CHEMICAL ENGINEERING

For additional information concerning heat transfer and fluid mechanics, refer to the **HEAT TRANSFER**, **THERMODYNAMICS**, **MECHANICAL ENGINEERING** or **FLUID MECHANICS** sections.

For additional information concerning chemical process control, refer to the **COMPUTERS, MEASUREMENT, AND CONTROLS** section.

For additonal information concerning statistical data analysis, refer to the following.

Confidence Intervals
See the subsection in the **ENGINEERING PROBABILITY AND STATISTICS** section of this handbook.

Statistical Quality Control
See the subsection in the **INDUSTRIAL ENGINEERING** section of this handbook.

Linear Regression
See the subsection in the **ENGINEERING PROBABILITY AND STATISTICS** section of this handbook.

One-Way Analysis of Variance (ANOVA)
See the subsection in the **INDUSTRIAL ENGINEERING** section of this handbook.

SELECTED RULES OF NOMENCLATURE IN ORGANIC CHEMISTRY

Alcohols

Three systems of nomenclature are in general use. In the first the alkyl group attached to the hydroxyl group is named and the separate word *alcohol* is added. In the second system the higher alcohols are considered as derivatives of the first member of the series, which is called *carbinol*. The third method is the modified Geneva system in which (1) the longest carbon chain containing the hydroxyl group determines the surname, (2) the ending *e* of the corresponding saturated hydrocarbon is replaced by *ol*, (3) the carbon chain is numbered from the end that gives the hydroxyl group the smaller number, and (4) the side chains are named and their positions indicated by the proper number. Alcohols in general are divided into three classes. In *primary* alcohols the hydroxyl group is united to a primary carbon atom, that is, a carbon atom united directly to only one other carbon atom. *Secondary* alcohols have the hydroxyl group united to a secondary carbon atom, that is, one united to two other carbon atoms. *Tertiary* alcohols have the hydroxyl group united to a tertiary carbon atom, that is, one united to three other carbon atoms.

Ethers

Ethers are generally designated by naming the alkyl groups and adding the word *ether*. The group RO is known as an *alkoxyl group*. Ethers may also be named as alkoxy derivatives of hydrocarbons.

Carboxylic Acids

The name of each linear carboxylic acid is unique to the number of carbon atoms it contains. 1: (one carbon atom) Formic. 2: Acetic. 3: Propionic. 4: Butyric. 5: Valeric. 6: Caproic. 7: Enanthic. 8: Caprylic. 9: Pelargonic. 10: Capric.

Aldehydes

The common names of aldehydes are derived from the acids which would be formed on oxidation, that is, the acids having the same number of carbon atoms. In general the *ic acid* is dropped and *aldehyde* added.

Ketones

The common names of ketones are derived from the acid which on pryrolysis would yield the ketone. A second method, especially useful for naming mixed ketones, simply names the alkyl groups and adds the word *ketone*. The name is written as three separate words.

Common Names and Molecular Formulas of Some Industrial (Inorganic and Organic) Chemicals

Common Name	Chemical Name	Molecular Formula
Muriatic acid	Hydrochloric acid	HCl
Cumene	Isopropyl benzene	$C_6H_5CH(CH_3)_2$
Styrene	Vinyl benzene	$C_6H_5CH = CH_2$
—	Hypochlorite ion	OCl^{-1}
—	Chlorite ion	ClO_2^{-1}
—	Chlorate ion	ClO_3^{-1}
—	Perchlorate ion	ClO_4^{-1}
Gypsum	Calcium sulfate	$CaSO_4$
Limestone	Calcium carbonate	$CaCO_3$
Dolomite	Magnesium carbonate	$MgCO_3$
Bauxite	Aluminum oxide	Al_2O_3
Anatase	Titanium dioxide	TiO_2
Rutile	Titanium dioxide	TiO_2
—	Vinyl chloride	$CH_2=CHCl$
—	Ethylene oxide	C_2H_4O
Pyrite	Ferrous sulfide	FeS
Epsom salt	Magnesium sulfate	$MgSO_4$
Hydroquinone	p-Dihydroxy benzene	$C_6H_4(OH)_2$
Soda ash	Sodium carbonate	Na_2CO_3
Salt	Sodium chloride	$NaCl$
Potash	Potassium carbonate	K_2CO_3
Baking soda	Sodium bicarbonate	$NaHCO_3$
Lye	Sodium hydroxide	$NaOH$
Caustic soda	Sodium hydroxide	$NaOH$
—	Vinyl alcohol	$CH_2=CHOH$
Carbolic acid	Phenol	C_6H_5OH
Aniline	Aminobenzene	$C_6H_5NH_2$
—	Urea	$(NH_2)_2CO$
Toluene	Methyl benzene	$C_6H_5CH_3$
Xylene	Dimethyl benzene	$C_6H_4(CH_3)_2$
—	Silane	SiH_4
—	Ozone	O_3
Neopentane	2,2-Dimethylpropane	$CH_3C(CH_3)_2CH_3$
Magnetite	Ferrous/ferric oxide	Fe_3O_4
Quicksilver	Mercury	Hg
Heavy water	Deuterium oxide	$(H^2)_2O$
—	Borane	BH_3
Eyewash	Boric acid (solution)	H_3BO_3
—	Deuterium	H^2
—	Tritium	H^3
Laughing gas	Nitrous oxide	N_2O
—	Phosgene	$COCl_2$
Wolfram	Tungsten	W
—	Permanganate ion	MnO_4^{-1}
—	Dichromate ion	$Cr_2O_7^{-2}$
—	Hydronium ion	H_3O^{+1}
Brine	Sodium chloride (solution)	$NaCl$
Battery acid	Sulfuric acid	H_2SO_4

CHEMICAL THERMODYNAMICS

Vapor-Liquid Equilibrium

For a multi-component mixture at equilibrium

$$\hat{f}_i^{V} = \hat{f}_i^{L}, \text{ where}$$

$\hat{f}_i^{V} =$ fugacity of component i in the vapor phase, and

$\hat{f}_i^{L} =$ fugacity of component i in the liquid phase.

Fugacities of component i in a mixture are commonly calculated in the following ways:

For a liquid $\quad \hat{f}_i^{L} = x_i \gamma_i f_i^{L}$, where

$x_i =$ mole fraction of component i,

$\gamma_i =$ activity coefficient of component i, and

$f_i^{L} =$ fugacity of pure liquid component i.

For a vapor $\quad \hat{f}_i^{V} = y_i \hat{\Phi}_i P$, where

$y_i =$ mole fraction of component i in the vapor,

$\hat{\Phi}_i =$ fugacity coefficient of component i in the vapor, and

$P =$ system pressure.

The activity coefficient γ_i is a correction for liquid phase non-ideality. Many models have been proposed for γ_i such as the Van Laar model:

$$\ln\gamma_1 = A_{12}\left(1 + \frac{A_{12}x_1}{A_{21}x_2}\right)^{-2}$$

$$\ln\gamma_2 = A_{21}\left(1 + \frac{A_{21}x_2}{A_{12}x_1}\right)^{-2}, \text{ where}$$

$\gamma_1 =$ activity coefficient of component 1 in a two-component system,

$\gamma_2 =$ activity coefficient of component 2 in a two-component system, and

$A_{12}, A_{21} =$ constants, typically fitted from experimental data.

The pure component fugacity is calculated as:

$$f_i^{L} = \Phi_i^{\text{sat}} P_i^{\text{sat}} \exp\{v_i^{L}(P - P_i^{\text{sat}})/(RT)\}, \text{ where}$$

$\Phi_i^{\text{sat}} =$ fugacity coefficient of pure saturated i,

$P_i^{\text{sat}} =$ saturation pressure of pure i,

$v_i^{L} =$ specific volume of pure liquid i, and

$R =$ Ideal Gas Law Constant.

Often at system pressures close to atmospheric:

$$f_i^{L} \cong P_i^{\text{sat}}$$

The fugacity coefficient $\hat{\Phi}_i$ for component i in the vapor is calculated from an equation of state (e.g., Virial). Sometimes it is approximated by a pure component value from a correlation. Often at pressures close to atmospheric, $\hat{\Phi}_i = 1$. The fugacity coefficient is a correction for vapor phase non-ideality.

For sparingly soluble gases the liquid phase is sometimes represented as

$$\hat{f}_i^{L} = x_i k_i$$

where k_i is a constant set by experiment (Henry's constant). Sometimes other concentration units are used besides mole fraction with a corresponding change in k_i.

Reactive Systems

Conversion: moles reacted/moles fed

Extent: For each species in a reaction, the mole balance may be written:

$\text{moles}_{i,\text{out}} = \text{moles}_{i,\text{in}} + v_i \xi$ where

ξ is the **extent** in moles and v_i is the stoichiometric coefficient of the ith species, sign of which is negative for reactants and positive for products.

Limiting reactant: reactant that would be consumed first if reaction proceeded to completion. Other reactants are **excess reactants**.

Selectivity: moles of desired product formed/moles of undesired product formed.

Yield: moles of desired product formed/moles that would have been formed if there were no side reactions and limiting reactant had reacted completely.

Chemical Reaction Equilibrium

For reaction
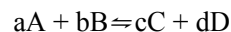
$$aA + bB \rightleftharpoons cC + dD$$
$$\Delta G^{\text{o}} = -RT \ln K_a$$
$$K_a = \frac{(\hat{a}_C^c)(\hat{a}_D^d)}{(\hat{a}_A^a)(\hat{a}_B^b)} = \prod_i (\hat{a}_i)^{v_i}, \text{ where}$$

$\hat{a}_i =$ activity of component i $= \dfrac{\hat{f}_i}{f_i^{\text{o}}}$

$f_i^{\text{o}} =$ fugacity of pure i in its standard state

$v_i =$ stoichiometric coefficient of component i

$\Delta G^{\text{o}} =$ standard Gibbs energy change of reaction

$K_a =$ chemical equilibrium constant

For mixtures of ideal gases:

f_i^o = unit pressure, often 1 bar

$$\hat{f}_i = y_i P = p_i$$

where p_i = partial pressure of component i.

Then $K_a = K_p = \dfrac{\left(p_C^c\right)\left(p_D^d\right)}{\left(p_A^a\right)\left(p_B^b\right)} = P^{c+d-a-b}\dfrac{\left(y_C^c\right)\left(y_D^d\right)}{\left(y_A^a\right)\left(y_B^b\right)}$

For solids $\hat{a}_i = 1$

For liquids $\hat{a}_i = x_i \gamma_i$

The effect of temperature on the equilibrium constant is

$$\frac{d\ln K}{dT} = \frac{\Delta H^o}{RT^2}$$

where ΔH^o = standard enthalpy change of reaction.

HEATS OF REACTION

For a chemical reaction the associated energy can be defined in terms of heats of formation of the individual species $\left(\Delta\hat{H}_f^o\right)$ at the standard state

$$\left(\Delta\hat{H}_r^o\right) = \sum_{\text{products}} \upsilon_i\left(\Delta\hat{H}_f^o\right)_i - \sum_{\text{reactants}} \upsilon_i\left(\Delta\hat{H}_f^o\right)_i$$

The standard state is 25°C and 1 bar.

The heat of formation is defined as the enthalpy change associated with the formation of a compound from its atomic species as they normally occur in nature (i.e., $O_{2(g)}$, $H_{2(g)}$, $C_{(solid)}$, etc.)

The heat of reaction for a combustion process using oxygen is also known as the heat of combustion. The principal products are $CO_{2(g)}$ and $H_2O_{(\ell)}$.

CHEMICAL REACTION ENGINEERING

A chemical reaction may be expressed by the general equation

$$a\text{A} + b\text{B} \leftrightarrow c\text{C} + d\text{D}.$$
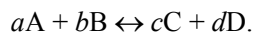
The rate of reaction of any component is defined as the moles of that component formed per unit time per unit volume.

$$-r_A = -\frac{1}{V}\frac{dN_A}{dt} \qquad \text{[negative because A disappears]}$$

$$-r_A = \frac{-dC_A}{dt} \qquad \text{if V is constant}$$

The rate of reaction is frequently expressed by

$$-r_A = kf_r\,(C_A, C_B,....), \text{ where}$$

k = reaction rate constant and

C_I = concentration of component I.

In the conversion of A, the fractional conversion X_A is defined as the moles of A reacted per mole of A fed.

$$X_A = (C_{Ao} - C_A)/C_{Ao} \qquad \text{if V is constant}$$

The Arrhenius equation gives the dependence of k on temperature

$$k = Ae^{-E_a/\bar{R}T}, \text{ where}$$

A = pre-exponential or frequency factor,

E_a = activation energy (J/mol, cal/mol),

T = temperature (K), and

$\bar{R}$ = gas law constant = 8.314 J/(mol·K).

For values of rate constant (k_i) at two temperatures (T_i),

$$E_a = \frac{RT_1T_2}{(T_1 - T_2)}\ln\left(\frac{k_1}{k_2}\right)$$

Reaction Order

If $-r_A = kC_A^x C_B^y$

the reaction is x order with respect to reactant A and y order with respect to reactant B. The overall order is

$$n = x + y$$

BATCH REACTOR, CONSTANT T AND V

Zero-Order Reaction

$-r_A$	$=$	$kC_A^o = k\,(1)$	
$-dC_A/dt$	$=$	k	or
C_A	$=$	$C_{Ao} - kt$	
dX_A/dt	$=$	k/C_{Ao}	or
$C_{Ao}X_A$	$=$	kt	

First-Order Reaction

$-r_A$	$=$	kC_A	
$-dC_A/dt$	$=$	kC_A	or
$\ln(C_A/C_{Ao})$	$=$	$-kt$	
dX_A/dt	$=$	$k\,(1 - X_A)$	or
$\ln(1 - X_A)$	$=$	$-kt$	

Second-Order Reaction

$-r_A$	$=$	kC_A^2	
$-dC_A/dt$	$=$	kC_A^2	or
$1/C_A - 1/C_{Ao}$	$=$	kt	
dX_A/dt	$=$	$kC_{Ao}\,(1 - X_A)^2$	or
$X_A/[C_{Ao}\,(1 - X_A)]$	$=$	kt	

Batch Reactor, General

For a well-mixed, constant-volume, batch reactor

$$-\mathbf{r}_A = -dC_A/dt$$

$$t = -C_{Ao}\int_o^{X_A} dX_A/(-r_A)$$

If the volume of the reacting mass varies with the conversion (such as a variable-volume batch reactor) according to

$$V = V_{X_{A=0}}(1+\varepsilon_A X_A)$$

(ie., at constant pressure), where

$$\varepsilon_A = \frac{V_{X_A=1} - V_{X_A=0}}{V_{X_A=0}}$$

then at any time

$$C_A = C_{Ao}\left[\frac{1-X_A}{1+\varepsilon_A X_A}\right]$$

and

$$t = -C_{Ao}\int_o^{X_A} dX_A/[(1+\varepsilon_A X_A)(-r_A)]$$

For a first order irreversible reaction,

$$kt = -\ln(1-X_A) = -\ln\left(1-\frac{\Delta V}{\varepsilon_A V_{XA=O}}\right)$$

FLOW REACTORS, STEADY STATE

Space-time τ is defined as the reactor volume divided by the inlet volumetric feed rate. Space-velocity SV is the reciprocal of space-time, $SV = 1/\tau$.

Plug-Flow Reactor (PFR)

$$\tau = \frac{C_{Ao}V_{PFR}}{F_{Ao}} = C_{Ao}\int_o^{X_A}\frac{dX_A}{(-r_A)}, \text{ where}$$

F_{Ao} = moles of A fed per unit time.

Continuous Stirred Tank Reactor (CSTR)

For a constant volume, well-mixed, CSTR

$$\frac{\tau}{C_{Ao}} = \frac{V_{CSTR}}{F_{Ao}} = \frac{X_A}{-r_A}, \text{ where}$$

$-r_A$ is evaluated at exit stream conditions.

Continuous Stirred Tank Reactors in Series

With a first-order reaction $A \rightarrow R$, no change in volume.

$$\tau_{N\text{-reactors}} = N\tau_{individual}$$

$$= \frac{N}{k}\left[\left(\frac{C_{Ao}}{C_{AN}}\right)^{1/N} - 1\right], \text{ where}$$

N = number of CSTRs (equal volume) in series, and

C_{AN} = concentration of A leaving the Nth CSTR.

MASS TRANSFER

Diffusion

Molecular Diffusion

Gas: $\dfrac{N_A}{A} = \dfrac{p_A}{P}\left(\dfrac{N_A}{A} + \dfrac{N_B}{A}\right) - \dfrac{D_m}{RT}\dfrac{\partial p_A}{\partial z}$

Liquid: $\dfrac{N_A}{A} = x_A\left(\dfrac{N_A}{A} + \dfrac{N_B}{A}\right) - CD_m\dfrac{\partial x_A}{\partial z}$

in which $(p_B)_{lm}$ is the log mean of p_{B2} and p_{B1},

Unidirectional Diffusion of a Gas A Through a Second Stagnant Gas B ($N_b = 0$)

$$\frac{N_A}{A} = \frac{D_m P}{\overline{R}T(p_B)_{lm}} \times \frac{(p_{A2} - p_{A1})}{z_2 - z_1}$$

in which $(p_B)_{lm}$ is the log mean of p_{B2} and p_{B1},

N_i = diffusive flow (mole/time) of component i through area A, in z direction, and

D_m = mass diffusivity.

EQUIMOLAR COUNTER-DIFFUSION (GASES)

($N_B = -N_A$)

$$N_A/A = D_m/(\overline{R}T) \times \left[(p_{A1} - p_{A2})/(\Delta z)\right]$$

$$N_A/A = D_m(C_{A1} - C_{A2})/\Delta z$$

CONVECTION

Two-Film Theory (for Equimolar Counter-Diffusion)

$$
\begin{aligned}
N_A/A &= k'_G(p_{AG} - p_{Ai}) \\
&= k'_L(C_{Ai} - C_{AL}) \\
&= K'_G(p_{AG} - p_A^*) \\
&= K'_L(C_A^* - C_{AL})
\end{aligned}
$$

where p_A^* is partial pressure in equilibrium with C_{AL}, and

C_A^* = concentration in equilibrium with p_{AG}.

Overall Coefficients

$$1/K'_G = 1/k'_G + H/k'_L$$

$$1/K'_L = 1/Hk'_G + 1/k'_L$$

Dimensionless Group Equation (Sherwood)

For the turbulent flow inside a tube the Sherwood number

$$\left(\frac{k_m D}{D_m}\right) \text{ is given by: } \left(\frac{k_m D}{D_m}\right) = 0.023\left(\frac{DV\rho}{\mu}\right)^{0.8}\left(\frac{\mu}{\rho D_m}\right)^{1/3}$$

where,

D = inside diameter,

D_m = diffusion coefficient,

V = average velocity in the tube,

ρ = fluid density, and

μ = fluid viscosity,

k_m = mass transfer coefficient.

Distillation

Definitions:

α = relative volatility,

B = molar bottoms-product rate,

D = molar overhead-product rate,

F = molar feed rate,

L = molar liquid downflow rate,

R_D = ratio of reflux to overhead product,

V = molar vapor upflow rate,

W = total moles in still pot,

x = mole fraction of the more volatile component in the liquid phase, and

y = mole fraction of the more volatile component in the vapor phase.

Subscripts:

B = bottoms product,

D = overhead product,

F = feed,

m = any plate in stripping section of column,

$m+1$ = plate below plate m,

n = any plate in rectifying section of column,

$n+1$ = plate below plate n, and

o = original charge in still pot.

Flash (or equilibrium) Distillation

Component material balance:

$$Fz_F = yV + xL$$

Overall material balance:

$$F = V + L$$

Differential (Simple or Rayleigh) Distillation

$$\ln\left(\frac{W}{W_o}\right) = \int_{x_o}^{x} \frac{dx}{y - x}$$

When the relative volatility α is constant,

$$y = \alpha x/[1 + (\alpha - 1)\,x]$$

can be substituted to give

$$\ln\left(\frac{W}{W_o}\right) = \frac{1}{(\alpha - 1)}\ln\left[\frac{x(1 - x_o)}{x_o(1 - x)}\right] + \ln\left[\frac{1 - x_o}{1 - x}\right]$$

For binary system following Raoult's Law

$$\alpha = (y/x)_a/(y/x)_b = p_a/p_b, \text{ where}$$

p_i = partial pressure of component i.

Continuous Distillation (binary system)

Constant molal overflow is assumed (trays counted downward)

OVERALL MATERIAL BALANCES

Total Material:

$$F = D + B$$

Component A:

$$Fz_F = Dx_D + Bx_B$$

OPERATING LINES

Rectifying Section

Total Material:

$$V_{n+1} = L_n + D$$

Component A:

$$V_{n+1}y_{n+1} = L_n x_n + Dx_D$$

$$y_{n+1} = [L_n/(L_n + D)]\,x_n + Dx_D/(L_n + D)$$

Stripping Section

Total Material:

$$L_m = V_{m+1} + B$$

Component A:

$$L_m x_m = V_{m+1}y_{m+1} + Bx_B$$

$$y_{m+1} = [L_m/(L_m - B)]\,x_m - Bx_B/(L_m - B)$$

Reflux Ratio

Ratio of reflux to overhead product

$$R_D = L_R/D = (V_R - D)/D$$

Minimum reflux ratio is defined as that value which results in an infinite number of contact stages. For a binary system the equation of the operating line is

$$y = \frac{R_{\min}}{R_{\min} + 1}x + \frac{x_D}{R_{\min} + 1}$$

*Feed Condition Line*

slope = $q/(q - 1)$, where

$$q = \frac{\text{heat to convert one mol of feed to saturated vapor}}{\text{molar heat of vaporization}}$$

Murphree Plate Efficiency

$$E_{ME} = (y_n - y_{n+1})/(y^*_n - y_{n+1}), \text{ where}$$

y = concentration of vapor above plate n,

y_{n+1} = concentration of vapor entering from plate below n, and

y^*_n = concentration of vapor in equilibrium with liquid leaving plate n.

A similar expression can be written for the stripping section by replacing n with m.

COST ESTIMATION

Cost Indexes
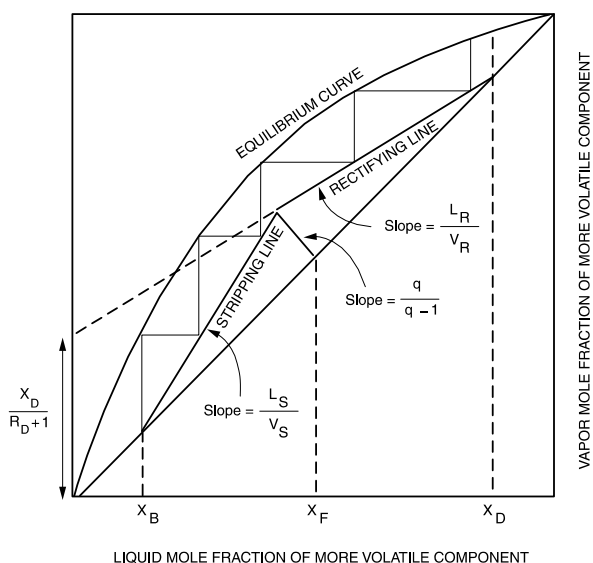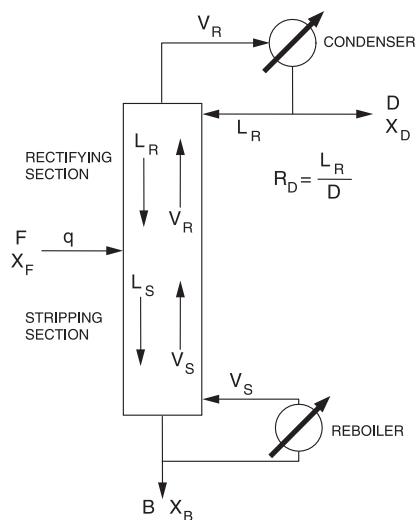
Cost Indexes as Annual Averages		
Year	Marshall and Swift installed-equipment index for the process industry, 1926 = 100	Chemical engineering plant cost index 1957–1959 = 100
1950	167	79
1960	237	102
1970	301	126
1980	675	261
1990	924	356
2000	1,108	394

Other Mass Transfer Operations

For additional information concerning solid/fluid separators, membrane separations, and air stripping, refer to the **ENVIRONMENTAL ENGINEERING** section.

Cost Segments of Fixed-Capital Investment

Component	Range
Direct costs	
Purchased equipment-delivered (including fabricated equipment and process machinery such as pumps and compressors)	100
Purchased-equipment installation	39–47
Instrumentation and controls (installed)	9–18
Piping (installed)	16–66
Electrical (installed)	10–11
Buildings (including services)	18–29
Yard improvements	10–13
Service facilities (installed)	40–70
Land (if purchase is required)	6
Total direct plant cost	264–346
Indirect costs	
Engineering and supervision	32–33
Construction expenses	34–41
Total direct and indirect plant costs	336–420
Contractor's fee (about 5% of direct and indirect plant costs)	17–21
Contingency (about 10% of direct and indirect plant costs)	36–42
Fixed-capital investment	387–483
Working capital (about 15% of total capital investment)	68–86
Total capital investment	455–569

Scaling of Equipment Costs

The cost of Unit A at one capacity related to the cost of a similar Unit B with X times the capacity of Unit A is approximately X^n times the cost of Unit B.

$$\text{Cost of Unit A} = \text{cost of Unit B}\left(\frac{\text{capacity of Unit A}}{\text{capacity of Unit B}}\right)^n$$

TYPICAL EXPONENTS (n) FOR EQUIPMENT COST VS. CAPACITY		
Equipment	**Size range**	**Exponent**
Dryer, drum, single vacuum	$10–10^2$ ft^2	0.76
Dryer, drum, single atmospheric	$10–10^2$ ft^2	0.40
Fan, centrifugal	$10^3–10^4$ ft^3/min	0.44
Fan, centrifugal	$2 \times 10^4 – 7 \times 10^4$ ft^3/min	1.17
Heat exchanger, shell and tube, floating head, c.s.	100–400 ft^2	0.60
Heat exchanger, shell and tube, fixed sheet, c.s.	100–400 ft^2	0.44
Motor, squirrel cage, induction, 440 volts, explosion proof	5–20 hp	0.69
Motor, squirrel cage, induction, 440 volts, explosion proof	20–200 hp	0.99
Tray, bubble cup, c.s.	3–10 ft diameter	1.20
Tray, sieve, c.s.	3–10 ft diameter	0.86

CHEMICAL PROCESS SAFETY

Threshold Limit Value (TLV)

TLV is the lowest dose (ppm by volume in the atmosphere) the body is able to detoxify without any detectable effects. Examples are:

Compound	TLV
Ammonia	25
Chlorine	0.5
Ethyl Chloride	1,000
Ethyl Ether	400

Flammability

LFL = lower flammability limit (volume % in air)

UFL = upper flammability limit (volume % in air)

A vapor-air mixture will only ignite and burn over the range of concentrations between LFL and UFL. Examples are:

Compound	LFL	UFL
Ethyl alcohol	3.3	19
Ethyl ether	1.9	36.0
Ethylene	2.7	36.0
Methane	5	15
Propane	2.1	9.5

Concentrations of Vaporized Liquids

Vaporization Rate (Q_m, mass/time) from a Liquid Surface

$$Q_m = [MKA_S P^{sat}/(R_g T_L)]$$

M = molecular weight of volatile substance
K = mass transfer coefficient
A_S = area of liquid surface
P^{sat} = saturation vapor pressure of the pure liquid at T_L
R_g = ideal gas constant
T_L = absolute temperature of the liquid

Mass Flow Rate of Liquid from a Hole in the Wall of a Process Unit

$$Q_m = A_H C_o (2\rho g_c P_g)^{1/2}$$

A_H = area of hole
C_o = discharge coefficient
ρ = density of the liquid
g_c = gravitational constant
P_g = gauge pressure within the process unit

Concentration (C_{ppm}) of Vaporized Liquid in
Ventilated Space

$$C_{ppm} = [Q_m R_g T \times 10^6/(kQ_V PM)]$$

T = absolute ambient temperature
k = nonideal mixing factor
Q_V = ventilation rate
P = absolute ambient pressure

Concentration in the Atmosphere

See "Atmospheric Dispersion Modeling" under
AIR POLLUTION in the **ENVIRONMENTAL ENGINEERING** section.

Sweep-Through Concentration Change in a Vessel

$$Q_V t = V\ln[(C_1 - C_o)/(C_2 - C_o)]$$

Q_V = volumetric flow rate
t = time
V = vessel volume
C_o = inlet concentration
C_1 = initial concentration
C_2 = final concentration