

SECOND EDITION

Chemical Process

DESIGN AND
INTEGRATION

Robin Smith



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Chemical Process

Design and Integration

Chemical Process **Design and Integration**

Second Edition

Robin Smith

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WILEY

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*To the next generation
George, Oliver, Ava and Freya*

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Preface to the Second Edition

PREFACE TO THE SECOND EDITION

This book deals with the design and integration of chemical processes. The Second Edition has been rewritten, restructured and updated throughout from the First Edition. At the heart of the book are the conceptual issues that are fundamental to the creation of chemical processes and their integration to form complete manufacturing systems. Compared with the First Edition, this edition includes much greater consideration of equipment and equipment design, including materials of construction, whilst not sacrificing understanding of the overall conceptual design. Greater emphasis has also been placed on physical properties, process simulation and batch processing. Increasing environmental awareness has dictated the necessity of a greater emphasis on environmental sustainability throughout. The main implication of this for process design is greater efficiency in the use of raw materials, energy and water and a greater emphasis on process safety. Consideration of integration has not been restricted to individual processes, but integration across processes has also been emphasized to create environmentally sustainable integrated manufacturing systems. Thus, the text integrates equipment, process and manufacturing system design. This edition has been rewritten to make it more accessible to undergraduate students of chemical engineering than the First Edition, as well as maintaining its usefulness to

postgraduate students of chemical engineering and to practicing chemical engineers.

As with the first edition, this edition as much as possible emphasizes understanding of process design methods, as well as their application. Where practical, the derivation of design equations has been included, as this is the best way to understand the limitations of those equations and to ensure their wise application.

The book is intended to provide a practical guide to chemical process design and integration for students of chemical engineering at all levels, practicing process designers and chemical engineers and applied chemists working in process development. For undergraduate studies, the text assumes basic knowledge of material and energy balances and thermodynamics, together with basic spreadsheeting skills. Worked examples have been included throughout the text. Most of these examples do not require specialist software and can be solved either by hand or using spreadsheet software. A suite of Excel spreadsheets has also been made available to allow some of the more complex example calculations to be performed more conveniently. Finally, a number of exercises has been added at the end of each chapter to allow the reader to practice the calculation procedures. A solutions manual is available.

Robin Smith

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Finally, gratitude is expressed to all of the member companies of the Process Integration Research Consortium, both past and present. Their support has made a considerable contribution to research in the area, and hence to this text.

Nomenclature

NOMENCLATURE

<i>a</i>	Activity (–), or constant in cubic equation of state ($\text{N} \cdot \text{m}^4 \cdot \text{kmol}^{-2}$), or correlating coefficient (units depend on application), or cost law coefficient (\$), or order of reaction (–)	<i>B_C</i>	Baffle cut for shell-and-tube heat exchangers (–)
<i>a_{mn}</i>	Group interaction parameter in the UNIFAC Model (K)	<i>BOD</i>	Biological oxygen demand ($\text{kg} \cdot \text{m}^{-3}$, $\text{mg} \cdot \text{l}^{-1}$)
<i>a₁, a₂</i>	Profile control parameters in optimization (–)	<i>c</i>	Capital cost law coefficient (–), or correlating coefficient (units depend on application), or order of reaction (–)
<i>A</i>	Absorption factor in absorption (–), or annual cash flow (\$), or constant in vapor pressure correlation ($\text{N} \cdot \text{m}^{-2}$, bar), or heat exchanger area (m^2)	<i>c_D</i>	Drag coefficient (–)
<i>A_C</i>	Cross-sectional area of column (m^2)	<i>c_f</i>	Fanning friction factor (–)
<i>A_{CF}</i>	Annual cash flow ($\$ \cdot \text{y}^{-1}$)	<i>c_{fS}</i>	Smooth tube Fanning friction factor (–)
<i>A_D</i>	Area occupied by distillation downcomer (m^2)	<i>c_L</i>	Loss coefficient for pipe or pipe fitting (–)
<i>A_{DCF}</i>	Annual discounted cash flow ($\$ \cdot \text{y}^{-1}$)	<i>C</i>	Concentration ($\text{kg} \cdot \text{m}^{-3}$, $\text{kmol} \cdot \text{m}^{-3}$, ppm), or constant in vapor pressure correlation (K), or number of components (separate systems) in network design (–)
<i>A_{FIN}</i>	Area of fins (m)	<i>C_B</i>	Base capital cost of equipment (\$)
<i>A_I</i>	Heat transfer area on the inside of tubes (m^2), or interfacial area (m^2 , $\text{m}^2 \cdot \text{m}^{-3}$)	<i>C_e</i>	Environmental discharge concentration (ppm)
<i>A_M</i>	Membrane area (m^2)	<i>C_E</i>	Equipment capital cost (\$), or unit cost of energy ($\$ \cdot \text{kW}^{-1}$, $\$ \cdot \text{MW}^{-1}$)
<i>A_{NETWORK}</i>	Heat exchanger network area (m^2)	<i>C_F</i>	Fixed capital cost of complete installation (\$)
<i>A_O</i>	Heat transfer area on the outside of tubes (m^2)	<i>C_P</i>	Specific heat capacity at constant pressure ($\text{kJ} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$, $\text{kJ} \cdot \text{kmol}^{-1} \cdot \text{K}^{-1}$)
<i>A_{ROOT}</i>	Exposed outside root area of a finned tube (m)	\overline{CP}	Mean heat capacity at constant pressure ($\text{kJ} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$, $\text{kJ} \cdot \text{kmol}^{-1} \cdot \text{K}^{-1}$)
<i>A_{SHELL}</i>	Heat exchanger area for an individual shell (m^2)	<i>C_S</i>	Corrected superficial velocity in distillation ($\text{m} \cdot \text{s}^{-1}$)
<i>AF</i>	Annualization factor for capital cost (–)	<i>C_V</i>	Specific heat capacity at constant volume ($\text{kJ} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$, $\text{kJ} \cdot \text{kmol}^{-1} \cdot \text{K}^{-1}$)
	capital cost law coefficient (units depend on cost law), or constant in cubic equation of state ($\text{m}^3 \cdot \text{kmol}^{-1}$), or correlating coefficient (units depend on application), or order of reaction (–)	<i>C*</i>	Solubility of solute in solvent ($\text{kg} \cdot \text{kg solvent}^{-1}$)
<i>b_i</i>	Bottoms flowrate of Component <i>i</i> ($\text{kmol} \cdot \text{s}^{-1}$, $\text{kmol} \cdot \text{h}^{-1}$)	<i>CC</i>	Cycles of concentration for a cooling tower (–)
<i>B</i>	Baffle spacing in shell-and-tube heat exchangers (m), or Bottoms flowrate in distillation ($\text{kg} \cdot \text{s}^{-1}$, $\text{kg} \cdot \text{h}^{-1}$, $\text{kmol} \cdot \text{s}^{-1}$, $\text{kmol} \cdot \text{h}^{-1}$), or breadth of device (m), or constant in vapor pressure correlation ($\text{N} \cdot \text{K} \cdot \text{m}^{-2}$, bar · K), or moles remaining in batch distillation (kmol)	<i>CC_{STEAM}</i>	Cumulative cost ($\$ \cdot \text{t}^{-1}$)
		<i>COD</i>	Chemical oxygen demand ($\text{kg} \cdot \text{m}^{-3}$, $\text{mg} \cdot \text{l}^{-1}$)
		<i>COP</i>	Coefficient of performance (–)
		<i>COP_{AHP}</i>	Coefficient of performance of an absorption heat pump (–)
		<i>COP_{AHT}</i>	Coefficient of performance of an absorption heat transformer (–)
		<i>COP_{AR}</i>	Coefficient of performance of absorption refrigeration (–)
		<i>COP_{CHP}</i>	Coefficient of performance of a compression heat pump (–)
		<i>COP_{HP}</i>	Coefficient of performance of a heat pump (–)
		<i>COP_{REF}</i>	Coefficient of performance of a refrigeration system (–)
		<i>CP</i>	Capacity parameter in distillation ($\text{m} \cdot \text{s}^{-1}$) or heat capacity flowrate ($\text{kW} \cdot \text{K}^{-1}$, $\text{MW} \cdot \text{K}^{-1}$)

CP_{EX}	Heat capacity flowrate of heat engine exhaust ($\text{kW} \cdot \text{K}^{-1}$, $\text{MW} \cdot \text{K}^{-1}$)	F_{TC}	Correction factor for tube count in shell-and-tube heat exchangers (–)
CW	Cooling water	F_{Tmin}	Minimum acceptable F_T for noncountercurrent heat exchangers (–)
d	Diameter (μm , m), or correlating coefficient (units depend on application)	F_{XY}	Factor to allow for inclination in structured packing (–)
d_C	Column inside diameter (m)	F_σ	Factor to allow for inadequate wetting of packing (–)
d_i	Distillate flowrate of Component i ($\text{kmol} \cdot \text{s}^{-1}$, $\text{kmol} \cdot \text{h}^{-1}$)	g	Acceleration due to gravity ($9.81 \text{ m} \cdot \text{s}^{-2}$)
d_I	Inside diameter of pipe or tube (m)	g_{ij}	Energy of interaction between Molecules i and j in the NRTL equation ($\text{kJ} \cdot \text{kmol}^{-1}$)
d_P	Distillation and absorption packing size (m)	G	Free energy (kJ), or gas flowrate ($\text{kg} \cdot \text{s}^{-1}$, $\text{kmol} \cdot \text{s}^{-1}$)
d_R	Outside tube diameter for a finned tube at the root of fins (m)	\bar{G}_i	Partial molar free energy of Component i ($\text{kJ} \cdot \text{kmol}^{-1}$)
D	Distillate flowrate ($\text{kg} \cdot \text{s}^{-1}$, $\text{kg} \cdot \text{h}^{-1}$, $\text{kmol} \cdot \text{s}^{-1}$, $\text{kmol} \cdot \text{h}^{-1}$)	\bar{G}_i^O	Standard partial molar free energy of Component i ($\text{kJ} \cdot \text{kmol}^{-1}$)
D_B	Tube bundle diameter for shell-and-tube heat exchangers (m)	GCV	Gross calorific value of fuel ($\text{J} \cdot \text{m}^{-3}$, $\text{kJ} \cdot \text{m}^{-3}$, $\text{J} \cdot \text{kg}^{-1}$, $\text{kJ} \cdot \text{kg}^{-1}$)
D_S	Inside shell diameter for shell-and-tube heat exchangers (m)	h	Settling distance of particles (m)
$DCFRR$	Discounted cash flowrate of return (%)	h_B	Boiling heat transfer coefficient for the tube bundle ($\text{W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$, $\text{kW} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$)
e	Wire diameter (m)	h_C	Condensing film heat transfer coefficient ($\text{W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$, $\text{kW} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$)
E	Activation energy of reaction ($\text{kJ} \cdot \text{kmol}^{-1}$), or entrainer flowrate in azeotropic and extractive distillation ($\text{kg} \cdot \text{s}^{-1}$, $\text{kmol} \cdot \text{s}^{-1}$), or exchange factor in radiant heat transfer (–), or extract flowrate in liquid–liquid extraction ($\text{kg} \cdot \text{s}^{-1}$, $\text{kmol} \cdot \text{s}^{-1}$), or stage efficiency in separation (–)	h_I	Film heat transfer coefficient for the inside ($\text{W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$, $\text{kW} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$)
E_O	Overall stage efficiency in distillation and absorption (–)	h_{IF}	Fouling heat transfer coefficient for the inside ($\text{W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$, $\text{kW} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$)
EP	Economic potential ($\$ \cdot \text{y}^{-1}$)	h_L	Head loss in a pipe or pipe fitting (m)
f	Fuel-to-air ratio for gas turbine (–)	h_{NB}	Nucleate boiling heat transfer coefficient ($\text{W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$, $\text{kW} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$)
f_i	Capital cost installation factor for Equipment i (–), or feed flowrate of Component i ($\text{kmol} \cdot \text{s}^{-1}$, $\text{kmol} \cdot \text{h}^{-1}$), or fugacity of Component i ($\text{N} \cdot \text{m}^{-2}$, bar)	h_O	Film heat transfer coefficient for the outside ($\text{W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$, $\text{kW} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$)
f_P	Capital cost factor to allow for design pressure (–)	h_{OF}	Fouling heat transfer coefficient for the outside ($\text{W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$, $\text{kW} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$)
f_T	Capital cost factor to allow for design temperature (–)	h_{RAD}	Radiant heat transfer coefficient ($\text{W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$, $\text{kW} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$)
F	Feed flowrate ($\text{kg} \cdot \text{s}^{-1}$, $\text{kg} \cdot \text{h}^{-1}$, $\text{kmol} \cdot \text{s}^{-1}$, $\text{kmol} \cdot \text{h}^{-1}$), or future worth a sum of money allowing for interest rates (\$), or number of degrees of freedom (–), or volumetric flowrate ($\text{m}^3 \cdot \text{s}^{-1}$, $\text{m}^3 \cdot \text{h}^{-1}$)	h_W	Heat transfer coefficient for the tube wall ($\text{W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$, $\text{kW} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$)
F_{FOAM}	Foaming factor in distillation (–)	H	Enthalpy (kJ, $\text{kJ} \cdot \text{kg}^{-1}$, $\text{kJ} \cdot \text{kmol}^{-1}$), or height (m), or Henry's Law Constant ($\text{N} \cdot \text{m}^{-2}$, bar , atm), or stream enthalpy ($\text{kJ} \cdot \text{s}^{-1}$, $\text{MJ} \cdot \text{s}^{-1}$)
F_{LV}	Liquid–vapor flow parameter in distillation (–)	H_F	Height of fin (m)
F_{RAD}	Fraction of heat absorbed in fired heater radiant section (–)	H_T	Tray spacing (m)
F_{SC}	Correction factor for shell construction in shell-and-tube heat exchangers (–)	\bar{H}_i^O	Standard heat of formation of Component i ($\text{kJ} \cdot \text{kmol}^{-1}$)
F_T	Correction factor for noncountercurrent flow in shell-and-tube heat exchangers (–)	ΔH^O	Standard heat of reaction (J, kJ)
		ΔH_{COMB}	Heat of combustion ($\text{J} \cdot \text{kmol}^{-1}$, $\text{kJ} \cdot \text{kmol}^{-1}$)
		ΔH_{COMB}^O	Standard heat of combustion at 298 K ($\text{J} \cdot \text{kmol}^{-1}$, $\text{kJ} \cdot \text{kmol}^{-1}$)
		ΔH_{FUEL}	Heat to bring fuel to standard temperature ($\text{J} \cdot \text{kmol}^{-1}$, $\text{kJ} \cdot \text{kg}^{-1}$)
		ΔH_{IS}	Isentropic enthalpy change of an expansion ($\text{J} \cdot \text{kmol}^{-1}$, $\text{kJ} \cdot \text{kg}^{-1}$)

ΔH_P	Heat to bring products from standard temperature to the final temperature ($\text{J} \cdot \text{kmol}^{-1}$, $\text{kJ} \cdot \text{kg}^{-1}$)	m	Mass flowrate ($\text{kg} \cdot \text{s}^{-1}$), or molar flowrate ($\text{kmol} \cdot \text{s}^{-1}$), or number of items (–)
ΔH_R	Heat to bring reactants from their initial temperature to standard temperature ($\text{J} \cdot \text{kmol}^{-1}$, $\text{kJ} \cdot \text{kmol}^{-1}$)	m_C	Mass flowrate of water contaminant ($\text{g} \cdot \text{h}^{-1}$, $\text{g} \cdot \text{d}^{-1}$)
ΔH_{STEAM}	Enthalpy difference between generated steam and boiler feedwater (kW, MW)	m_{COND}	Mass of condensate (kg)
ΔH_{VAP}	Latent heat of vaporization ($\text{kJ} \cdot \text{kg}^{-1}$, $\text{kJ} \cdot \text{kmol}^{-1}$)	m_{EX}	Mass flowrate of exhaust ($\text{kg} \cdot \text{s}^{-1}$)
$HETP$	Height equivalent of a theoretical plate (m)	m_{FUEL}	Mass of fuel (kg)
HP	High pressure	m_{max}	Maximum mass flowrate ($\text{kg} \cdot \text{s}^{-1}$)
HR	Heat rate for gas turbine ($\text{kJ} \cdot \text{kWh}^{-1}$)	m_{STEAM}	Mass flowrate of steam ($\text{kg} \cdot \text{s}^{-1}$)
i	Fractional rate of interest on money (–), or number of ions (–)	m_W	Mass flowrate of pure water ($\text{t} \cdot \text{h}^{-1}$, $\text{t} \cdot \text{d}^{-1}$)
I	Total number of hot streams (–)	m_{WL}	Limiting mass flowrate of pure water ($\text{t} \cdot \text{h}^{-1}$, $\text{t} \cdot \text{d}^{-1}$)
J	Total number of cold streams (–)	m_{Wmin}	Minimum mass flowrate of fresh water ($\text{t} \cdot \text{h}^{-1}$, $\text{t} \cdot \text{d}^{-1}$)
k	Reaction rate constant (units depend on order of reaction), or step number in a numerical calculation (–), or thermal conductivity ($\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$, $\text{kW} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$)	m_{WT}	Target mass flowrate of fresh water ($\text{t} \cdot \text{h}^{-1}$, $\text{t} \cdot \text{d}^{-1}$)
k_F	Fin thermal conductivity ($\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$, $\text{kW} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$)	m_{WTLOSS}	Target mass flowrate of fresh water involving a water loss ($\text{t} \cdot \text{h}^{-1}$, $\text{t} \cdot \text{d}^{-1}$)
$k_{G,i}$	Mass transfer coefficient in the gas phase ($\text{kmol} \cdot \text{m}^{-2} \cdot \text{Pa}^{-1} \cdot \text{s}^{-1}$)	M	Constant in capital cost correlations (–), or molar mass ($\text{kg} \cdot \text{kmol}^{-1}$), or number of variables (–)
k_{ij}	Interaction parameter between Components i and j in an equation of state (–)	MP	Medium pressure
$k_{L,i}$	Mass transfer coefficient of Component i in the liquid phase ($\text{m} \cdot \text{s}^{-1}$)	MC_{STEAM}	Marginal cost of steam ($\$ \cdot \text{t}^{-1}$)
k_0	Frequency factor for heat of reaction (units depend on order of reaction)	n	Number of items (–), or number of years (–), or polytropic coefficient (–), or slope of Willans Line ($\text{kJ} \cdot \text{kg}^{-1}$, $\text{MJ} \cdot \text{kg}^{-1}$)
k_W	Wall thermal conductivity ($\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$, $\text{kW} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$)	N	Number of compression stages (–), or number of independent equations (–), or number of moles (kmol), or number of theoretical stages (–), or rate of transfer of a component ($\text{kmol} \cdot \text{s}^{-1} \cdot \text{m}^{-3}$), or rotational speed (s^{-1} , min^{-1})
K	Overall mass transfer coefficient ($\text{kmol} \cdot \text{Pa}^{-1} \cdot \text{m}^{-2} \cdot \text{s}^{-1}$), or rate constant for fouling ($\text{m}^2 \cdot \text{K} \cdot \text{W}^{-1} \cdot \text{day}^{-1}$), or total number of enthalpy intervals in heat exchanger networks (–)	N_F	Number of fins per unit length (m^{-1})
K_a	Equilibrium constant of reaction based on activity (–)	N_i	Number of moles of Component i (kmol)
K_i	Ratio of vapor-to-liquid composition at equilibrium for Component i (–)	N_{i0}	Initial number of moles of Component i (kmol)
$K_{M,i}$	Equilibrium partition coefficient of membrane for Component i (–)	N_{min}	Minimum number of theoretical stages (–)
K_p	Equilibrium constant of reaction based on partial pressure in the vapor phase (–)	N_P	Number of tube passes (–)
K_T	Parameter for terminal settling velocity ($\text{m} \cdot \text{s}^{-1}$)	N_R	Number of tube rows (–)
K_x	Equilibrium constant of reaction based on mole fraction in the liquid phase (–)	N_{SHELLS}	Number of number of 1–2 shells in shell-and-tube heat exchangers (–)
K_y	Equilibrium constant of reaction based on mole fraction in vapor phase (–)	N_R	Number of tube rows (–)
L	length (m), or liquid flowrate ($\text{kg} \cdot \text{s}^{-1}$, $\text{kmol} \cdot \text{s}^{-1}$), or number of independent loops in a network (–)	N_S	Specific speed of centrifugal pump (–)
L_W	Distillation tray weir length (m)	N_T	Number of tubes (–)
LP	Low pressure	N_{TR}	Number of tubes per row (–)
		N_{UNITS}	Number of units in a heat exchanger network (–)
		NC	Number of components in a multicomponent mixture (–)
		NCV	Net calorific value of fuel ($\text{J} \cdot \text{m}^{-3}$, $\text{kJ} \cdot \text{m}^{-3}$, $\text{J} \cdot \text{kg}^{-1}$, $\text{kJ} \cdot \text{kg}^{-1}$)
		$NPSH$	Net positive suction head (m)
		NPV	Net present value (\$)
		Nu	Nusselt number (–)
		p	Partial pressure ($\text{N} \cdot \text{m}^{-2}$, bar), or helical pitch (m)

p_C	Pitch configuration factor for tube layout (–)	Q_{INPUT}	Heat input from fuel (kW, MW)
p_T	Tube pitch (m)	Q_{HP}	Heat duty on high-pressure steam (kW, MW), or heat pump heat duty (kW, MW)
P	Present worth of a future sum of money (\$), or pressure ($N \cdot m^{-2}$, bar), or probability (–), or thermal effectiveness of 1–2 shell-and-tube heat exchanger (–)	Q_{LP}	Heat duty on low-pressure steam (kW, MW)
P_C	Critical pressure ($N \cdot m^{-2}$, bar)	Q_{LOSS}	Stack loss from furnace, boiler, or gas turbine (kW, MW)
P_{max}	Maximum thermal effectiveness of 1–2 shell-and-tube heat exchangers (–)	Q_{OUTPUT}	Heat output to steam generation (kW, MW)
$P_{M,i}$	Permeability of Component i for a membrane ($kmol \cdot m \cdot s^{-1} \cdot m^{-2} \cdot bar^{-1}$, $kg \text{ solvent} \cdot m^{-1} \cdot s^{-1} \cdot bar^{-1}$)	Q_{RAD}	Radiant heat duty (kW, MW)
$\bar{P}_{M,i}$	Permeance of Component i for a membrane ($m^3 \cdot m^{-2} \cdot s^{-1} \cdot bar^{-1}$)	Q_{REACT}	Reactor heating or cooling duty (kW, MW)
P_{N-2N}	Thermal effectiveness over N_{SHELLS} number of 1–2 shell-and-tube heat exchangers in series (–)	Q_{REB}	Reboiler heat duty (kW, MW)
P_{1-2}	Thermal effectiveness over each 1–2 shell-and-tube heat exchanger in series (–)	Q_{REC}	Heat recovery (kW, MW)
P^{SAT}	Saturated liquid–vapor pressure ($N \cdot m^{-2}$, bar)	Q_{SITE}	Site heating demand (kW, MW)
Pr	Prandtl number (–)	Q_{STEAM}	Heat input for steam generation (kW, MW)
ΔP	Pressure drop ($N \cdot m^{-2}$, bar)	r	Molar ratio (–), or pressure ratio (–), or radius (m)
ΔP_{FLOOD}	Pressure drop under flooding conditions ($N \cdot m^{-2}$, bar)	r_i	Pure component property measuring the molecular van der Waals volume for Molecule i in the UNIQUAC Equation and UNIFAC Model (–), or rate of reaction of Component i ($kmol^{-1} \cdot s^{-1}$), or recovery of Component i in separation (–)
q	Heat flux ($W \cdot m^{-2}$, $kW \cdot m^{-2}$), or thermal condition of the feed in distillation (–), or Wegstein acceleration parameter for the convergence of recycle calculations (–)	R	Fractional recovery of a component in separation (–), or heat capacity ratio of 1–2 shell-and-tube heat exchanger (–), or raffinate flowrate in liquid–liquid extraction ($kg \cdot s^{-1}$, $kmol \cdot s^{-1}$), or ratio of heat capacity flowrates (–), or reflux ratio in distillation (–), or removal ratio in water treatment (–), or residual error (units depend on application), or universal gas constant ($8314.5 N \cdot m \cdot kmol^{-1} \cdot K^{-1} = J \cdot kmol^{-1} \cdot K^{-1}$, $8.3145 kJ \cdot kmol^{-1} \cdot K^{-1}$)
q_C	Critical heat flux ($W \cdot m^{-2}$, $kW \cdot m^{-2}$)	R_{AF}	Mass ratio of air to fuel (–)
q_{C1}	Critical heat flux for a single tube ($W \cdot m^{-2}$, $kW \cdot m^{-2}$)	R_{min}	Minimum reflux ratio (–)
q_i	Individual stream heat duty for Stream i ($kJ \cdot s^{-1}$), or pure component property measuring the molecular van der Waals surface area for Molecule i in the UNIQUAC Equation of UNIFAC Model (–)	R_F	Fouling resistance in heat transfer ($m^{-2} \cdot K \cdot W^{-1}$), or ratio of actual to minimum reflux ratio (–)
q_{RAD}	Radiant heat flux ($W \cdot m^{-2}$, $kW \cdot m^{-2}$)	R_{SITE}	Site power-to-heat ratio (–)
Q	Heat duty (kW, MW)	ROI	Return on investment (%)
Q_{ABS}	Absorber heat duty (kW, MW)	Re	Reynolds number (–)
Q_C	Cooling duty (kW, MW)	s	Reactor space velocity (s^{-1} , min^{-1} , h^{-1}), or steam-to-air ratio for gas turbine (–)
Q_{Cmin}	Target for cold utility (kW, MW)	S	Entropy ($kJ \cdot K^{-1}$, $kJ \cdot kg^{-1} \cdot K^{-1}$, $kJ \cdot kmol^{-1} \cdot K^{-1}$), or number of streams in a heat exchanger network (–), or reactor selectivity (–), or reboil ratio for distillation (–), or selectivity of a reaction (–), or slack variable in optimization (units depend on application), or solvent flowrate ($kg \cdot s^{-1}$, $kmol \cdot s^{-1}$), or stripping factor in absorption (–)
Q_{COND}	Condenser heat duty (kW, MW)		
Q_{CONV}	Convective heat duty (kW, MW)		
Q_{EVAP}	Evaporator heat duty (kW, MW)		
Q_{EX}	Heat duty for heat engine exhaust (kW, MW)		
Q_{FEED}	Heat duty to the feed (kW, MW)		
Q_{FUEL}	Heat from fuel in a furnace, boiler, or gas turbine (kW, MW)		
Q_{GEN}	Heat pump generator heat duty (kW, MW)		
Q_H	Heating duty (kW, MW)		
Q_{Hmin}	Target for hot utility (kW, MW)		
Q_{HE}	Heat engine heat duty (kW, MW)		
Q_{HEN}	Heat exchanger network heat duty (kW, MW)		

S_C	Number of cold streams (–)	W_{LOSS}	Power loss in gas or steam turbines (kW, MW)
S_H	Number of hot streams (–)	W_{SITE}	Site power demand (kW, MW)
S_W	Dimensionless swirl parameter (–)	x	Control variable in optimization problem (units depend on application), or liquid-phase mole fraction (–)
t	Batch time (s, h), or time (s, h)	x_F	Final value of control variable in optimization problem (units depend on application), or mole fraction in the feed (–)
T	Temperature (°C, K)	x_B	Mole fraction in the distillation bottoms (–)
T_{ABS}	Absorber temperature (°C, K)	x_D	Mole fraction in the distillate (–)
T_{BPT}	Normal boiling point (°C, K)	x_0	Initial value of control variable in optimization problem (units depend on application)
T_C	Critical temperature (K), or temperature of heat sink (°C, K)	X	Reactor conversion (–), or wetness fraction of steam (–)
T_{COND}	Condenser temperature (°C, K)	X_E	Equilibrium reactor conversion (–)
T_E	Equilibrium temperature (°C, K)	X_{OPT}	Optimal reactor conversion (–)
T_{EVAP}	Evaporation temperature (°C, K)	X_P	Fraction of maximum thermal effectiveness P_{max} allowed in a 1–2 shell-and-tube heat exchanger (–)
T_{FEED}	Feed temperature (°C, K)	XP	Cross-pinch heat transfer in heat exchanger network (kW, MW)
T_{GEN}	Heat pump generator temperature (°C, K)	y	Integer variable in optimization (–), or twist ratio for twisted tape (–), or vapor-phase mole fraction (–)
T_H	Temperature of heat source (°C, K)	y_F	Distance between fins (m)
T_R	Reduced temperature T/T_C (–)	z	Elevation (m), or feed mole fraction (–)
T_{REB}	Reboiler temperature (°C, K)	Z	Compressibility of a fluid (–)
T_S	Stream supply temperature (°C)		
T_{SAT}	Saturation temperature of boiling liquid (°C, K)		
T_T	Stream target temperature (°C)		
T_{TFT}	Theoretical flame temperature (°C, K)		
T_W	Wall temperature (°C, K)		
T_{WBT}	Wet bulb temperature (°C)		
T^*	Interval temperature (°C)		
ΔT_{LM}	Logarithmic mean temperature difference (°C, K)		
ΔT_{min}	Minimum temperature difference (°C, K)		
$\Delta T_{THRESHOLD}$	Threshold temperature difference (°C, K)		
TAC	Total annual cost ($\$ \cdot y^{-1}$)		
TOD	Total oxygen demand ($kg \cdot m^{-3}$, $mg \cdot l^{-1}$)		
u_{ij}	Interaction parameter between Molecule i and Molecule j in the UNIQUAC Equation ($kJ \cdot kmol^{-1}$)		
U	Overall heat transfer coefficient ($W \cdot m^{-2} \cdot K^{-1}$, $kW \cdot m^{-2} \cdot K^{-1}$)		
v	Velocity ($m \cdot s^{-1}$)		
v_D	Downcomer liquid velocity ($m \cdot h^{-1}$)		
v_S	Shell-side fluid velocity ($m \cdot s^{-1}$), or superficial vapor velocity ($m \cdot s^{-1}$)		
v_T	Terminal settling velocity ($m \cdot s^{-1}$), or tube-side tube velocity ($m \cdot s^{-1}$)		
v_V	Superficial vapor velocity in empty column ($m \cdot s^{-1}$)		
V	Molar volume ($m^3 \cdot kmol^{-1}$), or vapor flowrate ($kg \cdot s^{-1}$, $kmol \cdot s^{-1}$), or volume (m^3), or volume of gas or vapor adsorbed ($m^3 \cdot kg^{-1}$)		
V_{min}	Minimum vapor flow ($kg \cdot s^{-1}$, $kmol \cdot s^{-1}$)		
VF	Vapor fraction (–)		
w	Mass of adsorbate per mass of adsorbent (–)		
W	Shaft power (kW, MW), or shaft work (kJ, MJ)		
W_{GEN}	Power generated (kW, MW)		
W_{GT}	Power generated by gas turbine (kW, MW)		
W_{INT}	Intercept of Willans Line (kW, MW)		

Greek Letters

α	Constant in cubic equation of state (–), or constants in vapor pressure correlation (units depend on which constant), or fraction open of a valve (–), or helix angle of wire to the tube axis (degrees), or relative volatility between a binary pair (–)
α_{ij}	Ideal separation factor or selectivity of membrane between Components i and j (–), or parameter characterizing the tendency of Molecule i and Molecule j to be distributed in a random fashion in the NRTL equation (–), or relative volatility between Components i and j (–)
α_{LH}	Relative volatility between light and heavy key components (–)
α_P	Packing surface area ($m^2 \cdot m^3$)
β_{ij}	Separation factor between Components i and j (–)
γ	Logic variable in optimization (–), or ratio of heat capacities for gases and vapors (–)
γ_i	Activity coefficient for Component i (–)
δ	Thickness (m)
δ_F	Fin thickness (m)
δ_M	Membrane thickness (m)
ϵ	Emissivity (–), or extraction factor in liquid-liquid extraction (–), or

	pipe roughness (mm)	<i>e</i>	Enhanced, or
η	Carnot factor (–), or efficiency (–)		end zone on the shell side of a heat exchanger, or environment, or equivalent
η_{AHP}	Absorber heat pump efficiency (–)	<i>E</i>	Evaporation, or
η_{AHT}	Absorber heat transformer efficiency (–)		extract in liquid–liquid extraction
η_{BOILER}	Boiler efficiency (–)	<i>EVAP</i>	Evaporator conditions
η_C	Carnot efficiency (–)	<i>EX</i>	Exhaust
η_{CHP}	Compression heat pump efficiency (–)	<i>final</i>	Final conditions in a batch
η_{COGEN}	Cogeneration efficiency (–)	<i>F</i>	Feed, or final, or fluid
η_F	Fin efficiency (–)		
η_{GT}	Efficiency of gas turbine (–)	<i>FIN</i>	Fin on a finned tube
η_{IS}	Isentropic efficiency of compression or expansion (–)	<i>FG</i>	Flue gas
η_{MECH}	Mechanical efficiency of steam turbine (–)	<i>G</i>	Gas phase
η_P	Polytropic efficiency of compression or expansion (–)	<i>H</i>	Hot stream
η_{POWER}	Power generation efficiency (–)	<i>HP</i>	Heat pump, or high pressure
η_{ST}	Efficiency of steam turbine (–)	<i>i</i>	Component number, or stream number
η_W	Weighted fin efficiency (–)		
θ	Angle (degrees), or fraction of feed permeated through membrane (–), or root of the Underwood Equation (–)	<i>in</i>	Inlet
ϑ	Logic variable in optimization (–)	<i>I</i>	Inside
λ	Ratio of latent heats of vaporization (–)	<i>IF</i>	Inside fouling
λ_{ij}	Energy parameter characterizing the interaction of Molecule <i>i</i> with Molecule <i>j</i> ($\text{kJ} \cdot \text{kmol}^{-1}$)	<i>IMP</i>	Impeller
μ	Fluid viscosity ($\text{kg} \cdot \text{m}^{-1} \cdot \text{s}^{-1}$, $\text{mN} \cdot \text{s} \cdot \text{m}^{-2} = \text{cP}$)	<i>IS</i>	Isentropic
π	Osmotic pressure ($\text{N} \cdot \text{m}^{-2}$, bar)	<i>J</i>	Component number, or stream number
ρ	Density ($\text{kg} \cdot \text{m}^{-3}$, $\text{kmol} \cdot \text{m}^{-3}$)	<i>K</i>	Enthalpy interval number in heat exchanger networks
σ	Stephan–Boltzmann constant ($\text{W} \cdot \text{m}^{-2} \cdot \text{K}^{-4}$), or surface tension ($\text{mN} \cdot \text{m}^{-1} = \text{mJ} \cdot \text{m}^{-2} = \text{dyne} \cdot \text{cm}^{-1}$)	<i>L</i>	Liquid phase
τ	Reactor space time (s, min, h), or residence time (s, min, h)	<i>LP</i>	Low pressure
τ_W	Wall shear stress ($\text{N} \cdot \text{m}^{-2}$)	<i>M</i>	Stage number in distillation and absorption
v_k^i	Number of interaction Groups <i>k</i> in Molecule <i>i</i> (–)	<i>max</i>	Maximum
Φ	Fugacity coefficient (–), or logic variable in optimization (–)	<i>min</i>	Minimum
ω	Acentric factor (–)	<i>M</i>	Makeup
		<i>MIX</i>	Mixture
		<i>N</i>	Stage number in distillation and absorption
		<i>out</i>	Outlet
		<i>O</i>	Outside, or standard conditions
		<i>OF</i>	Outside fouling
		<i>p</i>	Stage number in distillation and absorption
		<i>prod</i>	Products of reaction
		<i>P</i>	Particle, or permeate
		<i>PINCH</i>	Pinch conditions
		<i>react</i>	Reactants
		<i>R</i>	Raffinate in liquid–liquid extraction
		<i>REACT</i>	Reaction
		<i>ROOT</i>	Root of a finned tube
		<i>S</i>	Solvent in liquid–liquid extraction
		<i>SAT</i>	Saturated conditions
		<i>SF</i>	Supplementary firing
		<i>SUP</i>	Superheated conditions
		<i>SW</i>	Swirl direction
		<i>T</i>	Treatment

Subscripts

<i>axial</i>	Axial direction
<i>B</i>	Blowdown, or bottoms in distillation
<i>BFW</i>	Boiler feedwater
<i>BW</i>	Bridgwall
<i>cont</i>	Contribution
<i>C</i>	Cold stream, or contaminant
<i>CN</i>	Condensing
<i>COND</i>	Condensing conditions
<i>CP</i>	Cold plane, or continuous phase
<i>CW</i>	Cooling water
<i>D</i>	Distillate in distillation
<i>DS</i>	De-superheating

<i>Te</i>	Tube side enhanced
<i>TW</i>	Treated water
<i>V</i>	Vapor phase
<i>w</i>	Window section on the shell side of a heat exchanger
<i>W</i>	Conditions at the tube wall, or water
<i>WBT</i>	Wet bulb conditions
<i>WW</i>	Waste water
∞	Conditions at distillate pinch point

Superscripts

<i>I</i>	Phase <i>I</i>
<i>II</i>	Phase <i>II</i>
<i>III</i>	Phase <i>III</i>
<i>IDEAL</i>	Ideal behavior
<i>L</i>	Liquid phase
<i>O</i>	Standard conditions
<i>V</i>	Vapor phase
*	Adjusted parameter

The Nature of Chemical Process Design and Integration

1.1 Chemical Products

Chemical products are essential to modern living standards. Almost all aspects of everyday life are supported by chemical products in one way or another. However, society tends to take these products for granted, even though a high quality of life fundamentally depends on them.

When considering the design of processes for the manufacture of chemical products, the market into which they are being sold fundamentally influences the objectives and priorities in the design. Chemical products can be divided into three broad classes:

- 1) *Commodity or bulk chemicals*. These are produced in large volumes and purchased on the basis of chemical composition, purity and price. Examples are sulfuric acid, nitrogen, oxygen, ethylene and chlorine.
- 2) *Fine chemicals*. These are produced in small volumes and purchased on the basis of chemical composition, purity and price. Examples are chloropropylene oxide (used for the manufacture of epoxy resins, ion-exchange resins and other products), dimethyl formamide (used, for example, as a solvent, reaction medium and intermediate in the manufacture of pharmaceuticals), *n*-butyric acid (used in beverages, flavorings, fragrances and other products) and barium titanate powder (used for the manufacture of electronic capacitors).
- 3) *Specialty or effect or functional chemicals*. These are purchased because of their effect (or function), rather than their chemical composition. Examples are pharmaceuticals, pesticides, dyestuffs, perfumes and flavorings.

Because commodity and fine chemicals tend to be purchased on the basis of their chemical composition alone, they can be

considered to be *undifferentiated*. For example, there is nothing to choose between 99.9% benzene made by one manufacturer and that made by another manufacturer, other than price and delivery issues. On the other hand, specialty chemicals tend to be purchased on the basis of their effect or function and therefore can be considered to be *differentiated*. For example, competitive pharmaceutical products are differentiated according to the efficacy of the product, rather than chemical composition. An adhesive is purchased on the basis of its ability to stick things together, rather than its chemical composition, and so on.

However, in practice few products are completely undifferentiated and few completely differentiated. Commodity and fine chemical products might have impurity specifications as well as purity specifications. Traces of impurities can, in some cases, give some differentiation between different manufacturers of commodity and fine chemicals. For example, 99.9% acrylic acid might be considered to be an undifferentiated product. However, traces of impurities, at concentrations of a few parts per million, can interfere with some of the reactions in which it is used and can have important implications for some of its uses. Such impurities might differ between different manufacturing processes. Not all specialty products are differentiated. For example, pharmaceutical products like aspirin (acetylsalicylic acid) are undifferentiated. Different manufacturers can produce aspirin, and there is nothing to choose between these products, other than the price and differentiation created through marketing of the product. Thus, the terms undifferentiated and differentiated are more relative than absolute terms.

The scale of production also differs between the three classes of chemical products. Fine and specialty chemicals tend to be produced in volumes less than $1000 \text{ t}\cdot\text{y}^{-1}$. By contrast, commodity chemicals tend to be produced in much larger volumes than this. However, the distinction is again not so clear. Polymers are differentiated products because they are purchased on the basis of their mechanical properties, but can be produced in quantities significantly higher than $1000 \text{ t}\cdot\text{y}^{-1}$.

When a new chemical product is first developed, it can often be protected by a patent in the early years of its commercial exploitation. For a product to be eligible to be patented, it must be novel, useful and unobvious. If patent protection can be obtained, this effectively gives the producer a monopoly for commercial exploitation of the product until the patent expires. Patent protection lasts for 20 years from the filing date of the patent. Once the patent expires, competitors can join in and manufacture the product. If competitors cannot wait until the patent expires, then alternative competing products must be developed.

Another way to protect a competitive edge for a new product is to protect it by secrecy. The formula for Coca-Cola has been kept a secret for over 100 years. Potentially, there is no time limit on such protection. However, for the protection through secrecy to be viable, competitors must not be able to reproduce the product from chemical analysis. This is likely to be the case only for certain classes of specialty chemicals and food products for which the properties of the product depend on both the chemical composition and the method of manufacture.

Figure 1.1 illustrates different product *life cycles* (Sharratt, 1997; Brennan, 1998). The general trend is that when a new product is introduced into the market, the sales grow slowly until the market is established and then more rapidly once the market is established. If there is patent protection, then competitors will not be able to exploit the same product commercially until the patent expires, when competitors can produce the same product and take market share. It is expected that competitive products will cause sales to diminish later in the product life cycle until sales become so low that a company would be expected to withdraw from the market. In Figure 1.1, Product A appears to be a poor

product that has a short life with low sales volume. It might be that it cannot compete well with other competitive products and alternative products quickly force the company out of that business. However, a low sales volume is not the main criterion to withdraw a product from the market. It might be that a product with low volume finds a market niche and can be sold for a high value. On the other hand, if it were competing with other products with similar functions in the same market sector, which keeps both the sale price and volume low, then it would seem wise to withdraw from the market. Product B in Figure 1.1 appears to be a better product, showing a longer life cycle and higher sales volume. This has patent protection but sales decrease rapidly after patent protection is lost, leading to loss of market through competition. Product C in Figure 1.1 is an even better product. This shows high sales volume with the life of the product extended through reformulation of the product (Sharratt, 1997). Finally, Product D in Figure 1.1 shows a product life cycle that is typical of commodity chemicals. Commodity chemicals tend not to exhibit the same kind of life cycles as fine and specialty chemicals. In the early years of the commercial exploitation, the sales volume grows rapidly to a high volume, but then volume does not decline and enters a mature period of slow growth, or, in some exceptional cases, slow decline. This is because commodity chemicals tend to have a diverse range of uses. Even though competition might take away some end uses, new end uses are introduced, leading to an extended life cycle.

The different classes of chemical products will have very different *added value* (the difference between the selling price of the product and the purchase cost of raw materials). Commodity chemicals tend to have low added value, whereas fine and specialty chemicals tend to have high added value. Commodity chemicals tend to be produced in large volumes with low added value, while fine and specialty chemicals tend to be produced in small volumes with high added value.

Because of this, when designing a process for a commodity chemical, it is usually important to keep operating costs as low as possible. The capital cost of the process will tend to be high relative to a process for fine or specialty chemicals because of the scale of production.

When designing a process for specialty chemicals, priority tends to be given to the product, rather than to the process. This is because the unique function of the product must be protected. The process is likely to be small scale and operating costs tend to be less important than with commodity chemical processes because of the scale. The capital cost of the process will be low relative to commodity chemical processes because of the scale. The time to market for the product is also likely to be important with specialty chemicals, especially if there is patent protection. If this is the case, then anything that shortens the time from basic research, through product testing, pilot plant studies, process design, construction of the plant to product manufacture will have an important influence on the overall project profitability.

All this means that the priorities in process design are likely to differ significantly, depending on whether a process is being designed for the manufacture of a commodity, fine or specialty chemical. In commodity chemicals, there is likely to be relatively little product innovation, but intensive process innovation. Also,

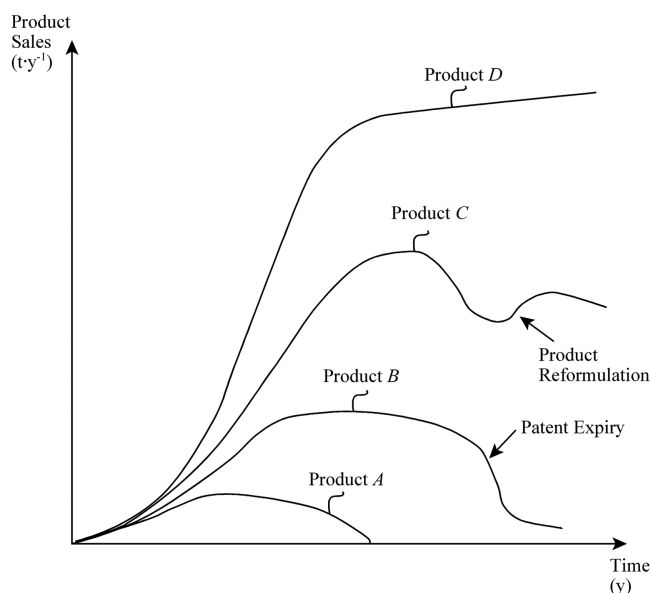


Figure 1.1

Product life cycles. (Adapted from Sharratt PN, 1997, Handbook of Batch Process Design, Chapman & Hall, reproduced by permission.)

equipment will be designed for a specific process step. On the other hand, the manufacture of fine and specialty chemicals might involve:

- selling into a market with low volume;
- a short product life cycle;
- a demand for a short time to market, and therefore less time is available for process development, with product and process development proceeding simultaneously.

As a result, the manufacture of fine and specialty chemicals is often carried out in multipurpose equipment, perhaps with different chemicals being manufactured in the same equipment at different times during the year. The life of the equipment might greatly exceed the life of the product.

The development of pharmaceutical products demands that high-quality products must be manufactured during the development of the process to allow safety and clinical studies to be carried out before full-scale production. Pharmaceutical production represents an extreme case of process design in which the regulatory framework controlling production makes it difficult to make process changes, even during the development stage. Even if significant improvements to processes for pharmaceuticals can be suggested, it might not be feasible to implement them, as such changes might prevent or delay the process from being licensed for production.

1.2 Formulation of Design Problems

Before a process design can be started, the design problem must be formulated. Formulation of the design problem requires a product specification. If a well-defined chemical product is to be manufactured, then the specification of the product might appear straightforward (e.g. a purity specification). However, if a specialty product is to be manufactured, it is the functional properties that are important, rather than the chemical properties, and this might require a *product design* stage in order to specify the product (Seider *et al.*, 2010; Cussler and Moggridge, 2011).

The initial statement of the design problem is often ill defined. For example, the design team could be asked to expand the production capacity of an existing plant that produces a chemical that is a precursor to a polymer product, which is also produced by the company. This results from an increase in the demand for the polymer product and the plant producing the precursor currently being operated at its maximum capacity. The design team might well be given a specification for the expansion. For example, the marketing department might assess that the market could be expanded by 30% over a two-year period, which would justify a 30% expansion in the process for the precursor. However, the 30% projection can easily be wrong. The economic environment can change, leading to the projected increase being either too large or too small. It might also be possible to sell the polymer precursor in the market to other manufacturers of the polymer and justify an expansion even larger than 30%. If the polymer precursor can be sold in the marketplace, is the current purity specification of the

company suitable for the marketplace? Perhaps the marketplace demands a higher purity than the current company specification. Perhaps the current specification is acceptable, but if the specification could be improved, the product could be sold for a higher value and/or at a greater volume. An option might be to not expand the production of the polymer precursor to 30%, but instead to purchase it from the market. If it is purchased from the market, is it likely to be up to the company specifications or will it need some purification before it is suitable for the company's polymer process? How reliable will the market source be? All these uncertainties are related more to market supply and demand issues than to specific process design issues.

Closer examination of the current process design might lead to the conclusion that the capacity can be expanded by 10% with a very modest capital investment. A further increase to 20% would require a significant capital investment, but an expansion to 30% would require an extremely large capital investment. This opens up further options. Should the plant be expanded by 10% and a market source identified for the balance? Should the plant be expanded to 20% similarly? If a real expansion in the marketplace is anticipated and expansion to 30% would be very expensive, why not be more aggressive and, instead of expanding the existing process, build an entirely new process? If a new process is to be built, then what should be the process technology? New process technology might have been developed since the original plant was built that enables the same product to be manufactured at a much lower cost. If a new process is to be built, where should it be built? It might make more sense to build it in another country that would allow lower operating costs, and the product could be shipped back to be fed to the existing polymer process. At the same time, this might stimulate the development of new markets in other countries, in which case, what should be the capacity of the new plant?

Thus, from the initial ill-defined problem, the design team must create a series of very specific options and these should then be compared on the basis of a common set of assumptions regarding, for example, raw materials and product prices. Having specified an option, this gives the design team a well-defined problem to which the methods of engineering and economic analysis can be applied.

In examining a design option, the design team should start out by examining the problem at the highest level, in terms of its feasibility with the minimum of detail to ensure the design option is worth progressing (Douglas, 1985). Is there a large difference between the value of the product and the cost of the raw materials? If the overall feasibility looks attractive, then more detail can be added, the option re-evaluated, further detail added, and so on. Byproducts might play a particularly important role in the economics. It might be that the current process produces some byproducts that can be sold in small quantities to the market. However, as the process is expanded, there might be market constraints for the new scale of production. If the byproducts cannot be sold, how does this affect the economics?

In summary, the original problem posed to process design teams is often ill defined, even though it might appear to be well defined in the original design specification. The design team must then formulate a series of plausible design options to be screened by the methods of engineering and economic analysis.

These design options are formulated into very specific design problems. In this way, the design team turns the ill-defined problem into a series of well-defined design options for analysis.

1.3 Synthesis and Simulation

In a chemical process, the transformation of raw materials into desired chemical products usually cannot be achieved in a single step. Instead, the overall transformation is broken down into a number of steps that provide intermediate transformations. These are carried out through reaction, separation, mixing, heating, cooling, pressure change, particle size reduction or enlargement for solids. Once individual steps have been selected, they must be interconnected to carry out the overall transformation (Figure 1.2a). Thus, the *synthesis* of a chemical process involves two broad activities. First, individual transformation steps are selected. Second, these individual transformations are interconnected to form a complete process that achieves the required overall transformation. A *flowsheet* or *process flow diagram* (PFD) is a diagrammatic representation of the process steps with their interconnections.

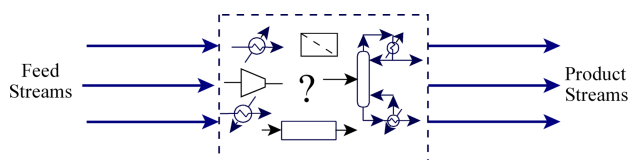
Once the flowsheet structure has been defined, a *simulation* of the process can be carried out. A simulation is a mathematical model of the process that attempts to predict how the process would behave if it was constructed (Figure 1.2b). Material and energy balances can be formulated to give better definition to the inner workings of the process and a more detailed process design can be developed. Having created a model of the process, the flowrates, compositions, temperatures and pressures of the feeds can be

assumed. The simulation model then predicts the flowrates, compositions, temperatures, pressures and properties of the products. It also allows the individual items of equipment in the process to be sized and predicts, for example, how much raw material is being used or how much energy is being consumed. The performance of the design can then be evaluated.

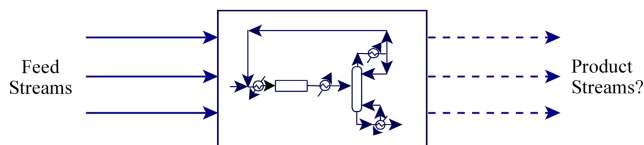
1) *Accuracy of design calculations.* A simulation adds more detail once a design has been synthesized. The design calculations for this will most often be carried out in a general purpose simulation software package and solved to a high level of precision. However, a high level of precision cannot usually be justified in terms of the operation of the plant after it has been built. The plant will almost never work precisely at its original design flowrates, temperatures, pressures and compositions. This might be because the raw materials are slightly different from what is assumed in the design. The physical properties assumed in the calculations might have been erroneous in some way, or operation at the original design conditions might create corrosion or fouling problems, or perhaps the plant cannot be controlled adequately at the original conditions, and so on, for a multitude of other possible reasons. The instrumentation on the plant will not be able to measure the flowrates, temperatures, pressures and compositions as accurately as the calculations performed. High precision might be required in the calculations for certain specific parts of the design. For example, a polymer precursor might need certain impurities to be very tightly controlled, perhaps down to the level of parts per million, or it might be that some contaminant in a waste stream might be exceptionally environmentally harmful and must be extremely well defined in the design calculations.

Even though a high level of precision cannot be justified in many cases in terms of the plant operation, the design calculations will normally be carried out to a reasonably high level of precision. The value of precision in design calculations is that the consistency of the calculations can be checked to allow errors or poor assumptions to be identified. It also allows the design options to be compared on a valid like-for-like basis.

Because of all the uncertainties in carrying out a design, the specifications are often increased beyond those indicated by the design calculations and the plant is *overdesigned*, or *contingency* is added, through the application of *safety factors* to the design. For example, the designer might calculate the number of distillation plates required for a distillation separation using elaborate calculations to a high degree of precision, only to add an arbitrary extra 10% to the number of plates for contingency. This allows for the feed to the unit not being exactly as specified, errors in the physical properties, upset conditions in the plant, control requirements, and so on. If too little contingency is added, the plant might not work. If too much contingency is added, the plant will not only be unnecessarily expensive but too much overdesign might make the plant difficult to operate and might lead to a less efficient plant. For example, the designer might calculate the size of a heat exchanger and then add in a large contingency and significantly oversize the heat exchanger. The lower fluid velocities encountered by the oversized heat exchanger can



(a) Process design starts with the synthesis of a process to convert raw materials into desired products.



(b) Simulation predicts how a process would behave if it was constructed.

Figure 1.2

Synthesis is the creation of a process to transform feed streams into product streams. Simulation predicts how it would behave if it was constructed.

cause it to have a poorer performance and to foul-up more readily than a smaller heat exchanger.

Too little overdesign might lead to the plant not working. Too much overdesign will lead to the plant becoming unnecessarily expensive, and perhaps difficult to operate and less efficient. A balance must be made between different risks.

2) *Physical properties in process design.* Almost all design calculations require physical properties of the solids, liquids and gases being fed, processed and produced. Physical properties can be critical to obtaining meaningful, economic and safe designs. When carrying out calculations in computer software packages there is most often a choice to be made for the physical property correlations and data. However, if poor decisions are made by the designer regarding physical properties, the design calculations can be meaningless or even dangerous, even though the calculations have been performed to a high level of precision. Using physical property correlations outside the ranges of conditions for which they were intended can be an equally serious problem. Appendix A discusses physical properties in process design in more detail.

3) *Evaluation of performance.* There are many facets to the evaluation of performance. Good economic performance is an obvious first criterion, but it is certainly not the only one. Chemical processes should be designed to maximize the *sustainability* of industrial activity. Maximizing sustainability requires that industrial systems should strive to satisfy human needs in an economically viable, environmentally benign and socially beneficial way (Azapagic, 2014). For chemical process design, this means that processes should make use of materials of construction that deplete the resource as little as practicable. Process raw materials should be used as efficiently as is economic and practicable, both to prevent the production of waste that can be environmentally harmful and to preserve the reserves of manufacturing raw materials as much as possible. Processes should use as little energy as is economic and practicable, both to prevent the build-up of carbon dioxide in the atmosphere from burning fossil fuels and to preserve the reserves of fossil fuels. Water must also be consumed in sustainable quantities that do not cause deterioration in the quality of the water source and the long-term quantity of the reserves. Aqueous and atmospheric emissions must not be environmentally harmful and solid waste to landfill must be avoided. The boundary of consideration should go beyond the immediate boundary of the manufacturing facility to maximize the benefit to society to avoid adverse health effects, unnecessarily high burdens on transportation, odour, noise nuisances, and so on.

The process must also meet required health and safety criteria. Start-up, emergency shutdown and ease of control are other important factors. Flexibility, that is, the ability to operate under different conditions, such as differences in feedstock and product specification, may be important. Availability, that is, the portion of the total time that the process meets its production requirements, might also be critically important.

Uncertainty in the design, for example, resulting from poor design data, or uncertainty in the economic data might guide the design away from certain options. Some of these factors, such as economic performance, can be readily quantified; others, such as safety, often cannot. Evaluation of the factors that are not readily quantifiable, the intangibles, requires the judgment of the design team.

4) *Materials of construction.* Choice of materials of construction affects both the mechanical design and the capital cost of equipment. Many factors enter into the choice of the materials of construction. Among the most important are (see Appendix B):

- mechanical properties (particularly yield and tensile strength, compressive strength, ductility, toughness, hardness, fatigue limit and creep resistance);
- effect of temperature on mechanical properties (both low and high temperatures),
- ease of fabrication (machining, welding, and so on);
- corrosion resistance;
- availability of standard equipment in the material;
- cost (e.g. if materials of construction are particularly expensive, it might be desirable to use a cheaper material together with a lining on the process side to reduce the cost).

Estimation of the capital cost and preliminary specification of equipment for the evaluation of performance requires decisions to be made regarding the materials of construction. The discussion of the more commonly used materials of construction is given in Appendix B.

5) *Process safety.* When evaluating a process design, process safety should be the prime consideration. Safety considerations must not be left until the design has been completed. Safety systems need to be added to the design later for the relief of overpressure, to trip the process under dangerous conditions, etc. However, by far the largest impact on process safety can be made early in the design through measures to make the design *inherently safer*. This will be discussed in detail in Chapter 28. Inherently safer design means avoiding the need for hazardous materials if possible, or using less of them, or using them at lower temperatures and pressures or diluting them with inert materials. One of the principal approaches to making a process inherently safer is to limit the inventory of hazardous material. The inventories to be avoided most of all are flashing flammable or toxic liquids, that is, liquids under pressure above their atmospheric boiling points (see Chapter 28).

6) *Optimization.* Once the basic performance of the design has been evaluated, changes can be made to improve the performance; the process is *optimized*. These changes might involve the synthesis of alternative structures, that is, *structural optimization*. Thus, the process is simulated and evaluated again, and so on, optimizing the structure. Each structure can be subjected to *parameter optimization* by changing operating conditions within that structure. This is illustrated in Figure 1.3.

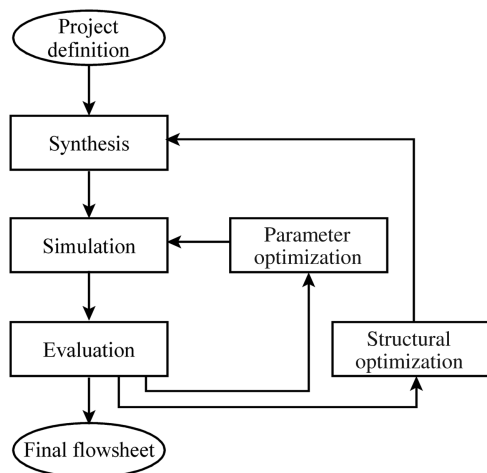


Figure 1.3

Optimization can be carried out as structural or parameter optimization to improve the evaluation of the design.

From the project definition an initial design is synthesized. This can then be simulated and evaluated. Once evaluated, the design can be optimized in a parameter optimization through changing the continuous parameters of flowrate, composition, temperature and pressure to improve the evaluation. However, this parameter optimization only optimizes the initial design configuration, which might not be an optimal configuration. So the design team might return to the synthesis stage to explore other configurations in a structural optimization. Also, if the parameter optimization adjusts the settings of the conditions to be significantly different from the original assumptions, then the design team might return to the synthesis stage to consider other configurations in the structural optimization. The different ways this design process can be followed will be considered later in this chapter.

- 7) *Keeping design options open.* To develop a design concept requires design options to be first generated and then evaluated. There is a temptation to carry out preliminary evaluation early in the development of a design and eliminate options early that initially appear to be unattractive. However, this temptation must be avoided. In the early stages of a design the uncertainties in the evaluation are often too serious for early elimination of options, unless it is absolutely clear that a design option is not viable. Initial cost estimates can be very misleading and the full safety and environmental implications of early decisions are only clear once detail has been added. If it was possible to foresee everything that lay ahead, decisions made early might well be different. There is a danger in focusing on one option without rechecking the assumptions later for validity when more information is available. The design team must not be boxed in early by preconceived ideas. This means that design options should be left open as long as practicable until it is clear that options can be closed down. All options should be considered, even if they appear unappealing at first.

1.4 The Hierarchy of Chemical Process Design and Integration

Consider the process illustrated in Figure 1.4 (Smith and Linnhoff, 1988). The process requires a reactor to transform the *FEED* into *PRODUCT* (Figure 1.4a). Unfortunately, not all the *FEED* reacts. Also, part of the *FEED* reacts to form *BYPRODUCT* instead of the desired *PRODUCT*. A separation system is needed to isolate the *PRODUCT* at the required purity. Figure 1.4b shows one possible separation system consisting of two distillation columns. The unreacted *FEED* in Figure 1.4b is recycled and the *PRODUCT* and *BYPRODUCT* are removed from the process. Figure 1.4b shows a flowsheet where all heating and cooling is provided by external *utilities* (steam and cooling water in this case). This flowsheet is probably too inefficient in its use of energy and heat should be recovered. Thus, *heat integration* is carried out to exchange heat between those streams that need to be cooled and those that need to be heated. Figure 1.5 (Smith and Linnhoff, 1988) shows two possible designs for the *heat exchanger network*, but many other heat integration arrangements are possible.

The flowsheets shown in Figure 1.5 feature the same reactor design. It could be useful to explore the changes in reactor design. For example, the size of the reactor could be increased to increase the amount of *FEED* that reacts (Smith and Linnhoff, 1988). Now there is not only much less *FEED* in the reactor effluent but also more *PRODUCT* and *BYPRODUCT*. However, the increase in *BYPRODUCT* is larger than the increase in *PRODUCT*. Thus, although the reactor has the same three components in its effluent as the reactor in Figure 1.4a, there is less *FEED*, more *PRODUCT* and significantly more *BYPRODUCT*. This change in reactor design generates a different task for the separation system and it is possible that a separation system different from that shown in Figures 1.4 and 1.5 is now appropriate. Figure 1.6 shows a possible alternative. This also uses two distillation columns, but the separations are carried out in a different order.

Figure 1.6 shows a flowsheet without any heat integration for the different reactor and separation system. As before, this is probably too inefficient in the use of energy, and heat integration schemes can be explored. Figure 1.7 (Smith and Linnhoff, 1988) shows two of the many possible flowsheets involving heat recovery.

Different complete flowsheets can be evaluated by simulation and costing. On this basis, the flowsheet in Figure 1.5b might be more promising than the flowsheets in Figures 1.5a and 1.7a and b. However, the best flowsheet cannot be identified without first optimizing the operating conditions for each. The flowsheet in Figure 1.7b might have greater scope for improvement than that in Figure 1.5b, and so on.

Thus, the complexity of chemical process synthesis is two-fold. First, can all possible structures be identified? It might be considered that all the structural options can be found by inspection, at least all of the significant ones. The fact that

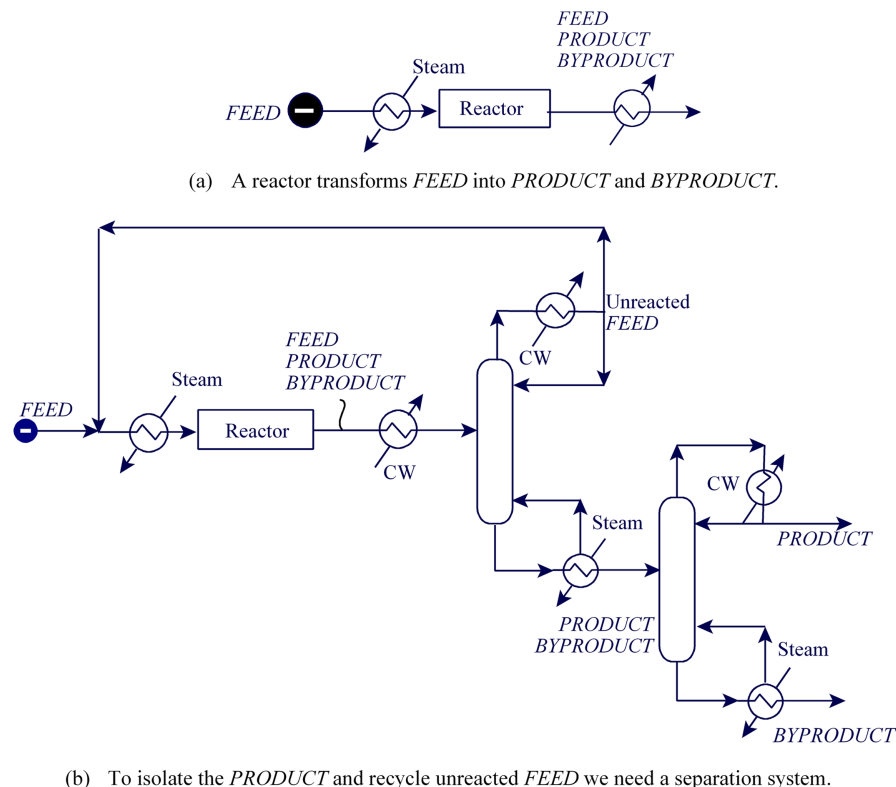


Figure 1.4

Process design starts with the reactor. The reactor design dictates the separation and recycle problem. (Reproduced from Smith R and Linnhoff B, 1998, *Trans IChemE ChERD*, 66: 195 by permission of the Institution of Chemical Engineers.)

even long-established processes are still being improved bears evidence to just how difficult this is. Second, can each structure be optimized for a valid comparison? When optimizing the structure, there may be many ways in which each individual task can be performed and many ways in which the individual tasks can be interconnected. This means that the operating conditions for a multitude of structural options must be simulated and optimized. At first sight, this appears to be an overwhelmingly complex problem.

It is helpful when developing a methodology if there is a clear picture of the nature of the problem. If the process requires a reactor, this is where the design starts. This is likely to be the only place in the process where raw material components are converted into components for the products. The chosen reactor design produces a mixture of unreacted feed materials, products and byproducts that need separating. Unreacted feed material is recycled. The reactor design dictates the separation and recycle problem. Thus, design of the separation and recycle system follows the reactor design. The reactor and separation and recycle system designs together define the process for heating and cooling duties. Thus, the heat exchanger network design comes next. Those heating and cooling duties that cannot be satisfied by heat recovery dictate the need for external heating and cooling *utilities*

(furnace heating, use of steam, steam generation, cooling water, air cooling or refrigeration). Thus, utility selection and design follows the design of the heat recovery system. The selection and design of the utilities is made more complex by the fact that the process will most likely operate within the context of a site comprising a number of different processes that are all connected to a common utility system. The process and the utility system will both need water, for example, for steam generation, and will also produce aqueous effluents that will have to be brought to a suitable quality for discharge. Thus, the design of the water and aqueous effluent treatment system comes last. Again, the water and effluent treatment system must be considered at the site level as well as the process level.

This hierarchy can be represented symbolically by the layers of the “onion diagram” shown in Figure 1.8 (Linnhoff *et al.*, 1982). The diagram emphasizes the sequential, or hierarchical, nature of process design. Other ways to represent the hierarchy have also been suggested (Douglas, 1985).

Some processes do not require a reactor, for example, some processes just involve separation. Here, the design starts with the separation system and moves outward to the heat exchanger network, utilities, and so on. However, the same basic hierarchy prevails.

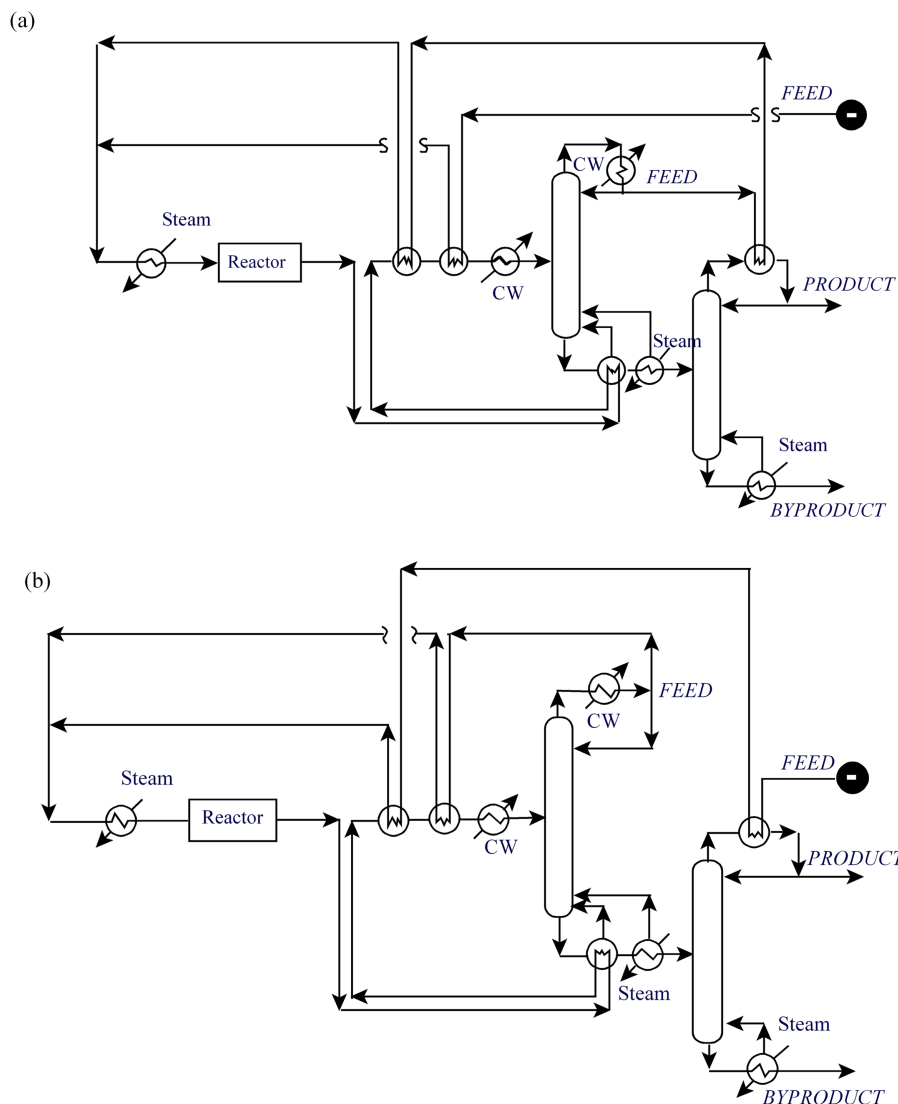


Figure 1.5

For a given reactor and separator design there are different possibilities for heat integration. (Reproduced from Smith R and Linnhoff B, 1998, *Trans IChemE ChERD*, 66: 195 by permission of the Institution of Chemical Engineers.)

The synthesis of the correct structure and the optimization of parameters in the design of the reaction and separation systems are often the most important tasks of process design. Usually there are many options, and it is impossible to fully evaluate them unless a complete design is furnished for the “outer layers” of the onion model. For example, it is not possible to assess which is better, the basic scheme from Figure 1.4b or that from Figure 1.6, without fully evaluating all possible designs, such as those shown in Figures 1.5a and b and 1.7a and b, all completed, including utilities. Such a complete search is normally too time-consuming to be practical.

Later, in Chapter 17, an approach will be presented in which some early decisions (i.e. decisions regarding reactor and separator options) can be evaluated without a complete design for the “outer layers”.

1.5 Continuous and Batch Processes

When considering the processes in Figures 1.4 to 1.6, an implicit assumption was made that the processes operated continuously. However, not all processes operate continuously. In a *batch* process, the main steps operate discontinuously. In contrast with a continuous process, a batch process does not deliver its product continuously but in discrete amounts. This means that heat, mass, temperature, concentration and other properties vary with time. In practice, most batch processes are made up of a series of batch and *semi-continuous* steps. A semi-continuous step runs continuously with periodic start-ups and shutdowns.

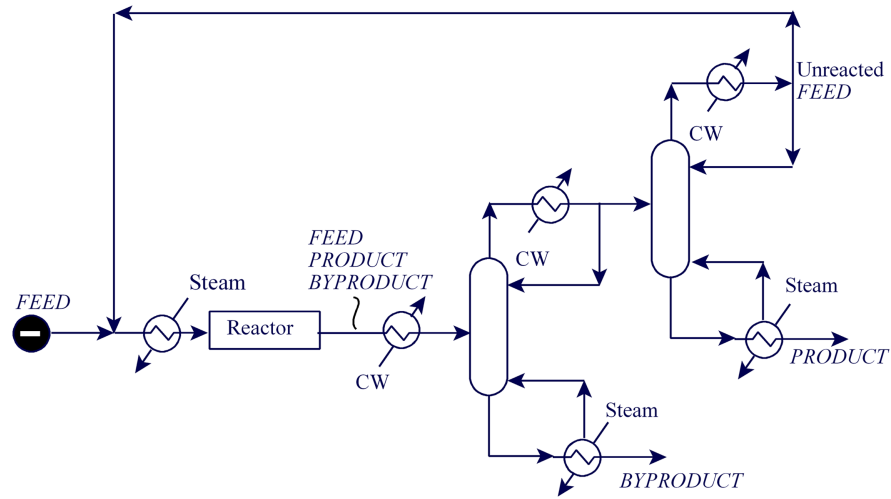


Figure 1.6

Changing the reactor dictates a different separation and recycle problem. (Reproduced from Smith R and Linnhoff B, 1998, *Trans IChemE ChERD*, 66: 195 by permission of the Institution of Chemical Engineers.)

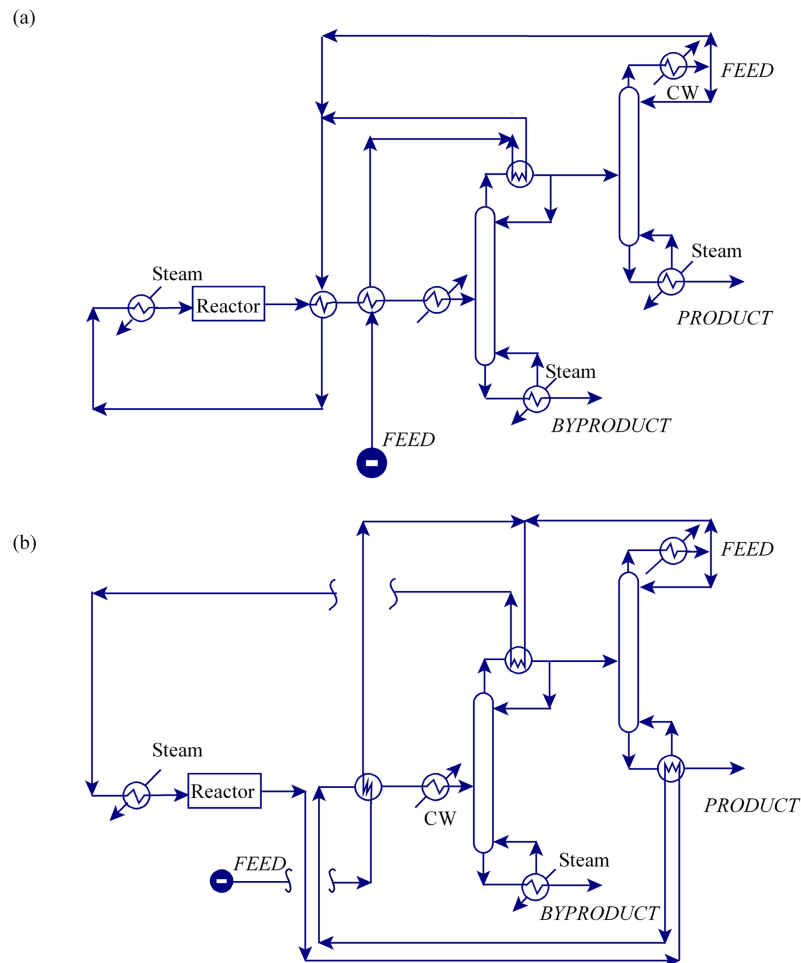


Figure 1.7

A different reactor design not only leads to a different separation system but additional possibilities for heat integration. (Reproduced from Smith R and Linnhoff B, 1998, *Trans IChemE ChERD*, 66: 195 by permission of the Institution of Chemical Engineers.)