the spirit receiver. Again, toward the end of the distillation, the spirit begins to fall off in strength and quality. It is then no longer collected as spirit but drawn off and kept, together with the first running, for redistillation with the next low wines.

Pot-still distillation is a batch process.

Grain Whisky

The patent still process by which grain whisky is made is continuous in operation and differs from the pot still process in four other ways.

a. The mash consists of a proportion of malted barley together with unmalted cereals.
b. Any unmalted cereals used are cooked under steam pressure in converters for about 3½ hours. During this time the mixture of grain and water is agitated by stirrers inside the cooker.
c. The starch cells in the grain burst, and when this liquid is transferred to the mash tun, with the malted barley, the diastase in the latter converts the starch into sugar.
d. The wort is collected at a specific gravity lower than in the case of the pot still process.
e. Distillation is carried out in a patent or Coffey still, and the spirit collected at a much higher strength.

Storage and aging of the whisky are also an important part of the overall process but need not be considered for this problem. Storage occurs in oak barrels that previously stored either sherry or bourbon (or both, in the case of double-aged whisky). The length of storage in the barrel determines the vintage of the whisky. Unlike wine, the time after bottling does not count, and so a 15-year-old scotch that was bought in 1960 is today still a 15-year-old scotch.

CHAPTER

3

Batch Processing

WHAT YOU WILL LEARN

- Batch processing is very different from continuous processing.
- The design equations are different and require the solution of transient balances.
- Scheduling of equipment is important.
- There are different types of scheduling patterns.

Some key reasons for choosing to manufacture a product using a batch process were discussed in Chapter 2. These include small production volume, seasonal variations in product demand, a need to document the production history of each batch, and so on. When designing a batch plant, there are many other factors an engineer must consider. The types of design calculations are very different for batch compared with continuous processes. Batch calculations involve transient balances, which are different from the steady-state design calculations taught in much of the traditional chemical engineering curriculum. Batch **sequencing**—the order and timing of the processing steps—is probably the most important factor to be considered. Determining the optimal batch sequence depends on a variety of factors. For example, will there be more than one product made using the same equipment? What is the optimal size of the equipment? How long must the equipment run to make each different product? What is the trade-off between economics and operability of the plant? In this chapter, these questions will be addressed, and an introduction to other problems that arise when considering the design and operation of batch processes will be provided.

3.1 DESIGN CALCULATIONS FOR BATCH PROCESSES

Design calculations for batch processes are different from the steady-state design calculations taught in most unit operations classes. The batch nature of the process makes all the design calculations unsteady state. This is best demonstrated by example; Example 3.1 illustrates the types of design calculations required for batch processing.

Example 3.1

In the production of an API (active pharmaceutical ingredient), the following batch recipe is used.

Step 1: 500 kg of reactant A (MW = 100 kg/kmol) is added to 5000 kg of a mixture of organic solvent (MW = 200 kg/kmol) containing 60% excess of a second reactant B (MW = 125 kg/kmol) in a jacketed reaction vessel (R-301), the reactor is sealed, and the mixture is stirred and heated (using steam in the jacket) until the temperature has risen to 95°C. The density of the reacting mixture is 875 kg/m^3 (time taken = 1.5 h).

Step 2: Once the reaction mixture has reached 95°C, a solid catalyst is added, and reaction takes place while the batch of reactants is stirred. The required conversion is 94% (time taken = 2.0 h).

Step 3: The reaction mixture is drained from the reactor and passed through a filter screen (Sc-301) that removes the catalyst and stops any further reaction (time taken = 0.5 h).

Step 4: The reaction mixture (containing API, solvent, and unused reactants) is transferred to a distillation column, T-301, where it is distilled under vacuum. Virtually all of the unused reactants and approximately 50% of the solvent are removed as overhead product (time taken = 3.5 h). The end point for the distillation is when the solution remaining in the still contains less than 1 mol% of reactant B. This ensures that the crystallized API, produced in Step 5, meets specification.

Step 5: The material remaining in the still is pumped to a crystallizer, CR-301, where the mixture is cooled under vacuum and approximately 60% of the API from Step 2 crystallizes out (time taken = 2.0 h).

Step 6: The API is filtered from the crystallizer and placed in a tray dryer, TD-301, where any entrapped solvent is removed (time taken = 4 h).

Step 7: The dried API is sealed and packaged in a packing machine, PK-301, and sent to a warehouse for shipment to the customer (time taken = 1.0 h).

Perform a preliminary design on the required equipment items for this batch process.

Solution

The equipment items will be designed in sequence.

Step 1: Reaction Vessel—Preheat

The reaction vessel, which is used to preheat the reactants and subsequently run the reaction, is designed first. For the batch size specified, the volume of the liquid in the tank, V, and the volume required for the reaction vessel, V_{tank}, are given by Equations (E3.1a) and (E3.1b), in which it is assumed that the vessel is approximately 60% full during operation.

$$V = \frac{5500\,[\text{kg}]}{875\,[\text{kg/m}^3]} = 6.286\,\text{m}^3 \tag{E3.1a}$$

$$V_{required} = \frac{5500\,[\text{kg}]}{875\,[\text{kg/m}^3]}\frac{1}{0.6} = 10.48\,\text{m}^3 = 2768\,\text{gal} \tag{E3.1b}$$

Because reactors of this sort come in standard sizes, a 3000 gal (V_{tank}) reactor is selected.

The heat transfer characteristics of this vessel are then checked. For a jacketed vessel, the unsteady-state design equation is

$$\rho V C_p \frac{dT}{dt} = UA\left(T_s - T\right) \tag{E3.1c}$$

where ρ is the liquid density, C_p is the liquid heat capacity, T is the temperature of the liquid in the tank (95°C is the desired value in 1.5 h), U is the overall heat transfer coefficient from the jacket to the liquid in the tank, A is the heat transfer area of the jacket (cylinder surface), and T_s is the temperature

of the condensing steam. (Normally, there is also a jacketed bottom to such a vessel, but this added heat transfer area is ignored in this example for simplification.) Integration of this equation yields

$$\ln\frac{\left(T_s - T_{final}\right)}{\left(T_s - T_o\right)} = -\frac{UA\Delta t}{\rho V C_p} \tag{E3.1d}$$

where T_o is the initial temperature in the tank (assumed to be 25°C). The following "typical" values are assumed for this design:

$C_p = 2000$ J/kg°C
$T_s = 120$°C (200 kPa Saturated Steam)
$U = 300$ W/m^2°C
Tank Height to Diameter Ratio = 3/1 (so $H = 3D$)

Assuming the tank to be cylindrical and ignoring the volume of the bottom elliptical head, the tank volume is $V_{tank} = \pi D^2 H/4 = 3\pi D^3/4$. Thus, the tank diameter, D, is 1.689 m. The height of fill is $H_{fill} = 4V/(\pi D^2) = 2.806$ m. The area for heat transfer is $A = \pi D H_{fill} = 14.89$ m^2, because it was assumesd there was negligible heat transfer to the vapor space. When these values are used in Equation (E3.1d), it is found that the time required for preheating the reactor, Δt, is 3288 s (55 min). Thus, the step time requirement of 1.5 h for this step is met. The additional time is required for filling, sealing, and inspecting the vessel prior to heating. It should be noted that there may be process issues that require a slower temperature ramp, which can be accomplished by controlling the steam pressure. Note also that it is assumed that the time requirement for cleaning the vessels in this example is included in the step times given in the problem statement.

Step 2: Reaction Vessel—Reaction

It is assumed that the reaction of one mole each of A and B to form one mole of the product is second order (first order in each reactant) and that the rate constant is 7.09×10^{-4} m^3/kmol s. The relationship for a batch reactor is

$$\frac{dC_A}{dt} = -kC_A C_B \tag{E3.1e}$$

where A and B are the two reactants, and A is the limiting reactant. The standard analysis for conversion in a reactor yields Equations (E3.1f–h):

$$C_A = C_{Ao}\left(1 - X\right) \tag{E3.1f}$$

$$C_B = C_{Ao}\left(\Theta - X\right) \tag{E3.1g}$$

$$\frac{dX}{dt} = kC_{Ao}\left(1 - X\right)\left(\Theta - X\right) \tag{E3.1h}$$

where $C_{Ao} = (500 \text{ kg}/100 \text{ kg/kmol})(875 \text{ kg/m}^3)/5500 \text{ kg} = 0.796$ kmol/m^3. Because reactant B is present in 60% excess, $\Theta = 1.6$. The desired conversion, X_{final}, is 0.94. Integration of Equation (E3.1h) with an initial condition of zero conversion at time zero yields

$$\frac{1}{\Theta - 1}\left[\ln\frac{\Theta - X_{final}}{1 - X_{final}}\right] = kC_{Ao}\Delta t \tag{E3.1i}$$

When all of the values are inserted into Equation (E3.1i), the time (Δt) is found to be 7082 s, or 118 min, which is just less than the desired 2 h allotted for the reaction. For simplicity, the additional reaction time that occurs after the mixture leaves the reactor until the catalyst is removed from the reacting mixture has been ignored.

Step 3: Draining Reaction Vessel and Catalyst Filtration

This step will be modeled as a draining tank, which may significantly underestimate the actual required time for draining and filtering. In reality, experimental data on the filter medium and inclusion of the exit pipe frictional resistance would have to be included to determine the actual time for a specific tank. Generally, the filter is the bottleneck in such a step. Here, a 2-in schedule-40 exit pipe, with a cross-sectional area of 0.00216 m^2, is assumed.

For a draining tank, the model is

$$\frac{dm}{dt} = \frac{d(\rho A_t H)}{dt} = -m = -\rho A_p v_p \tag{E3.1j}$$

where ρ is the density of the liquid in the tank, A_t is the cross-sectional area of the tank, H is the height of liquid in the tank, A_p is the cross-sectional area of the exit pipe, and v_p is the velocity of liquid in the exit pipe, which, from Bernoulli's equation (turbulent flow), is $(2gH)^{1/2}$, where g is the gravitational acceleration. Therefore, Equation (E3.1j) becomes

$$\frac{dH}{dt} = -\frac{(2g)^{1/2} A_p}{A_t} H^{1/2} \tag{E3.1k}$$

Integrating from $H = 2.806$ m at $t = 0$ to find the time when $H = 0$ yields

$$-2H^{0.5}\Big|_{2.806\,m}^{0} = \frac{2^{0.5}(9.81[\mathrm{m/s^2}])^{0.5}(0.00216[\mathrm{m^2}])}{\frac{\pi(1.689[\mathrm{m}])^2}{4}}\Delta t \tag{E3.1l}$$

which gives $\Delta t = 785$ s = 13 min, which is rounded up to 30 minutes for this step. Note that this time can be further reduced by pressurizing the vessel with an inert gas.

Step 4: Distillation of Reaction Products

A material balance on the reactor at the end of Step 2 yields the following:

Component, i	kmoles	x_i	MW	mass (kg)
Reactant A	$= (1 - 0.94)(5.0) = 0.3$	0.0106	100	30.0
Reactant B	$= (1.6)(5) - (5.0 - 0.3) = 3.3$	0.1166	125	412.5
Solvent S	20.0	0.7067	200	4000.0
Product P	$= (0.94)(5.0) = 4.7$	0.1661	225	1057.5
Total	**28.3**	**1.0000**		**5500.0**

Initially, the reaction mixture is heated to its boiling point of 115°C at the operating pressure. This is done by condensing steam in a heat exchanger located in the still of the column. The time to heat the mixture from 95°C (the temperature leaving the reactor, assuming no heat loss in the filter) to 115°C is given by Equation (E3.1d) with the following variable values:

$T_s = 120$°C
$\rho = 875$ kg/m^3
$C_p = 2000$ J/kg°C
$U = 420$ W/m^2°C
$A = 10$ m^2

Solving for the unknown time gives $t = 4215$ s = 70.3 min.

The distillation is performed using a still with three theoretical stages ($N = 3$), a boil-up rate, $V = 30$ kmol/h, and a reflux ratio, $R = 4.5$. The volatilities of each component relative to the product are given as follows:

$\alpha_{AP} = 3.375$
$\alpha_{BP} = 2.700$
$\alpha_{SP} = 1.350$
$\alpha_{PP} = 1.000$

The solution methodology involves a numerical integration using the method of Sundaram and Evans [1]. The overall material and component balances are given by

$$-\frac{dW}{dt} = D = \frac{V}{1+R}$$

or in finite difference form,

$$W^{(k+1)} = W^{(k)} - \left(\frac{V}{1+R}\right)\Delta t \tag{E3.1m}$$

$$\frac{d\left(Wx_{W_i}\right)}{dt} = x_{D_i}\frac{dW}{dt}$$

or in finite difference form,

$$x_{W_i}^{(k+1)} = x_{W_i}^{(k)} + \left(x_{D_i}^{(k)} - x_{W_i}^{(k)}\right)\frac{W^{(k+1)} - W^{(k)}}{W^{(k)}} \tag{E3.1n}$$

where W is the total moles in the still; x_{D_i} and x_{W_i} are the mole fractions of component i, at any time t, in the overhead product and in the still, respectively; k is the index for time in the finite difference representation; and Δt is the time step. These equations are solved in conjunction with the sum of the gas-phase mole fraction equaling unity and the Fenske-Underwood-Gilliland method for multicomponent distillation. This leads to the following additional equations:

$$x_{D_r} = \frac{x_{W_r}}{\sum_{i=1}^{C} x_{W_i}\,{}^{\circ}{}_{1,C}^{N_{min}}} \text{ and } x_{D_i} = x_{W_i}\left(\frac{x_{D_i}}{x_{w_i}}\right){}^{\circ}{}_{i,r}^{N_{min}} \tag{E3.1o}$$

$$R_{min} = \frac{{}^{\circ}{}_{1,C}^{N_{min}} - {}^{\circ}{}_{1,c}}{\left({}^{\circ}{}_{1,C} - 1\right)\sum_{i=1}^{C} x_{w_i}\,{}^{\circ}{}_{1,C}^{N_{min}}} \text{ and } \frac{N - N_{min}}{N+1} = 0.75\left[1 - \left(\frac{R - R_{min}}{R+1}\right)^{0.5668}\right] \tag{E3.1p}$$

where R_{min} and N_{min} are the minimum values for the reflux ratio and the number of theoretical stages, respectively. The solution of these equations is explained in detail by Seader and Henley [2], and the results for this example are shown in Figures E3.1(a) and E.3.1(b).

From Figures E3.1(a) and (b), the mole fraction of reactant B is seen to drop to less than the specification of 0.01 (1 mol%) at a time of approximately 2.3 h. This time, coupled with the heating time of 70.2 min, gives a total of 3.5 h. However, note that only about 75% of the product remains in the still to be recovered in the next step.

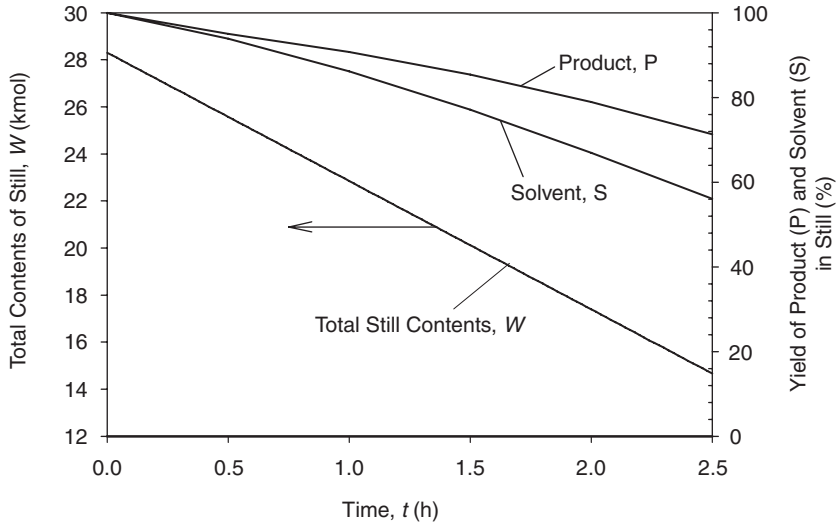

Figure E3.1(a) Change of Still Contents and Yields of P and S with Time

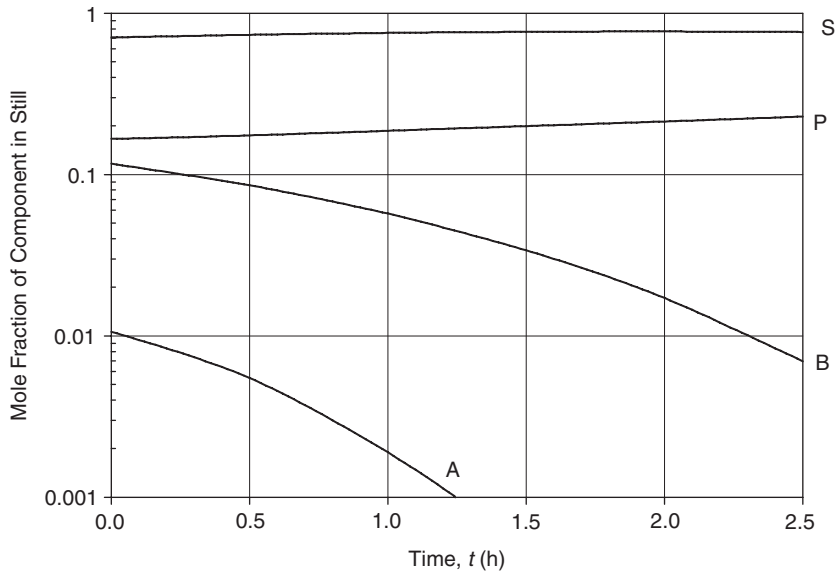

Figure E3.1(b) Change in Composition of Still Material with Time

Step 5: Cooling and Crystallization of Product

The analysis of the crystallization, filtration, drying, and packaging steps is beyond the scope of this analysis. Therefore, it is assumed that the times for each of these steps have been determined through laboratory-scale experiments, and those times are simply stated here. The amount of product crystallized is 80% of the product recovered from the still, or 60% of the 1057.5 kg produced in the reactor (634.5 kg). The time required to cool and crystallize is 2 h.

Step 6: Filtration and Drying

The time required for filtration and drying is 4 h.

Step 7: Packaging

The time required for packaging is 1 h.

There are several unique features of batch operations observed in Example 3.1. First, the heating, reaction, and separations steps are unsteady state, which is different from the typical steady-state analysis with which most undergraduate chemical engineers are familiar. Secondly, it is observed that no provision was made to recycle the unreacted raw materials. In Chapter 2, recycle was shown to be a key element of a steady-state chemical process. Raw materials are almost always the largest item in the cost of manufacturing; therefore, recycling unreacted raw materials is essential to ensure profitability. So, how is this done in a batch process? In Example 3.1, the overhead product from the batch distillation contains unreacted raw material and product in the solvent. This could be sent to a holding tank and periodically mixed with a stream containing pure solvent and just enough reactants A and/or B to make up a single charge to the process in Step 1. However, the recycling of product to the reactor would have to be investigated carefully to determine whether unwanted side reactions take place at higher product concentrations. Even though an additional tank would need to be purchased, it is almost certain that the cost benefit of recycling the raw materials would far outweigh the cost of the additional tank. Third, it is observed that, overall, only 60% of the product made in the reactor is crystallized out in Step 5. This means that the **mother liquor** (solution containing product to be crystallized after some has crystallized out) contains significant amounts of valuable product. Additional crystallization steps could recover some, if not most, of the valuable product. The strategy for accomplishing this could be as simple as scheduling a second or third cooling or crystallization step, or it could involve storing the mother liquor from several batch processes until a sufficient volume is available for another cooling or crystallization step. These additional crystallization steps are tantamount to adding additional separation stages.

3.2 GANTT CHARTS AND SCHEDULING

Gantt charts (see, for example, Dewar [3]) are tabular representations used to illustrate a series of tasks (rows) that occur over a period of time (columns). These charts graphically represent completion dates, milestone achievements, current progress, and so on [3] and are discussed further in Chapter 28 as a planning tool for completing large design projects. In this chapter, a simplified Gantt chart is used to represent the scheduling of equipment needed to produce a given batch product. Example 3.2 illustrates the use of Gantt charts to show the movement of material as it passes through several pieces of equipment during a batch operation.

Example 3.2

Draw a Gantt chart that illustrates the sequence of events in the production of the API in Example 3.1.

Solution

Gantt charts for this process are shown in Figure E3.2. Note that in both charts, Steps 1 and 2 have been consolidated into one operation because they occur sequentially in the same piece of

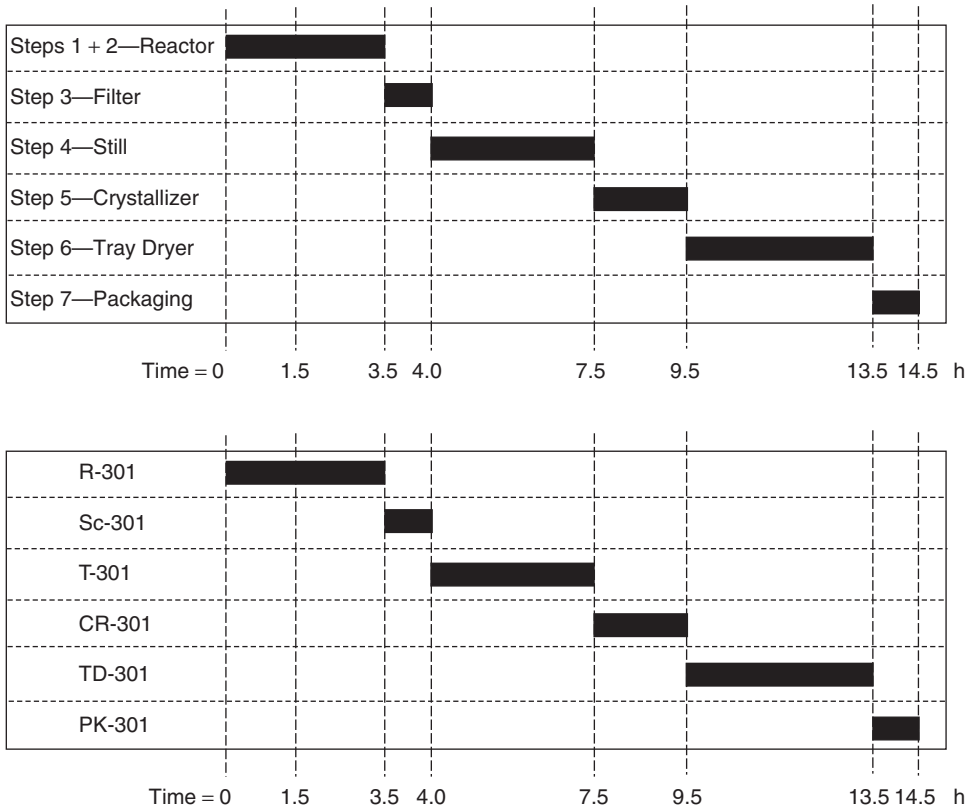

Figure E3.2 Gantt Chart Showing Sequence of Events for the Manufacture of API in Example 3.1

equipment. The top chart shows the row names as tasks, and the bottom figure simply identifies each row with the equipment number. In general, the notation used in the bottom figure will be adopted.

3.3 NONOVERLAPPING OPERATIONS, OVERLAPPING OPERATIONS, AND CYCLE TIMES

In general, product is produced throughout an extended period of time by using a repeating sequence of operations. For example, the batch process described in Example 3.1 produces a certain amount of crystallized API, namely, 634.5 kg. If it is desired to produce 5000 kg, then the sequence of steps must be repeated $5000/634.5 \cong 8$ times. There are several ways to repeat the sequence of tasks needed to make one batch, in order to make the desired total amount of product (5000 kg). An example of one such **nonoverlapping** scheme is shown in Figure 3.1.

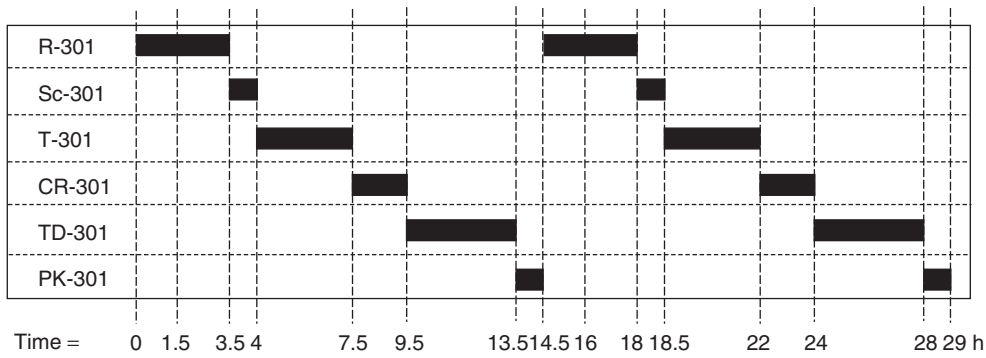

Figure 3.1 Example of a Nonoverlapping Sequence of Batch Operations

For the nonoverlapping (designated by the subscript *NO*) scheme, the total processing time is the number of batches multiplied by the time to process a single batch:

$$T_{NO} = n\sum_{i=1}^{m} t_i \tag{3.1}$$

where T_{NO} is the total time to process n batches without overlapping, each batch having m steps of duration $t_1, t_2, \ldots, t_m$. For this example, the total time is equal to (8)(3.5 + 0.5 + 3.5 + 2 + 4.0 + 1.0) = (8)(14.5) = 116.0 h.

For the process described in Figure 3.1, using the nonoverlapping scheme, the equipment is used infrequently, and the total processing time is unduly long. However, such a scheme might be employed in plants that operate only a single shift per day. In such cases, the production of a single batch might be tailored to fit an 8 or 10 h shift (for this example, the shift would have to be 14.5 h), with the limitation that only one batch would be produced per day. Although such a scheme does not appear to be very efficient, it eliminates prolonged storage of intermediate product and certainly makes the scheduling problem easy.

The total time to process all the batches can be reduced by starting a batch before the preceding batch has finished. This is equivalent to shifting backward the time blocks representing the steps in the batch process, as shown in Figure 3.2.

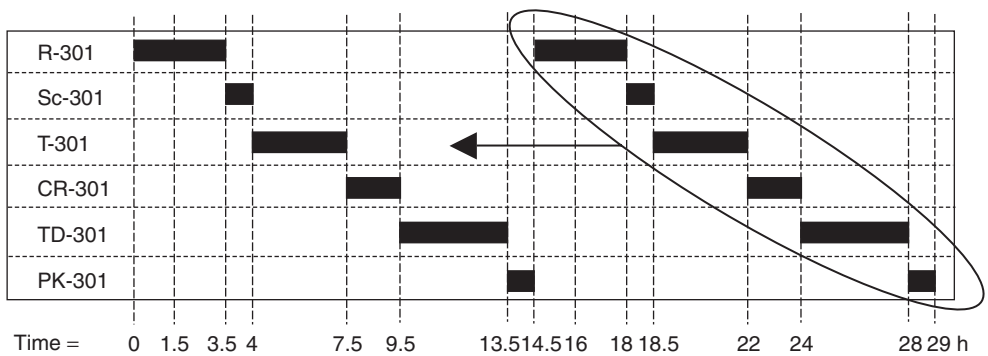

Figure 3.2 Backward Shifting of Batches, Giving Rise to Overlapping Sequencing

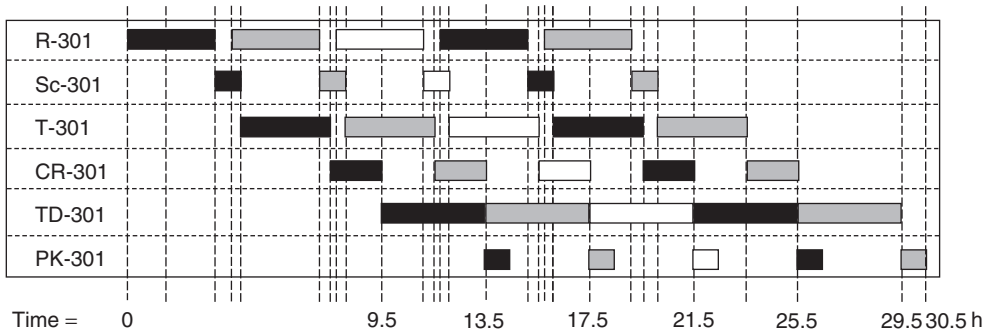

Figure 3.3 The Limiting Case for Overlapping Batch Sequencing

This shifting of batches backward in time leads to the concept of **overlapping** sequencing of batches. The limit of this shifting or overlapping process occurs when two time blocks in consecutive batches just touch each other (assuming that cleaning, inspection, and charging times are included). This situation is shown in Figure 3.3.

From Figure 3.3, it can be seen that the limiting case for overlapping occurs when the step taking the longest time (here, the tray drying step in TD-301, which takes 4 h to complete) repeats itself without a waiting time between batches. The time to complete n batches using this limiting overlapping scheme is given by

$$T_O = T = (n-1)\max_{i=1,\ldots,m}(t_i) + \sum_{i=1}^{m} t_i \tag{3.2}$$

where T_O is the minimum total (overlapping) time, and [max (t_i)] is the maximum individual time step for the batch process. The subscript O that denotes overlapping will be dropped, and T will be used as the total processing time from this point on. For the example, $T = (8-1)(4.0) + (14.5) = 42.5$ h.

Comparing Figures 3.1 and 3.3, the use of overlapping sequencing reduces the processing time significantly (from 116 to 42.5 h) and makes much better use of the equipment; specifically, the equipment is operated for a higher fraction of time in the overlapping scheme compared with the nonoverlapping scheme.

In batch operations, the concept of **cycle time** is used to refer to the average time required to cycle through all necessary steps to produce a batch. The formal definition is found by dividing the total time to produce a number of batches by the number of batches. Thus, from Equations (3.1) and (3.2),

$$t_{cycle,NO} = \frac{T_{NO}}{n} = \frac{n\sum_{i=1}^{m} t_i}{n} = \sum_{i=1}^{m} t_i \tag{3.3}$$

$$t_{cycle,O} = t_{cycle} = \frac{T}{n} = \frac{(n-1)\max_{i=1,\ldots,m}(t_i) + \sum_{i=1}^{m} t_i}{n} \tag{3.4}$$

For the overlapping scheme, when the number of batches (n) to be produced is large, the cycle time is approximated by

$$t_{cycle} \cong \max_{i=1,\ldots,m} \{t_i\} \tag{3.5}$$

Therefore, using the approximation in Equation (3.5) for Example 3.1, the nonoverlapping and overlapping cycle times are 14.5 h and 4 h, respectively.

3.4 FLOWSHOP AND JOBSHOP PLANTS

Thus far, the discussion has focused on the production of only a single product. However, most batch plants produce multiple products. All these products may require the same processing steps, or more often will require only a subset of all possible steps. Moreover, the order in which a batch process uses different equipment might also differ from product to product.

3.4.1 Flowshop Plants

Consider a plant that must make three products: A, B, and C. Figure 3.4 shows an example of the sequence of equipment used to produce these three products. In Figure 3.4, all the products use the same equipment in the same order or sequence, but not necessarily for the same lengths of time. This type of plant is sometimes referred to as a **flowshop** plant [4]. The total time for operation of overlapping schedules depends on the number of runs of each product and how these runs are scheduled. One approach to scheduling multiple products is to run each product in a campaign during which only that product is made. Then the plant is set up to run the next product in a campaign, and so on. The case when multiple products, using the same equipment in the same order, are to be produced in separate campaigns is considered first. If the corresponding numbers of batches for products A, B, and C in a campaign are n_A, n_B, and n_C, respectively, then the total processing time, or production cycle time, can be found by adding the operation times for each product. If the number of batches per campaign is large (for example, >20), then the production cycle time can be approximated by an extension of Equation (3.5):

$$T = \sum_{j=A}^{C} n_j \{t_{cycle}\}_j \cong \sum_{j=A}^{C} n_j \left\{ \max_{i=1,\ldots,m} \{t_i\} \right\}_j \tag{3.6}$$

An illustration of a multiple-product process is given in Example 3.3.

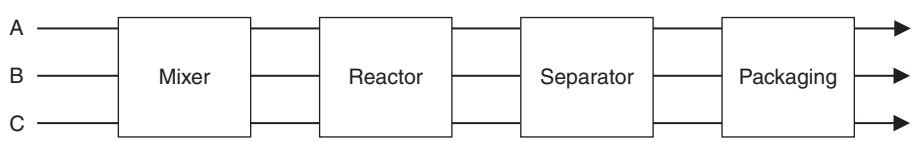

Figure 3.4 An Example of a Flowshop Plant for Three Products A, B, and C

Example 3.3

Consider three batch processes, producing products A, B, and C, as illustrated in Table E3.3. Each process uses the four pieces of equipment in the same sequence but for different times.

Market demand dictates that equal numbers of batches of the three products be produced over a prolonged period of time.

Determine the total number of batches that can be produced in a production cycle equal to one month of operation of the plant using separate campaigns for each product, assuming that a month of operation is equivalent to 500 h (based on 1/12 of a 6000 h year for a three-shift plant operating five days per week).

Table E3.3 Equipment Times (in Hours) Needed to Produce A, B, and C

Product	Time in Mixer	Time in Reactor	Time in Separator	Time in Packaging	Total Time
A	1.5	1.5	2.5	2.5	8.0
B	1.0	2.5	4.5	1.5	9.5
C	1.0	4.5	3.5	2.0	11.0

Solution

The time to produce each product is given by Equation (3.2). Assume that each product is run x times during the month:

$$T = 500 = \sum_{j=A}^{C} \left\{ (n-1) \max_{i=1,\ldots,m} \{t_i\} + \sum_{i=1}^{m} t_i \right\}_j$$

$$500 = \left[(x-1)(2.5) + 8\right] + \left[(x-1)(4.5) + 9.5\right] + \left[(x-1)(4.5) + 11\right]$$

$$500 = (x-1)(11.5) + 28.5 \Rightarrow x = \frac{(500-28.5)}{11.5} + 1 = 42$$

Thus, 42 batches each of A, B, and C can be run as campaigns in a 500 h period. The cycle times are $t_{cycle,A} = [(41)(2.5) + 8/(42)] = 2.631$ h, $t_{cycle,B} = 4.619$ h, and $t_{cycle,C} = 4.655$ h.

Using Equation (3.6) with the approximations $t_{cycle,A} = 2.5$, $t_{cycle,B} = 4.5$, and $t_{cycle,C} = 4.5$,

$$T = 500 = x(2.5 + 4.5 + 4.5) \Rightarrow x = \frac{500}{11.5} = 43$$

Equation (3.6) slightly overestimates the number of batches that can be run in the 500 h period but is a very good approximation. In general, Equation (3.6) will be used to estimate cycle times and other calculations for single-product campaigns for multiproduct plants.

Running campaigns for the production of the same product is efficient and makes scheduling relatively easy. However, this strategy suffers from a drawback: the longer the production cycle, the greater the amount of product that must be stored since an inventory should be kept on hand to ensure that customers can be provided with product at any time. The concept of product storage is addressed in the following section. However, the bottom line is that storage requires additional equipment or warehouse floor space that must be purchased or rented. On the other hand, a strategy of single-product campaigns may decrease cleaning times and costs, which generally are

greater when switching from one process to another. Therefore, the implementation of a batch sequencing strategy that uses sequences of single-product campaigns involves additional costs that should be included in any design and optimization. The extreme case for single-product batch campaigning occurs for seasonal produce (a certain vegetable oil, for example), where the feed material is available only for a short period of time and must be processed quickly, but the demand for the product lasts the whole year.

An alternative to running single-product campaigns (AAA…, BBB…, CCC…) over the production cycle is to run multiproduct campaigns—for example, ABCABCABC, ACBACBACB, AACBAACBAACB, and so on. In this strategy, products are run in a set sequence and the sequence is repeated. This approach is illustrated in Example 3.4.

Example 3.4

Consider the same processes given in Example 3.3. Determine the number of batches that can be produced in a month (500 h) using a multiproduct campaign strategy with the sequence ABCABCABC….

The Gantt chart for this sequence is shown in Figure E3.4.

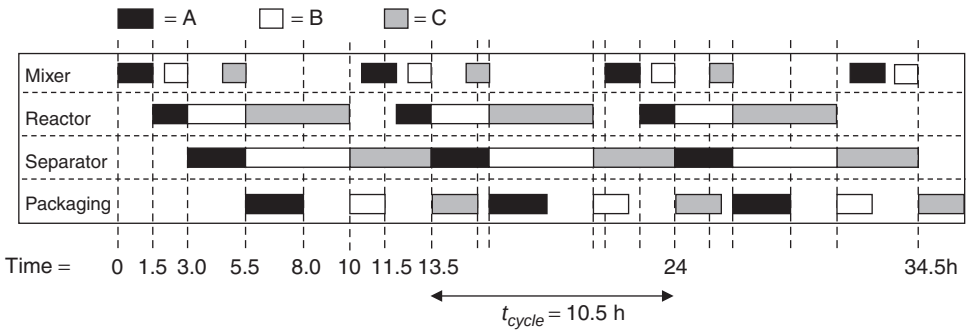

Figure E3.4 Gantt Chart Showing the Multiproduct Sequence ABCABCABC…

From Figure E3.4, it can be seen that the limiting equipment for this sequence is the separator. This means that the separator is used without downtime for the duration of the 500 h. If x batches are produced during the 500 h period, then

$$T = 500 = \left(3 + x\left(2.5 + 4.5 + 3.5\right) + 2\right) \Rightarrow x = \frac{(500-5)}{10.5} = 47$$

Therefore, an additional five batches of each product can be produced using this sequence compared with the single-product campaign discussed in Example 3.3, assuming there is no additional cleaning time. In general, it should be noted that other sequences, such as BACBACBAC, could be used, and these may give more or fewer batches than the sequence used here.

3.4.2 Jobshop Plants

The flowshop plant discussed previously is one example of a batch plant that processes multiple products. When not all products use the same equipment or the sequence of using the equipment is different for different products, then the plant is referred to as a **jobshop** plant [4]. Figure 3.5 gives two examples of such plants. In Figure 3.5(a), all the products move from the left to the right—that is, they move in the same direction through the plant, but not all of them use the

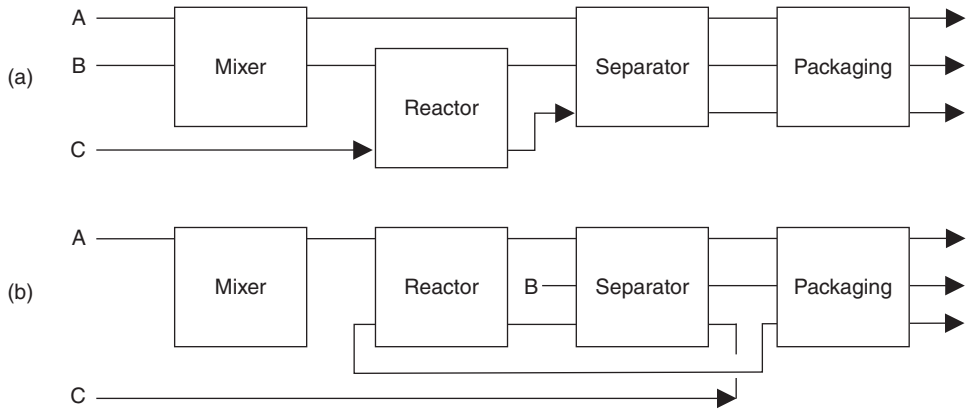

Figure 3.5 Two Examples of Jobshop Plants for Three Products A, B, and C

same equipment. In Figure 3.5(b), products A and B move from left to right, but product C uses the equipment in a different order from the other two products. The sequencing of multiproduct campaigns for this type of plant is more complex and is illustrated in Example 3.5. The relative efficiencies of different processing schemes for the plant shown in Figure 3.5(b) are calculated in Example 3.6.

Example 3.5

Consider the jobshop plant following the sequence shown in Figure 3.5(b) and described in Table E3.5. Construct the Gantt charts for overlapping single-product campaigns for products A, B, and C and for the multiproduct campaign with sequence ABCABCABC….

Table E3.5 Equipment Processing Times (in Hours) for Processes A, B, and C

Process	Mixer	Reactor	Separator	Packaging
A	1.0	5.0	4.0	1.5
B	—	—	4.5	1.0
C	—	3.0	5.0	1.5

Solution

The Gantt charts for the three processes are shown in Figure E3.5. The top chart shows the timing sequences for each batch, and the next three charts show overlapping campaigns for products A, B, and C, respectively. It can be seen that the rules and equations for overlapping campaigns given previously still apply. The bottom chart shows the overlapping multiproduct campaign using the sequence ABCABCABC…. Note that there are many time gaps separating the use of the different pieces of equipment, and no one piece of equipment is used all the time. This situation is common in jobshop plants, and strategies to increase equipment usage become increasingly important and complicated as the number of products increases.

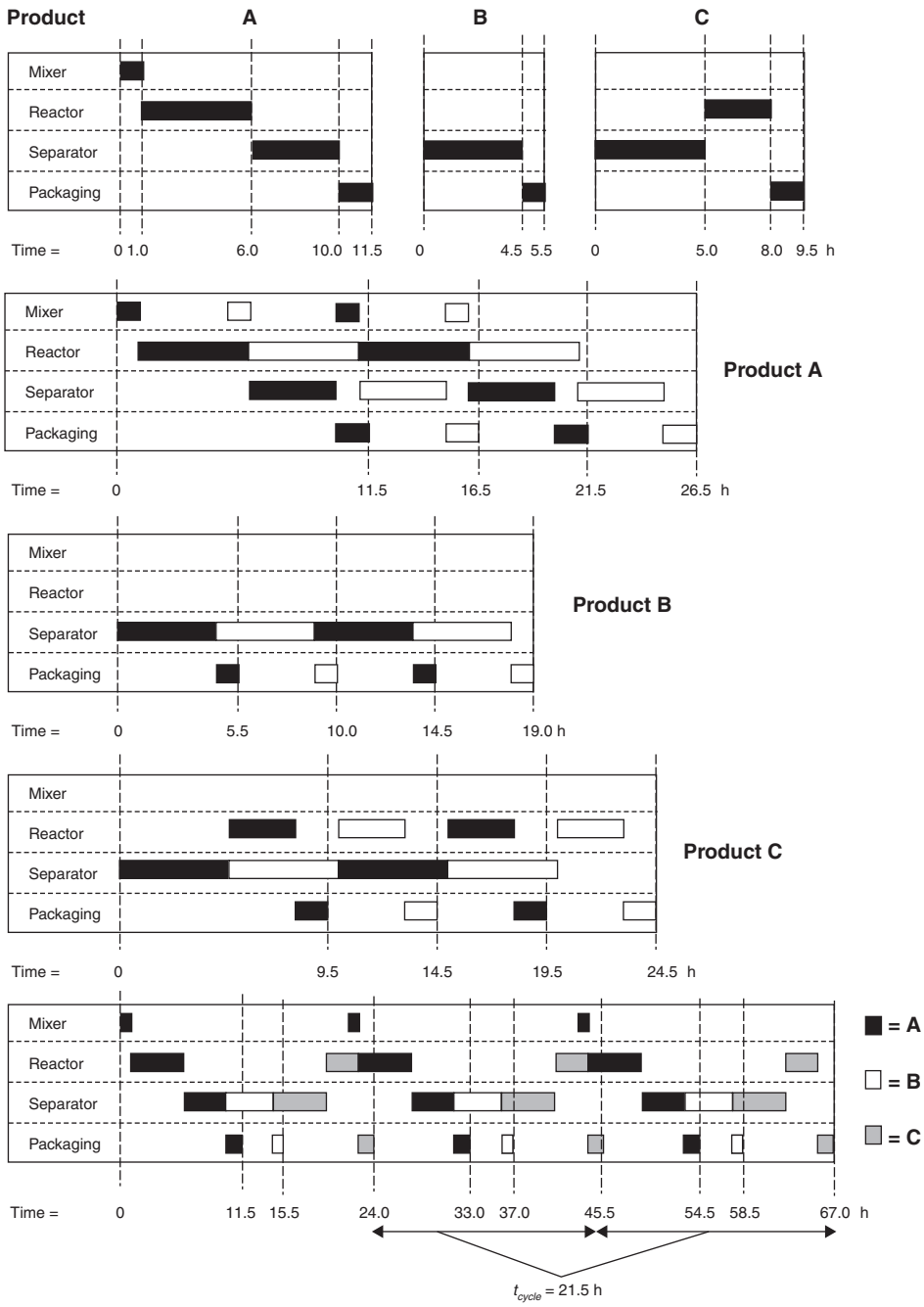

Figure E3.5 Gantt Charts for Single-Product and Multiproduct Campaigns

Example 3.6

It is desired to produce the same number of batches of A, B, and C. Using information from Example 3.5, determine the total number of batches of each product that can be produced in an operating period of 1 month = 500 h, using single-product campaigns and a multiproduct campaign following the sequence ABCABCABCABC….

Solution

For the single-product campaigns, the number of batches of each product, *s*, can be estimated using Equation (3.6). Thus

$$500 = x(5 + 4.5 + 5) \Rightarrow x = \frac{500}{14.5} = 34$$

Therefore, 34 batches of each product can be made in a 500 h period using single-product campaigns.

For the multiproduct campaign, referring to Figure E3.5, the cycle time for the sequence ABC is 21.5 h. This is found by determining the time between successive completions of say product C: 45.5 − 24 = 21.5 h, and 67 − 45.5 = 21.5 h. Therefore, the number of batches of A, B, and C that can be produced is given by

$$500 = x(21.5) \Rightarrow x = \frac{500}{21.5} = 23$$

This multiproduct sequence is clearly less efficient than the single-product campaign approach, but it does eliminate intermediate storage. It should be noted that different multiproduct sequences give rise to different results, and the ABCABC sequence may not be the most efficient sequence for the production of these products.

3.5 PRODUCT AND INTERMEDIATE STORAGE AND PARALLEL PROCESS UNITS

In this section, the effect of intermediate and product storage on the scheduling of batch processes and the use of parallel process units or equipment are investigated. Both of these concepts will, in general, increase the productivity of batch plants.

3.5.1 Product Storage for Single-Product Campaigns

When using combinations of single-product campaigns in a multiproduct plant, it is necessary to store product during the campaign. For example, considering the products produced in Example 3.3, the plant will produce 43 batches each of products A, B, and C in a 500 h period. If the required production rates for these three products are 10,000, 15,000, and 12,000 kg/month, respectively, then what is the amount of storage required? In practice, it is the volume, and not the weight, of each product that determines the required storage capacity. For this example, it is assumed that the densities of each product are the same and equal to 1000 kg/m^3. Considering product A first and assuming that demand is steady, the demand rate (r_d) is equal to 10,000/500 = 20 kg/h = 0.020 m^3/h. Note that the demand rate is calculated on the basis of plant operating hours, and not on the basis of a 24-hour day. During the campaign, 10,000 kg of A must be made in 43 batch runs, with each run taking $t_{cycle,\,A}$ = 2.5 h. Thus, during production, the production rate (r_p) of A is equal to 10,000/(43)(2.5) = 93.0 kg/h = 0.0930 m^3/h. Results for all the products are given in Table 3.1.

Table 3.1 Production and Demand Rates for Products A, B, and C in Example 3.3

Rate	Product A	Product B	Product C
Volume (m^3) of product required per month	10.0	15.0	12.0
Cycle time (h)	2.5*	4.5*	4.5*
Production rate, r_p (m^3/h)	(10)/[(43)(2.5)] = 0.0930	0.07752	0.06202
Demand rate, r_d (m^3/h)	(10)/(500) = 0.020	0.030	0.024

*These are approximate cycle times based on Equation (3.5).

When a campaign for a product is running, the rate of production is greater than the demand rate. When the campaign has stopped, the demand rate is greater than the production rate of zero. Therefore, the accumulation and depletion of product over the monthly period are similar to those shown in Figure 3.6. The changing inventory of material is represented on this figure by the bottom diagram. The maximum inventory, V_s, is the minimum storage capacity that is required for the product using this single-product campaign strategy. The expression for calculating V_s is

$$V_s = \left(r_p - r_d\right)t_{camp} \tag{3.7}$$

where t_{camp} is the campaign time. This assumes that the shipping rate of product from the plant is constant during plant operating hours. Because shipping is usually itself a batch process, the actual minimum storage capacity could be more or less than that calculated in Equation (3.7). The strategies for matching shipping schedules to minimize cost (including storage costs and missed-delivery risks) are known as logistics and are not covered here.

Determination of the minimum storage capacities for all products in Example 3.3 is given in Example 3.7.

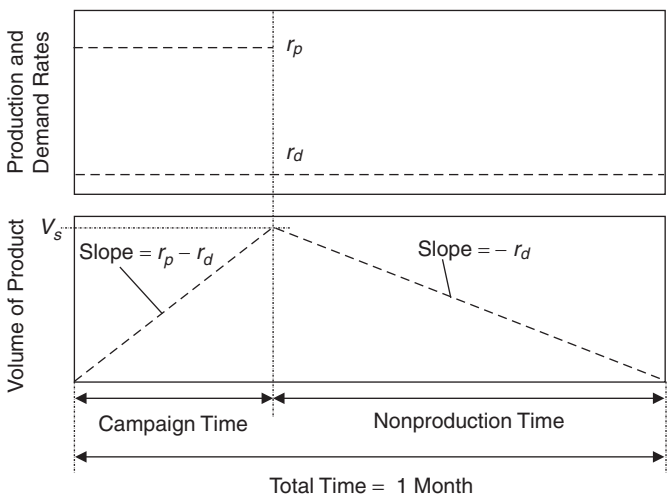

Figure 3.6 Changing Inventory of Product during Single-Product Campaign Run within a Multiproduct Process

Example 3.7

For the products A, B, and C in Example 3.3, determine the minimum storage capacities for the single-product campaign strategy outlined in Example 3.3.

Table E3.7 Results for the Estimation of Minimum Storage Volume from Equation (3.7)

Product	Campaign Time, t_{camp} (h)	$r_p - r_d$ (m^3/h)	V_s (m^3)
A	(43)(2.5) = 107.5	0.09302 – 0.020 = 0.07302	(0.07302)(107.5) = 7.85
B	(43)(4.5) = 193.5	0.07752 – 0.030 = 0.04752	(0.04752)(193.5) = 9.20
C	(43)(4.5) = 193.5	0.06202 – 0.024 = 0.03802	(0.03802)(193.5) = 7.36

Solution

Table E3.7 shows the results using data given in Example 3.3 and Table 3.1.

It should be noted that the production cycle time is equal to the sum of the campaign times, or (107.5 + 193.5 + 193.5) = 494.5 h, which is slightly less than 500 h. This discrepancy reflects the approximation of cycle times given by Equation (3.6). The actual cycle times for A, B, and C are found from Example 3.3 and are equal to 2.63, 4.62, and 4.65 h, respectively. The corresponding values of V_s are 7.79, 9.18, and 7.31 m^3. Clearly, these differences are small, and the approach using Equation (3.6) is acceptable when the number of production runs per campaign is 20 or more.

3.5.2 Intermediate Storage

Up to this point, it has been assumed that there is no intermediate product storage available. This type of process is also known as **a zero wait**, or a **zw process** [4]. Specifically, as soon as a unit operation is completed, the products are transferred to the next unit operation in the sequence, or they go to final product storage. The concept of storing the final product to match the supply with the demand was demonstrated in Example 3.7. However, it may also be beneficial to store the output from a given piece of equipment for a period of time to increase the overall efficiency of a process. It may be possible to store product in the equipment that has just been used. For example, if two feed streams are mixed in a vessel, the mixture could be stored until the next process unit in the production sequence becomes available. In this case, the storage time is limited based on the scheduling of equipment. This **holding-in-place** method may not work for some unit operations. For example, in a reactor, a side reaction may take place, and unless the reaction can be quenched, the product yield and selectivity will suffer. The upper limit of the intermediate storage concept occurs when there is **unlimited intermediate storage (uis)** available, and this is referred to as a **uis process** [4]. In general, cycle times can be shortened when intermediate product storage is available. This concept is illustrated in Figure 3.7, which is based on the information given in Table 3.2.

Without intermediate product storage, the shortest multiproduct campaign, as given by Equation (3.6), is 14 h, as shown in Figure 3.7. However, if the materials leaving the reactor and crystallizer are placed in storage prior to transfer to the crystallizer and dryer, respectively, then this time is reduced to 11 h. The limiting cycle time for a uis process is given by

$$t_{cycle,uis} = \max_{j=1,m} \sum_{i=1}^{N} nc_i t_{i,j} \tag{3.8}$$

where m is the number of unit operations, N is the number of products, and nc_i is the number of campaigns of product i produced in a single multiproduct sequence. For the case shown in

Table 3.2 and Figure 3.7, $n = 1$ (because only one campaign for each product [A, B, and C] is used in the multiproduct sequence), and Equation (3.8) is the maximum value given in the last row of Table 3.2, or 11.0 h.

Table 3.2 Equipment Times (in Hours) Required for Products A, B, and C

Product	Reactor	Crystallizer	Dryer	Total
A	2.0	5.0	2.0	9.0
B	6.0	4.0	4.0	14.0
C	2.0	2.0	3.0	7.0
Total Time per Equipment	10.0	11.0	9.0	

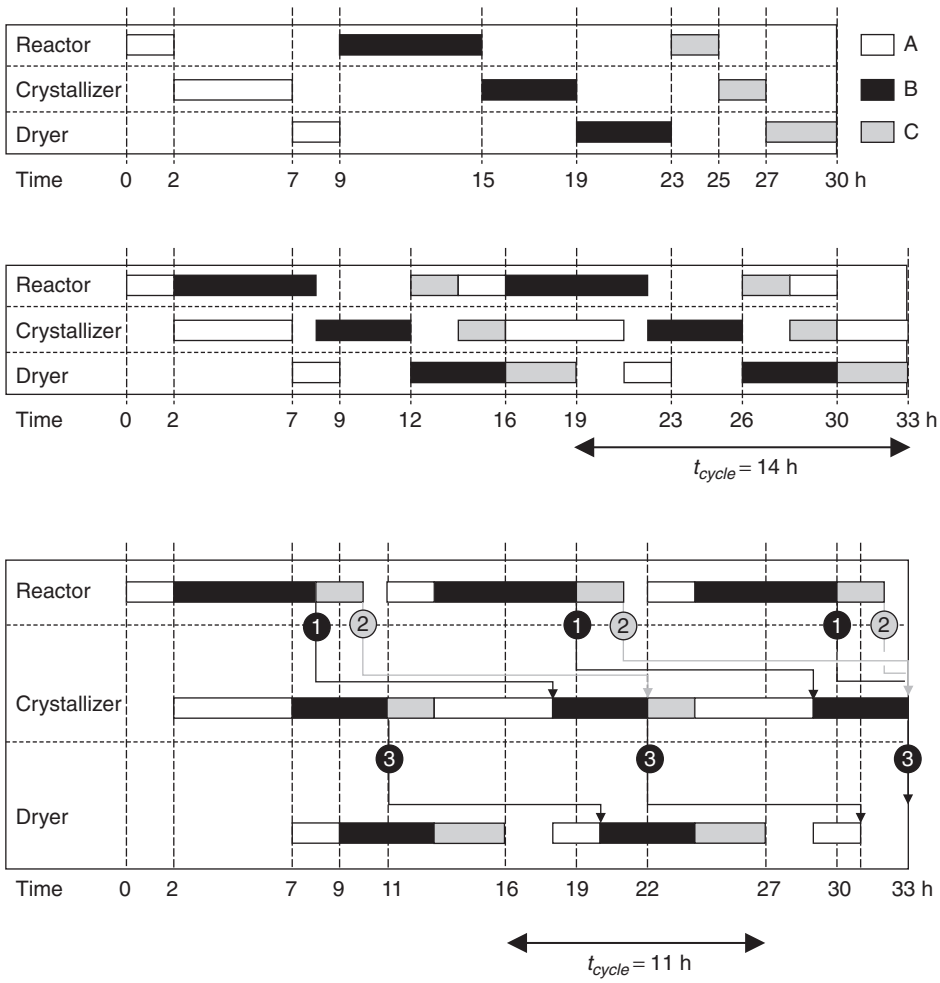

Figure 3.7 Multiproduct Sequence (ABC) for Products Given in Table 3.2 Showing Effect of Intermediate Storage (Storage Shown as Circles; Number Identifies Individual Tanks for Each Intermediate Product)

The total amount of storage required for this example is fairly small, because only three storage vessels are required, each dedicated to one intermediate product. The downside of this approach is that there are many more material transfers required, and the potential for product contamination and operator error increases significantly.

3.5.3 Parallel Process Units

Another strategy that can be employed to increase production is to use duplicate equipment. This strategy is most beneficial when there is a bottleneck involving a single piece of equipment that can be relieved by adding a second (or more) units in parallel. This strategy can be extended to a limiting case in which parallel trains of equipment are used for each product. This strategy eliminates the dependence of scheduling between the different products but is more expensive, because the number of pieces of equipment increases *m*-fold, where *m* is the number of products. An example of using parallel equipment is shown in Figure 3.8 based on the data in Table 3.3.

From the top chart in Figure 3.8 that shows the multiproduct sequence ABCABC…, the limiting piece of equipment is seen to be the crystallizer. The bottom chart shows the effect of adding a second crystallizer that processes product C. The effect is to reduce the cycle time from 21 h to 13 h, a considerable improvement in throughput. The determination of whether to make this change must be made using an appropriate economic criterion, such as net present value (NPV) or equivalent annual operating cost (EAOC), which are discussed in Chapter 10. The resulting trade-off is between increased product revenues and the cost of purchasing a second crystallizer plus additional operators to run the extra equipment.

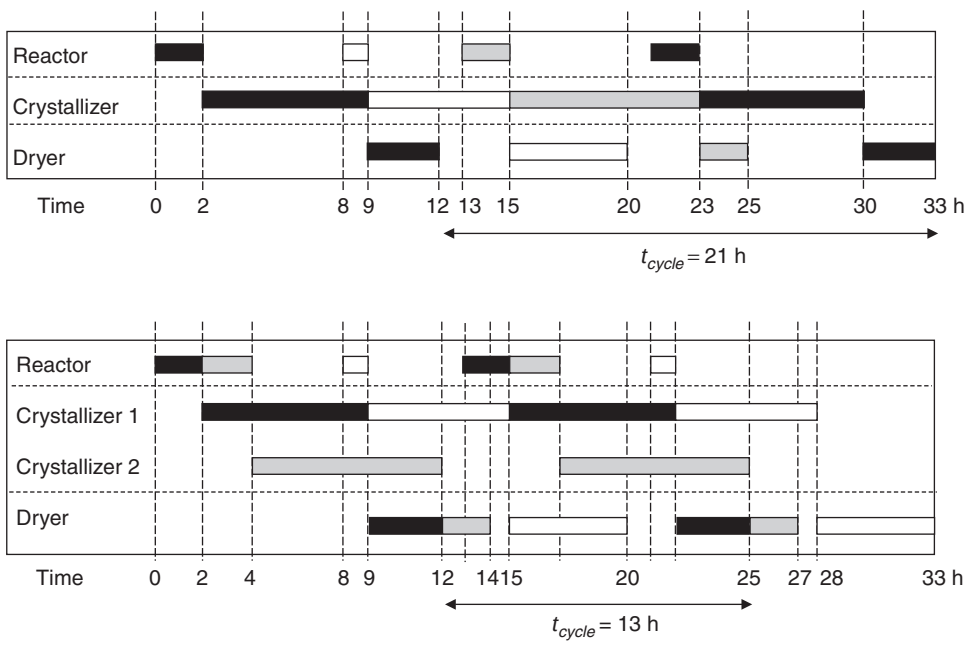

Figure 3.8 The Effect of Adding an Additional Crystallizer to the Process Given in Table 3.2