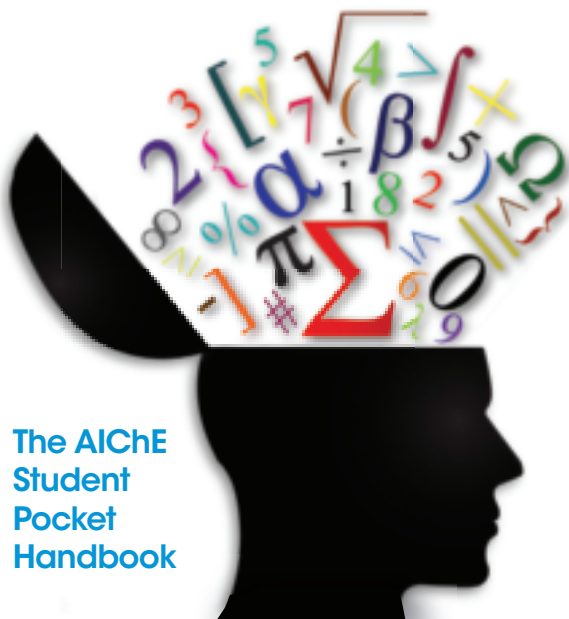


ChemE

Calculations

Formulas

Definitions



The AIChE
Student
Pocket
Handbook

The AIChE Pocket Handbook

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Foreword

The purpose of this handbook is to make readily available in a limited number of pages some of the more important chemical, biological, physical, safety, and mathematical data and concepts that are fundamental to the practice of the chemical engineering profession.

With these principles you should be able to solve many chemical engineering problems.

Good Luck!

AICHE would like to thank Professors David Murhammer, Chuck Coronella, Galen Suppes, and Joseph F. Louvar for their work on this Handbook.

INORGANIC CHEMISTRY

I. COMMON DEFINITIONS

Atomic number—the number of protons in the nucleus of an atom.

Avogadro's number—the number of molecules (6.023×10^{23}) in one gram-mole of a substance.

Equilibrium constants for the reaction $aA + bB = cC + dD$

where reaction is in solution,

$$K_c = \frac{[C]^c[D]^d}{[A]^a[B]^b} \quad ([] \text{ refers to molarity})$$

where reaction is in the gas phase,

$$K_p = \frac{p_C^c p_D^d}{p_A^a p_B^b} \quad (p = \text{partial pressure})$$

Gram equivalent weight—

A. (nonredox reaction) the mass in grams of a substance equivalent to 1 gram-atom of hydrogen, 0.5 gram-atom of oxygen, or 1 gram-ion of the hydroxyl ion. It can be determined by dividing the molecular weight by the number of hydrogen atoms or hydroxyl ions (or their equivalent) supplied or required by the molecule in a given reaction.

B. (redox reaction) the molecular weight in grams divided by the change in oxidation state.

Ion product of water (K_w)—the product of the hydrogen ion and hydroxyl ion concentrations in gram-ions per liter;

$$K_w = [H^+][OH^-]$$

Mass number—the number of protons plus the number of neutrons in the nucleus of an atom.

Molality (m)—(gram moles of solute)/(kilograms of solvent).

Molarity (M)—(gram moles of solute)/(liters of solution).

Normality (N)—(gram equivalents of solute)/(liters of solution).

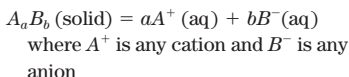
Oxidation—the loss of electrons by an atom or group of atoms.

pH—the negative logarithm (base 10) of the hydrogen ion concentration in gram ions per liter;

$$pH = -\log_{10}[H^+]$$

Reduction—the gain of electrons by an atom or group of atoms.

Solubility product (S.P. or K_{sp})—for the slightly soluble solid, A_aB_b , dissolving



S.P. or $K_{sp} = [A^+]^a[B^-]^b = \text{a constant at a given temperature}$

II. PROPERTIES OF CHEMICAL ELEMENTS

Name	Symbol	Atomic Number	Atomic Weight	Common Valence
Actinium	Ac	89	(227)	3
Aluminum	Al	13	26.9815	3
Americium	Am	95	(243)	6,5,4,3
Antimony	Sb	51	121.75	$\pm 3,5$

Name	Symbol	Atomic Number	Atomic Weight	Common Valence
Argon	Ar	18	39.948	0
Arsenic	As	33	74.9216	$\pm 3,5$
Astatine	At	85	(210)	$\pm 1,3,5,7$
Barium	Ba	56	137.34	2
Berkelium	Bk	97	(247)	4,3
Beryllium	Be	4	9.0122	2
Bismuth	Bi	83	208.980	3,5
Boron	B	5	10.811	3
Bromine	Br	35	79.904	$\pm 1,5$
Cadmium	Cd	48	112.40	2
Calcium	Ca	20	40.08	2
Californium	Cf	98	(249)	3
Carbon	C	6	12.01115	$\pm 4,2$
Cerium	Ce	58	140.12	3,4
Cesium	Cs	55	132.905	1
Chlorine	Cl	17	35.453	$\pm 1,3,5,7$
Chromium	Cr	24	51.996	6,2,3
Cobalt	Co	27	58.9332	2,3
Copper	Cu	29	63.546	2,1
Curium	Cm	96	(247)	3
Dysprosium	Dy	66	162.50	3
Einsteinium	Es	99	(254)	—
Erbium	Er	68	167.26	3
Europium	Eu	63	151.96	3,2
Fermium	Fm	100	(253)	—
Fluorine	F	9	18.9984	-1
Francium	Fr	87	(223)	1
Gadolinium	Gd	64	157.25	3
Gallium	Ga	31	69.72	3
Germanium	Ge	32	72.59	4
Gold	Au	79	196.967	3,1
Hafnium	Hf	72	178.49	4
Helium	He	2	4.0026	0
Holmium	Ho	67	164.930	3

Name	Symbol	Atomic Number	Atomic Weight	Common Valence
Hydrogen	H	1	1.00797	1
Indium	In	49	114.82	3
Iodine	I	53	126.9044	$\pm 1, 5, 7$
Iridium	Ir	77	192.2	2, 3, 4, 6
Iron	Fe	26	55.847	2, 3
Krypton	Kr	36	83.80	0
Lanthanum	La	57	138.91	3
Lawrencium	Lw	103	(257)	—
Lead	Pb	82	207.19	4, 2
Lithium	Li	3	6.939	1
Lutetium	Lu	71	174.97	3
Magnesium	Mg	12	24.312	2
Manganese	Mn	25	54.9380	7, 6, 4, 2, 3
Mendelevium	Md	101	(256)	—
Mercury	Hg	80	200.59	2, 1
Molybdenum	Mo	42	95.94	6, 5, 4, 3, 2
Neodymium	Nd	60	144.24	3
Neon	Ne	10	20.183	0
Neptunium	Np	93	(237)	6, 5, 4, 3
Nickel	Ni	28	58.71	2, 3
Niobium	Nb	41	92.906	5, 3
Nitrogen	N	7	14.0067	$\pm 3, 5, 4, 2$
Nobelium	No	102	(254)	—
Osmium	Os	76	190.2	2, 3, 4, 6, 8
Oxygen	O	8	15.9994	-2
Palladium	Pd	46	106.4	2, 4
Phosphorus	P	15	30.9738	$\pm 3, 5, 4$
Platinum	Pt	78	195.09	2, 4
Plutonium	Pu	94	(242)	6, 5, 4, 3
Polonium	Po	84	(210)	2, 4
Potassium	K	19	39.102	1
Praseodymium	Pr	59	140.907	3, 4
Promethium	Pm	61	(147)	3

Name	Symbol	Atomic Number	Atomic Weight	Common Valence
Protactinium	Pa	91	(231)	5,4
Radium	Ra	88	(226)	2
Radon	Rn	86	(222)	—
Rhenium	Re	75	186.2	7,6,4, 2, -1
Rhodium	Rh	45	102.905	2,3,4
Rubidium	Rb	37	85.47	1
Ruthenium	Ru	44	101.07	2,3,4,6,8
Samarium	Sm	62	150.35	3,2
Scandium	Sc	21	44.956	3
Selenium	Se	34	78.96	-2,4,5
Silicon	Si	14	28.086	4
Silver	Ag	47	107.870	1
Sodium	Na	11	22.9898	1
Strontium	Sr	38	87.62	2
Sulfur	S	16	32.064	± 2 ,4,6
Tantalum	Ta	73	180.948	5
Technetium	Tc	43	(98)	7
Tellurium	Te	52	127.60	-2,4,6
Terbium	Tb	65	158.924	3,4
Thallium	Tl	81	204.37	3,1
Thorium	Th	90	232.038	4
Thulium	Tm	69	168.934	3,2
Tin	Sn	50	118.69	4,2
Titanium	Ti	22	47.90	4,3
Tungsten	W	74	183.85	6,5,4,3,2
Uranium	U	92	238.03	6,5,4,3
Vanadium	V	23	50.942	5,4,3,2
Xenon	Xe	54	131.30	0
Ytterbium	Yb	70	173.04	3,2
Yttrium	Y	39	88.905	3
Zinc	Zn	30	65.37	2
Zirconium	Zr	40	91.22	4

III. COMMON ANIONS

Name	Symbol	Name	Symbol
Arsenite	AsO_3^-	Hydroxide	OH^-
Arsenate	AsO_4^-	Hypochlorite	OCl^-
Acetate	$\text{C}_2\text{H}_3\text{O}_2^-$	Iodide	I^-
Bicarbonate	HCO_3^-	Iodate	IO_3^-
Bisulfate	HSO_4^-	Molybdate	MoO_4^-
Bromate	BrO_3^-	Nitrate	NO_3^-
Bromide	Br^-	Nitrite	NO_2^-
Carbonate	CO_3^-	Oxalate	C_2O_4^-
Chlorate	ClO_3^-	Perchlorate	ClO_4^-
Chloride	Cl^-	Peroxide	O_2^-
Chromate	CrO_4^-	Permanganate	MnO_4^-
Cyanamide	CN_2^-	Phosphate	PO_4^-
Cyanide	CN^-	Sulfate	SO_4^-
Dichromate	Cr_2O_7^-	Sulfide	S^-
Dithionate	S_2O_6^-	Sulfite	SO_3^-
Ferricyanide	$\text{Fe}(\text{CN})_6^-$	Thiocyanate	CNS^-
Ferrocyanide	$\text{Fe}(\text{CN})_6^{--}$	Thiosulfate	S_2O_3^-
Formate	CHO_2^-		

ORGANIC CHEMISTRY

Note: For conciseness the following symbols are used:

R = H atom or saturated hydrocarbon group

R' = hydrocarbon group only

X = halogen

n = an integer

I. GENERAL CLASSES OF COMPOUNDS

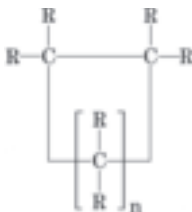
A. The straight and branched chain types of compounds

Type or Name	General Formula
1. Alkane or paraffin (also saturated hydrocarbons)	$ \begin{array}{c} \text{R} \quad \text{R} \\ \diagdown \quad \diagup \\ \text{C} \\ \diagup \quad \diagdown \\ \text{R} \quad \text{R} \end{array} $
2. Alkene or olefin (unsaturated hydrocarbons)	$ \begin{array}{c} \text{R} \quad \quad \text{R} \\ \diagdown \quad \diagup \\ \text{C} = \text{C} \\ \diagup \quad \diagdown \\ \text{R} \quad \quad \text{R} \end{array} $
3. Alkyne	$\text{R}-\text{C}\equiv\text{C}-\text{R}$
4. Alcohol	$ \begin{array}{c} \text{R} \quad \text{OH} \\ \diagdown \quad \diagup \\ \text{C} \\ \diagup \quad \diagdown \\ \text{R} \quad \text{R} \end{array} $
5. Ether	$\text{R}'-\text{O}-\text{R}'$
6. Aldehyde	$ \begin{array}{c} \text{H} \\ \\ \text{R}-\text{C}-\text{O} \end{array} $
7. Ketone	$ \begin{array}{c} \text{O} \\ \\ \text{R}'-\text{C}-\text{R}' \end{array} $
8. Carboxylic Acid	$ \begin{array}{c} \text{O} \\ \\ \text{R}-\text{C}-\text{OH} \end{array} $
9. Grignard reagent	$ \begin{array}{c} \text{R} \\ \\ \text{R}-\text{C}-\text{Mg}-\text{X} \\ \\ \text{R} \end{array} $
10. Acyl halide	$ \begin{array}{c} \text{O} \\ \\ \text{R}'-\text{C}-\text{X} \end{array} $

Type or Name	General Formula
11. Anhydride	$\text{R}-\overset{\text{O}}{\parallel}{\text{C}}-\text{O}-\overset{\text{O}}{\parallel}{\text{C}}-\text{R}$
12. Ester	$\text{R}-\overset{\text{O}}{\parallel}{\text{C}}-\text{O}-\underset{\text{R}}{\overset{\text{R}}{\text{C}}}-\text{R}$
13. Amide	$\text{R}-\overset{\text{O}}{\parallel}{\text{C}}-\text{NH}_2$
14. Amine (base)	$\begin{array}{c} \text{R} \quad \text{R} \\ \diagdown \quad \diagup \\ \text{C} \\ \diagup \quad \diagdown \\ \text{R} \quad \text{NH}_2 \end{array}$
15. Nitrile	$\begin{array}{c} \text{R} \quad \text{R} \\ \diagdown \quad \diagup \\ \text{C} \\ \diagup \quad \diagdown \\ \text{R} \quad \text{C}=\text{N} \end{array}$

B. Cyclic Compounds

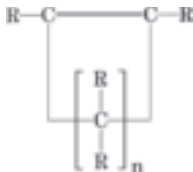
1. Cycloparaffin



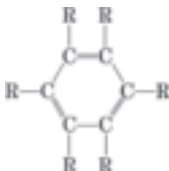
Type or Name

General Formula

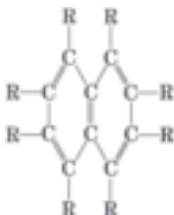
2. Cycloalkene



3. Aromatic



4. Naphthalenic



II. PERTINENT NOTES

- A. Markovnikov's (Markownikoff's) Rule for the addition of acids to acids to olefins: the negative group of the acid adds to the carbon atom having the fewest hydrogen atoms.

B. Mechanisms

1. Free radical (unshared electron)
(no charge)



2. Carbonium ion (deficient in electrons)
(positive charge)
(carbon with six electrons)



3. Carbanion
(excess of electrons)
(negative charge)
(carbon with eight electrons)



PHYSICAL CHEMISTRY

1. Amagat's Law of Partial Volumes—The volume of a mixture of gases is equal to the sum of the partial volumes of each component gas. The partial volume of a component gas is the volume which that component would occupy at the same temperature and pressure.
2. Boiling Point Elevation (ΔT_b)—The following equations hold for a dilute solution of a nonionic non-volatile solute.

$$\Delta T_b = K_b m$$

$$K_b = \frac{R(T_{bp})^2 M_a}{\Delta H_v (1000)}$$

where ΔH_v = molal heat of vaporization

K_b = molal boiling point elevation constant

m = molality

M_a = solvent molecular weight

R = ideal-gas constant

T_{bp} = solvent boiling point, absolute temperature

3. Clausius Equation

$$\frac{dp}{dT} = \frac{\Delta H_m}{(V - v)T}$$

where

p = pressure

T = absolute temperature

ΔH_m = molal heat of vaporization

V = molar vapor volume

v = molal liquid volume

4. Clausius-Clapeyron Equation—Where the volume of liquid can be ignored (or $v = 0$) and where the ideal-gas law holds (or $V = RT/p$) the Clausius equation becomes

$$\frac{d(\ln p)}{dT} = \frac{1}{p} \frac{dp}{dT} = \frac{\Delta H_m}{RT^2}$$

and with $\Delta H_m = \text{constant}$, integration yields

$$\ln \frac{p_2}{p_1} = \frac{\Delta H_m}{R} \left[\frac{T_2 - T_1}{T_1 T_2} \right]$$

The symbols are the same as in sections 2 and 3 above.

5. Dalton's Law of Partial Pressures—The pressure of a mixture of gases is equal to the sum of the partial pressures of each component gas. The partial pressure of a component gas is the pressure which that component would exert if it alone occupied the volume at the same temperature.

6. Faraday's Laws

First Law: The mass of a substance reacting at the electrodes is directly proportional to the quantity of electricity passed through the solution.

Second Law: The masses of different substances produced during electrolysis are directly proportional to their equivalent weights; 96,496 coulombs of electricity = 1 faraday = electricity to yield 1 gram equivalent of any substance.

7. Freezing Point Depression (ΔT_f)—The following equations hold for a dilute solution of a nonionic solute in which the solid phase is pure solvent.

$$\Delta T_f = K_f m$$
$$K_f = \frac{R(T_{fp})^2 M_a}{\Delta H_f (1000)}$$

where ΔH_f = molal heat of fusion of solvent

K_f = molal freezing point lowering constant

m = molality

M_a = solvent molecular weight

R = ideal-gas constant

T_{fp} = solvent freezing point, absolute temperature

8. Gibbs Phase Rule—At equilibrium the number of independent variables (F) required to specify the system is equal to the number of components (C) minus the number of phases (P) plus two, or symbolically $F = C - P + 2$. This form

of the phase rule applies to non-reactive systems.

9. Graham's Law of Diffusion—The rate of diffusion of a gas is inversely proportional to the square root of its density.
10. Henry's Law—At a constant temperature, the concentration of a gas dissolved in a liquid is directly proportional to the partial pressure of the gas above the liquid.
11. Raoult's Law

$$p_a = x_a P_a$$

where p_a = partial pressure of component A in vapor

x_a = mole fraction of A in liquid solution

P_a = vapor pressure of pure liquid A

12. van't Hoff Reaction Isochore

$$\frac{d(\ln K)}{dT} = \frac{\Delta H}{RT^2} \text{ at constant pressure}$$

where ΔH = heat of reaction

K = reaction equilibrium constant

R = ideal-gas constant

T = absolute temperature

If ΔH is constant,

$$\ln\left(\frac{K_2}{K_1}\right) = \frac{\Delta H}{R} \left[\frac{T_2 - T_1}{T_1 T_2} \right]$$

13. Molar Humidity—moles vapor/mole vaporfree gas

$$Y = \frac{y_a}{1 - y_a} = \frac{p_a}{P - p_a}$$

Humidity—pounds vapor/pound vapor-free gas

$$Y' = Y \frac{M_a}{M_b}$$

Relative Saturation—ratio of partial pressure of vapor to partial pressure of vapor at saturation (vapor pressure)

$$H_r = 100 \frac{p_a}{P_a}$$

Percentage of Saturation—ratio of vapor concentration to vapor concentration at saturation (ratio of molar humidity to saturated molar humidity)

$$H_p = 100 \frac{Y}{Y_{\text{sat}}} = 100 \frac{p_a(P - P_a)}{P_a(P - p_a)}$$

where p_a = partial pressure of component A in gas

P_a = vapor pressure of pure liquid A

P = total pressure

M_a = molecular weight of A

M_b = molecular weight of B

y_a = mole fraction of a gas

FLUID FLOW

I. DEFINITIONS AND GENERAL EQUATIONS

Mass velocity

$$G = \bar{V}\rho$$

Simple manometer equation

$$P_a - P_b = R_m \frac{g}{g_c} (\rho_a - \rho_b)$$

Hagen-Poiseuille equation (laminar flow in long horizontal tube)

$$P_a - P_b = \frac{32 L \bar{V} \mu}{g_c D^2}$$

Average velocity, $\bar{V}$

$$\bar{V} = \frac{q, \text{volumetric flow rate}}{s, \text{cross-sectional area}}$$

Reynolds number, N_{Re}

$$N_{Re} = \frac{D \bar{V} \rho}{\mu} = \frac{D \bar{V}}{\nu}$$

Mechanical energy balance

$$\frac{P_a}{\rho_a} + \frac{g}{g_c} Z_a + \frac{\bar{V}_a^2}{2g_c \alpha_a} - W_s = \frac{P_b}{\rho_b} + \frac{g}{g_c} Z_b + \frac{\bar{V}_b^2}{2g_c \alpha_b} + H_f$$

where $\alpha \approx 1$ for turbulent flow ($N_{Re} > 4,000$)

$\alpha = 0.5$ for laminar flow ($N_{Re} < 2,100$)

Hydraulic radius

$$r_H = \frac{s, \text{cross-sectional area}}{L_p, \text{the wetted perimeter}}$$

Equivalent diameter, D_e

$$D_e = 4 (\text{hydraulic radius, } r_H)$$

II. FRICTION

Skin friction

$$H_{fs} = \frac{2fL\bar{V}^2}{Dg_c}$$

Fanning friction factor, f (flow in smooth pipes)

$$\text{laminar} \quad f = \frac{16\mu}{DV\rho} = \frac{16}{N_{Re}}$$

$$\text{turbulent} \quad \frac{1}{f^{.5}} = 4.0 \log (N_{Re} f^{.5}) - 0.4$$

Friction of valves and fittings (Add to length of pipe to get total equivalent length.)

Fittings and Valves	Equivalent resistance, pipe diameters
45-degree elbows	15
90-degree elbows (standard radius)	32
90-degree square elbows	60
180-degree close return bends	75
T's (used as elbow, entering run)	60
T's (used as elbow, entering branch)	90
Couplings	Negligible
Unions	Negligible
Gate valves (open)	7
Globe valves (open)	300
Angle valves (open)	170

Friction loss from sudden expansion of cross section

$$H_{fe} = \frac{\bar{V}_a^2}{2g_c} \left(1 - \frac{s_a}{s_b} \right)^2$$

Friction loss from sudden contraction of cross section

$$H_{fc} = \frac{K_c \bar{V}_b^2}{2g_c}$$

Values of K_c are given on page 6-18, Perry's Chemical Engineers' Handbook, 7th ed., Don W. Green, ed., McGraw-Hill Book Co., New York, NY, 1997.

III. MEASUREMENT OF FLOWING FLUIDS

Venturi meter

$$\sqrt{V_b^2 - V_a^2} = C_v \sqrt{\frac{2g_c(p_a - p_b)}{\rho}} \quad (b \text{ is at throat of meter})$$

Orifice meter, design equation ($N_{Re} > 20,000$)

$$\bar{V}_o = \frac{0.61}{\sqrt{1 - \beta^4}} \sqrt{\frac{2g_c(p_a - p_b)}{\rho}}$$

Pilot tube (manometer measures $p_s - P$)

$$V = C_p \sqrt{\frac{2g_c(p_s - P)}{\rho}}$$

IV. SYMBOLS USED

C_u, C_p = coefficients of velocity

D = diameter

g = acceleration of gravity = 32.2 ft/s² = 9.81 m/s²

g_c = Newton's conversion factor = 32.2 ft-lb_m/(lb_f-s²)
= 1 m-kg/(N-s²)

H_f = head loss due to friction

H_{fs} = head loss due to skin friction

H_{fc} = head loss due to contraction of cross section

H_{fe} = head loss due to expansion of cross section
 K_e = expansion loss coefficient
 K_c = contraction loss coefficient
 L = length of pipe
 P = pressure
 P_a = upstream pressure
 P_b = downstream pressure
 p_w, p_b = pressure in arms of manometer
 p_s = static pressure
 R_m = manometer reading
 s = cross-sectional area
 V = velocity
 $\bar{V}$ = average velocity
 V_a = upstream velocity
 V_b = downstream velocity
 W_s = shaft work done by pump
 Z = elevation
 α = kinetic energy correction factor
 β = ratio of diameter of orifice to diameter of pipe
 ρ = fluid density, lb_m/ft^3
 ρ_a = density of manometer fluid
 ρ_b = density of fluid above manometer
 ν = kinematic viscosity = μ/ρ
 μ = viscosity

HEAT TRANSFER

I. CONDUCTION

Fourier's Law (constant k)
 steady state

$$q = \frac{-kA\Delta T}{\Delta x} = \frac{-\Delta T}{R}$$

unsteady state

$$\frac{\partial T}{\partial t} = \frac{k}{\rho C_p} x \frac{\partial^2 T}{\partial x^2}$$

Resistance in Series

$$\begin{aligned} q &= \frac{\Delta T}{\frac{x_A}{k_A A} + \frac{x_B}{k_B A} + \frac{x_C}{k_C A} + \dots} \\ &= \frac{\Delta T}{R_A + R_B + R_C + \dots} \end{aligned}$$

Radial Heat Flow Through a Cylinder

$$q = \frac{k(2\pi r_m)L\Delta T}{(r_o - r_i)} = \frac{kA_m\Delta T}{\Delta r}$$

where A_m = logarithmic mean area normal to heat flow

r_m = logarithmic mean radius

$$r_m = (r_o - r_i) / \ln [r_o / r_i]$$

II. CONVECTION

$$q = hA\Delta T$$

where $h = k' / \Delta x'$, heat transfer coefficient

k' = thermal conductivity of the fluid

$\Delta x'$ = thickness of the laminar film

III. COMBINED CONDUCTION AND CONVECTION

$$q = UA_{\text{avg}}(\Delta T)$$

where U = overall heat transfer coefficient

ΔT = overall temperature difference

$$\frac{1}{U} = \frac{A_r}{UA_r} = \frac{1}{h_i \frac{A_i}{A_r}} + \frac{x_m}{k_m \frac{A_m}{A_r}} + \frac{1}{h_o \frac{A_o}{A_r}} + \frac{1}{h_{Fi} \frac{A_i}{A_r}} + \frac{1}{h_{Fo} \frac{A_o}{A_r}}$$

where A_r = reference area, usually the area of the solid through which heat is being conducted
 h_{Fi}, h_{Fo} = inside and outside fouling factors

IV. RADIATION

$$q_{12} = \sigma AF(T_1^4 - T_2^4)$$

where q_{12} = net radiation between surfaces 1 and 2, Btu/hr
 T_1, T_2 = absolute temperature of surfaces 1, 2, °R.
 A = area of either surface, sq ft
 σ = Stefan-Boltzman Constant = 1.712×10^{-9} Btu/hr-sq ft-°R⁴
 F = geometric view factor

V. EMPIRICAL, DIMENSIONLESS CORRELATION

Turbulent Flow in Clean Smooth Pipes

$$\frac{h_i D}{k} = 0.023(N_{Re})^{0.8}(N_{Pr})^{0.33}(\mu/\mu_w)^{0.14}[1 + (D/L)^{0.7}]$$

where N_{Re} = the Reynolds Number = DG/μ
 N_{Pr} = the Prandtl Number = $C_p \mu/k$

Laminar Flow in Clean Smooth Pipes

$$\frac{h_i D}{k} = 1.86(N_{Re})^{0.33}(N_{Pr})^{0.33}(\mu/\mu_w)^{0.14}(D/L)^{0.33}$$

where the Reynolds and Prandtl Numbers are as defined for turbulence

VI. HEAT TRANSFER TO AND FROM FLUIDS FLOWING NORMAL TO A SINGLE TUBE

$$\frac{h_o D_o}{k_f} = 0.35 + 0.56(N_{Re})^{0.52}$$

where N_{Re} = the Reynolds Number = $D_o G / \mu_f$

The subscript f calls attention to the fact that the correlation is based on the mean film temperature, T_f , which is defined as the arithmetic mean of the average fluid temperature and the wall temperature.

VII. HEAT TRANSFER TO AND FROM FLUIDS FLOWING PERPENDICULAR TO TUBE BANKS

$$\frac{h_{\text{avg}} D_o}{k_f} = b(N_{Re})^n \quad (b \text{ and } n \text{ depend on geometry})$$

where N_{Re} = the Reynolds Number = DG_{max} / μ_f

VIII. HEAT TRANSFER FROM CONDENSING VAPORS

Vertical Tubes

$$h_{\text{avg}} = 1.13 \left[\frac{k_f^3 \rho_f^2 g \lambda}{\Delta T_o L \mu_f} \right]^{0.25}$$

Horizontal Tubes

$$h_{\text{avg}} = 0.725 \left[\frac{k_f^3 \rho_f^2 g \lambda}{\Delta T_o D_o \mu_f} \right]^{0.25}$$

IX. NOTATION

- A = area, sq. ft.
 b = empirical constant
 C_p = specific heat at constant pressure, Btu/lb-°F
 D = diameter, ft
 G = mass velocity, lb_m/sq ft-sec
 $G_{\max}$ = mass velocity through minimum cross section in tube bundle
 g = acceleration of gravity, 32.2 ft/sec²
 h = heat transfer coefficient, Btu/sq ft-hr-°F
 k = thermal conductivity, Btu/sq ft-(°F/ft)-hr
 L = length of tube or cylinder, ft
 q = heat flow per unit of time, Btu/hr
 R = resistance
 r = radius, ft
 T = temperature, °F
 t = time, hr
 U = over-all heat transfer coefficient, Btu/sq ft-hr-°F
 x = distance in direction of heat flow; thickness of layer, ft
 λ = latent heat of condensation or vaporization, Btu/lb_m
 μ = viscosity, lb_m/ft-sec
 ρ = density, lb_m/ft³

Subscripts

- avg = average
 f = film
 i = inside
 o = outside
 r = reference

w = wall

m = mean or log mean

DISTILLATION

I. FLASH (OR EQUILIBRIUM) DISTILLATION

$$Fz_F = yV + xL \quad (\text{component material balance})$$

$$F = V + L \quad (\text{over-all material balance})$$

II. DIFFERENTIAL (SIMPLE OR RAYLEIGH) DISTILLATION

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

When the relative volatility α is constant $y = \alpha x / [1 + (\alpha - 1)x]$ can be substituted to give

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

For binary system following Raoult's Law

$$\alpha = \frac{(y/x)_a}{(y/x)_b} = \frac{p_a}{p_b}$$

where p_i = partial pressure of component i

III. CONTINUOUS DISTILLATION (BINARY SYSTEM) WHERE CONSTANT MOLAL OVERFLOW IS ASSUMED

Total Material Balance

$$F = D + B$$

$$Fz_F = Dx_D + Bx_B$$

Operating Lines

1. Rectifying Section

Total material: $V_{n+1} = L_n + D$

Component A: $V_{n+1}y_{n+1} = L_nx_n + Dx_D$

$$y_{n+1} = \frac{L_n}{L_n + D}x_n + \frac{Dx_D}{L_n + D}$$

2. Stripping Section

Total material: $L_m = V_{m+1} + B$

Component A: $L_{m+1}x_m = V_{m+1}y_{m+1} + Bx_B$

$$y_{m+1} = \frac{L_m}{L_m - B}x_m - \frac{Bx_B}{L_m - B}$$

3. Reflux Ratio

Ratio of reflux to overhead product

$$R_D = \frac{L}{D} = \frac{V - D}{D}$$

4. Feed Condition Line

Type of Feed	Slope of feed line
Superheated vapor	+ (downward to left)
Saturated vapor	0 (horizontal)
Liquid and vapor	− (upward to left)
Saturated liquid	∞ (vertical)
Cold liquid	+ (upward to right)

5. Murphree Plate Efficiency

$$E_{ME} = \frac{y_n - y_{n+1}}{y_n^* - y_{n+1}}$$

where y_n = concentration of vapor above plate n
 y_{n+1} = concentration of vapor entering from plate below n
 y_n^* = concentration of vapor in equilibrium with liquid leaving plate n

IV. NOTATION

α = relative volatility
 B = moles of bottoms product
 D = moles of overhead product
 F = moles of feed
 L = molar liquid downflow
 R_D = ratio of reflux to overhead product
 V = molar vapor upflow
 W = weight in still pot
 x = mole fraction of the more volatile component in the liquid phase
 y = mole fraction of the more volatile component in the vapor phase
 z_D = mole fraction of the more volatile component in the feed

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 stripping section of column
 $n + 1$ = plate below plate n
 o = original charge in still pot

MASS TRANSFER

I. DIFFUSION

1. Molecular Diffusion

$$\frac{N_A}{A} = \frac{p_A}{P} \left[\frac{N_A}{A} + \frac{N_B}{A} \right] - \frac{D}{RT} \frac{\partial p_A}{\partial z}$$

2. Unidirectional Diffusion of a Gas A Through a Second Stagnant Gas B ($N_B = 0$)

$$\frac{N_A}{A} = \frac{-DP}{RT(p_B)_{lm}} \times \frac{(p_{A_2} - p_{A_1})}{x_2 - x_1}$$

in which $(p_B)_{lm}$ is the log mean of p_{B_2} and p_{B_1}

3. Equimolar Countercurrent Diffusion ($N_B = -N_A$) (gases)

$$\frac{N_A}{A} = \frac{-D}{RT} \times \frac{(p_{A_2} - p_{A_1})}{z_2 - z_1}$$

4. Unsteady State Diffusion

$$\frac{\partial p_A}{\partial t} = D \frac{\partial^2 p_A}{\partial z^2}$$

II. CONVECTION

1. Two-Film Theory

$$\begin{aligned} \frac{N_A}{A} &= k_G (p_{AG} - p_{Ai}) = k_L (C_{Ai} - C_{AL}) \\ &= k_G (p_{AG} - p_A) = k_L (C_A - C_{AL}) \end{aligned}$$

2. Overall Coefficients

$$\frac{1}{K_G} = \frac{1}{k_G} + \frac{H}{k_L}$$
$$\frac{1}{K_L} = \frac{1}{Hk_G} + \frac{1}{k_L}$$

3. Transfer Unit

HTU—height of a transfer unit

$$H_{TG} = \frac{G}{K_G a}$$
$$H_{TL} = \frac{L}{K_L a}$$

NTU—number of transfer units

$$N_{TG} = \int_{y_1}^{y_2} \frac{dy}{y^* - y} + \frac{1}{2} \ln \frac{1 - y_2}{1 - y_1}$$
$$N_{TL} = \int_{x_1}^{x_2} \frac{dx}{x - x^*} + \frac{1}{2} \ln \frac{1 - x_1}{1 - x_2}$$

For dilute solutions (straight operating and equilibrium line)

$$N_{TG} = \frac{y_1 - y_2}{(y - y^*)_{lm}}$$

$$Z = N_{TG} H_{TG} = N_{TL} H_{TL} = \text{tower height}$$

4. Dimensionless Group Equation (Sherwood)

$$(N_{Sh}) = 0.023 (N_{Re})^{0.8} (N_{Sc})^{1/3}$$

III. MOMENTUM, HEAT, AND MASS TRANSFER ANALOGY

$$0.5f = j_H = j_D$$

where f = Fanning friction factor

$$j_H = \frac{h}{C_p G} \left[\frac{C_p \mu}{k} \right]^{0.667} \left[\frac{\mu_w}{\mu} \right]^{0.14}$$

$$j_M = \frac{k_c}{G} (N_{Sc})^{0.667}$$

IV. NOTATION

- A = area perpendicular to direction of diffusion
 a = interfacial area per unit volume
 C = concentration in liquid phase
 d = tube diameter
 D = molecular diffusivity
 G = gas mass velocity, mass/(time)(area)
 H = Henry's Law constant, $p_i = HC_i$
 h = heat transfer coefficient
 k = film coefficient of mass transfer
 K = overall coefficient of mass transfer
 L = liquid mass velocity, mass/(time)(area)
 N = moles of a substance per unit time
 p = partial pressure
 P = total pressure
 R = gas constant
 N_{Re} = Reynolds number = $du\rho/\mu$
 N_{Sc} = Schmidt number = $\mu/\rho D$
 N_{Sh} = Sherwood number = kd/D
 t = time
 T = absolute temperature
 u = velocity

lm = logarithm mean average

Greek Letters

ρ = density

μ = viscosity

Subscripts

A, B = components of mixture

G = gas phase

L = liquid phase

i = interface

x = mole fraction of liquid

y = mole fraction of gas

z = length in direction of travel

$*$ = equilibrium concentration

THERMODYNAMICS

I. DEFINITIONS

System—an arbitrarily chosen portion of space which is under consideration.

A. Closed system—one in which matter does not pass through its boundaries.

B. Open system—one in which matter flows across its boundaries.

C. Isolated system—one in which there is no interchange of energy or matter with the surroundings.

Boundaries—the envelope separating the system from the surroundings.

Universe—a system and its surroundings.

Total energy, E —the sum of the various forms of energy of the system: e.g., U , internal energy; E_k , kinetic energy; E_p , potential energy; Hence,

$$E = U + E_p + E_k + \dots$$

II. FIRST LAW

In an isolated system $\Delta E = E_2 - E_1 = 0$

In a closed system $\Delta E = Q - W$

In an open system $\Delta E + \Sigma(H + E_p + E_k) = Q - W$

where the summed terms refer to leaving (+) and entering (−) streams

In a steady state open system

$$\Delta E_{\text{system}} = 0$$

Hence for the entering and leaving streams

$$\Delta H + \Delta E_k + \Delta E_p = Q - W$$

III. SECOND LAW

For any real process the total entropy of the universe always increases

$$\Delta S_{\text{system}} + \Delta S_{\text{surroundings}} > 0$$

IV. THERMODYNAMIC FUNCTIONS: DEFINITIONS AND RELATIONSHIPS

Definition of entropy

$$\Delta S = \int \frac{dQ_{\text{rev}}}{T}$$

From First and Second Laws, with changes in E_k ,

E_p , and composition negligible,

$$dU = dQ_{\text{rev}} - PdV = TdS - PdV$$

Also

$$dH = dU + d(PV) = TdS + VdP$$

$$dG = dH - d(TS) = -SdT + VdP$$

$$dA = dU - d(TS) = -SdT - PdV$$

$$C_p = (\partial H/\partial T)_p; C_v = (\partial U/\partial T)_v; \gamma = (C_p/C_v)$$

P, V, T, S, U, H, G, A are state functions. Q and W are path functions and have no total derivatives.

V. PERFECT-GAS RELATIONSHIPS

$$\text{For any path: } \Delta H = \int_{T_1}^{T_2} C_p dT \text{ or } (\partial H/\partial P)_T = 0$$

$$\text{For any path: } \Delta U = \int_{T_1}^{T_2} C_v dT \text{ or } (\partial U/\partial V)_T = 0$$

For monoatomic gas: $C_p = 2.5 R$ and $C_v = 1.5 R$

For diatomic gas: $C_p = 3.5 R$ and $C_v = 2.5 R$

Adiabatic ($Q = 0$) and reversible path for system with $\Delta E_p = \Delta E_k = 0$.

$$(P_2/P_1) = (V_1/V_2)^\gamma = (T_2/T_1)^{\gamma/(\gamma-1)}$$

$$W_{\text{nonflow}} = \Delta U = \frac{-RT_1}{\gamma - 1} \left[\left(\frac{P_2}{P_1} \right)^{(\gamma-1)/\gamma} - 1 \right] \text{ (per mole)}$$

$$W_{\text{flow}} = \Delta H = \gamma [W_{\text{nonflow}}] \text{ (per mole)}$$

Isothermal path, flow or nonflow

$$\frac{P_2}{P_1} = \frac{V_1}{V_2}$$

$$W = RT \ln \frac{V_2}{V_1} = RT \ln \frac{P_1}{P_2} \quad (\text{per mole})$$

VI. CRITERIA FOR EQUILIBRIUM CHANGE

For system and surroundings: $dS_{\text{universe}} = 0$

For system alone: $dG = 0$ when $P, T = \text{constant}$

$dA = 0$ when $V, T = \text{constant}$

VII. CHEMICAL THERMODYNAMICS

A. Fugacity (f) and Activity (a)

$$\Delta G = RT \ln (f_2/f_1) = \int_1^2 V dP \quad (\text{per mole})$$

(constant-temperature path)

and the limit of f/P as P approaches 0 = 1.00

$$a = f/f_0$$

B. Equilibrium

Standard free energy at temperature T for the reaction



$$\begin{aligned} \Delta G^\circ &= rG_R^\circ + sG_S^\circ - aG_A^\circ - bG_B^\circ \\ &= RT \ln \frac{a_R^r a_S^s}{a_A^a a_B^b} = -RT \ln K_a \end{aligned}$$

C. Cells

At standard conditions

$$\Delta G^\circ = -\epsilon^\circ nF = -RT \ln K_a$$

At actual conditions

$$G = \epsilon nF = \epsilon^\circ nF - RT \ln \frac{a_R^r a_S^s}{a_A^a a_B^b}$$

VIII. NOTATION

$A = U - TS$, Helmholtz work function

a = activity

C = heat capacity

E = total energy of the system

E_k = kinetic energy of the system

E_p = potential energy of the system

ϵ = reversible voltage of cell

F = faradays per equivalent

f = fugacity

$G = H - TS$, Gibbs free energy

g_c = Newton's conversion factor

$H = U + PV$, enthalpy

h = enthalpy per pound

K = equilibrium constant for the reaction as written

K_a = equilibrium constant in terms of activity

K_f = equilibrium constant in terms of fugacity

K_p = equilibrium constant in terms of partial pressure

n = number of equivalents for the reaction as written

P = pressure

Q = heat, defined as positive when absorbed by system

R = gas constant

S = entropy

T = absolute temperature

U = internal energy of the system

u = velocity

V = volume

v = specific volume

W = work, defined as positive when done by system
on surroundings

Δ = final state minus initial state

$\gamma = (C_p/C_v)$

Superscript

$^{\circ}$ = standard state

KINETICS AND REACTOR DESIGN

I. RATE OF REACTION

The rate of reaction of any component A based on unit volume of fluid is

$$r_A = \frac{1}{V} \frac{dN_a}{dt}$$

and where density remains unchanged

$$r_A = \frac{dC_A}{dt}$$

Frequently, the rate can be described as a temperature-dependent term times a concentration-dependent term, or

$$r_A = k(T)f(C_A, C_B \dots)$$

A. Order, Molecularity, Elementary Reactions

Where the rate can be expressed as

$$-r_A = kC_A^a C_B^b \dots$$

the reaction is a th order with respect to A and n th order overall; $n = a + b + \dots$

NOTE: $a, b, \dots$ are empirically observed and are not necessarily equal to the stoichiometric coefficients. In the special case where $a, b, \dots$ are the stoichiometric coefficients, the reaction is elementary: unimolecular ($n = 1$), bimolecular ($n = 2$), trimolecular ($n = 3$)

B. Rate Constant k and Temperature Dependency of a Reaction

$$k = (\text{conc})^{1-n}(\text{time})^{-1}$$

From Arrhenius's Law the variation with temperature is

$$k = k_o e^{-E/RT} \text{ or } \ln \frac{k_2}{k_1} = \frac{E}{R} \left[\frac{1}{T_1} - \frac{1}{T_2} \right]$$

where E is the activation energy of the reaction

II. HOMOGENEOUS, CONSTANT FLUID DENSITY, BATCH KINETICS

A. Irreversible First-order Reaction

For the reaction $A \rightarrow \text{products}$, with rate

$$-\frac{dC_A}{dt} = kC_A \text{ or } \frac{dX_A}{dt} = k(1 - X_A)$$

the integrated form is

$$-\ln \frac{C_A}{C_{A0}} = -\ln(1 - X_A) = kt$$

B. Irreversible Second-order Reaction

For the reaction $A + B \rightarrow \text{products}$, with rate

$$-\frac{dC_A}{dt} = kC_AC_B$$

When $M = C_{B0}/C_{A0} \neq 1$, the integrated form is

$$\ln \frac{C_B C_{A0}}{C_{B0} C_A} = \ln \frac{M - X_A}{M(1 - X_A)} = (C_{B0} - C_{A0})kt$$

When $C_{A0} = C_{B0}$, the integrated form is

$$\frac{1}{C_A} - \frac{1}{C_{A0}} = \frac{1}{C_{A0}} \frac{X_A}{1 - X_A} = kt$$

C. Irreversible nth-order Reaction

For the reaction with rate

$$-\frac{dC_A}{dt} = kC_A^n$$

the integrated form for $n \neq 1$ is

$$C_A^{1-n} - C_{A0}^{1-n} = (n - 1)kt$$

D. Reversible First-order Reaction

For the reaction $A \xrightleftharpoons[2]{1} R$, $K = k_1/k_2$ with rate

$$-\frac{dC_A}{dt} = \frac{dC_R}{dt} = k_1C_A - k_2C_R$$

the integrated form is

$$-\ln \frac{X_{Ae} - X_A}{X_{Ae}} = -\ln \frac{C_A - C_{Ae}}{C_{A0} - C_{Ae}} = (k_1 + k_2)t$$

E. Integration of Rate in General

For the reaction with rate

$$-r_A = -\frac{dC_A}{dt} = kf(C_A, C_B, \dots),$$
$$t = C_{A0} \int_0^{X_A} \frac{dX_A}{(-r_A)} = \int_{C_{A0}}^{C_A} \frac{dC_A}{kf(C_A, C_B, \dots)}$$

which is to be solved analytically or graphically.

III. BATCH REACTION WITH CHANGING FLUID DENSITY

Where density change is proportional to the fractional conversion of any reactant A (isothermal systems),

$$\frac{C_A}{C_{A0}} = \frac{1 - X_A}{1 + \epsilon_A X_A}$$

where

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

The rate for any reactant A is then

$$-r_a = -\frac{1}{V} \frac{dN_A}{dt} = \frac{C_{A0}}{(1 + \epsilon_A X_A)} \frac{dX_A}{dt} = kf(C_A, C_B, \dots)$$

Integrating in the general case

$$t = C_{A0} \int_0^{X_A} \frac{dX_A}{(1 + \epsilon_A X_A)(-r_A)}$$

IV. FLOW REACTORS

A. Capacity Measures

Space time: τ = time required to process one reactor
volume of entering feed =
mean residence time

$$\tau = \frac{V}{v} = \frac{VC_{A0}}{F_{A0}} \quad (\text{units of time})$$

B. Design Equation for Plug Flow (Ideal Tubular) Reactor

In general

$$\tau = C_{A0} \int_0^{X_A} \frac{dX_A}{(-r_A)} \text{ or } \frac{V}{F_{A0}} = \int_0^{X_A} \frac{dX_A}{(-r_A)}$$

For irreversible first-order reactions (isothermal)

$$-k\tau = (1 + \epsilon_A) \ln(1 - X_A) + \epsilon_A X_A$$

For reversible first-order reactions $A \xrightleftharpoons{2} rR$

(isothermal)

$$-k_1\tau = \frac{\epsilon_A X_A}{N} + \frac{N + \epsilon_A}{N^2} \ln(1 - NX_A)$$

where

$$N = 1 + \frac{k_2}{k_1} (1 + \epsilon_A)$$

C. Design Equation for Back-Mix (Ideal Stirred

Tank) Reactor

$$\tau = \frac{C_{A0}X_A}{(-r_A)} \text{ or } \frac{V}{F_{A0}} = \frac{X_A}{(-r_A)}$$

For a first-order reaction in j equal-sized backmix reactors in series

$$\frac{C_A \text{ entering}}{C_A \text{ leaving}} = (1 + k\tau \text{ per reactor})^j$$

D. NOTATION

A, B, R , etc. = substance A , etc.

$a, b, \dots$ = exponents on concentration term of empirical rate expression

C_A = concentration of A , moles A /volume

C_{A0} = initial concentration of A , moles A /volume

F_{A0} = feed rate of A or flow rate of A entering the reactor, moles A /time

K = equilibrium constant

k = reaction rate constant, $(\text{conc}^{1-n})(\text{time}^{-1})$

n = order of reaction

N_A = moles of A

r_A = rate of reaction of any component A , moles A formed/time-volume

T = temperature

t = time

V = volume of fluid in batch reactor, volume of fluid in a flow reactor, or reactor volume

v = volumetric feed rate, volume of feed/
time

X_A = fraction of reactant A converted, dimensionless

Greek Symbols

ϵ_A = measure of density change with reaction, dimensionless

τ = space time based on entering feed, time

Subscripts

e = equilibrium value

CONVERSION FACTORS

Acceleration

$$\begin{aligned}1 \text{ ft/s}^2 &= 0.3048 \text{ m/s}^2 \\&= 0.6318 (\text{mile/hr})/\text{sec} \\&= 1.097 \text{ km/hr-s} \\&= 30.48 \text{ cm/s}^2\end{aligned}$$

$$\begin{aligned}1 \text{ rev/min}^2 &= 2.778 \times 10^{-4} \text{ rev/s}^2 \\&= 0.001745 \text{ rad/s}^2 \\&= 0.01667 \text{ rev/min-s}\end{aligned}$$

Density

$$\begin{aligned}1 \text{ lb}_m/\text{ft}^3 &= 16.02 \text{ kg/m}^3 \\&= 5.787 \times 10^{-4} \text{ lb}_m/\text{in}^3 \\&= 0.01602 \text{ g/cc}\end{aligned}$$

Flow

$$\begin{aligned}1 \text{ ft}^3/\text{min} &= 4.719 \times 10^{-4} \text{ m}^3/\text{s} \\&= 0.1247 \text{ gal/s}\end{aligned}$$

$$= 0.4720 \text{ liter/s}$$

$$= 472 \text{ cc/s}$$

Length

$$1 \text{ ft} = 0.3048 \text{ m}$$

$$= 1.894 \times 10^{-4} \text{ mile}$$

$$= 1/3 \text{ yd}$$

$$= 12 \text{ in}$$

$$= 30.48 \text{ cm}$$

$$= 3.05 \times 10^5 \text{ microns } (\mu)$$

$$1 \text{ \AA} = 10^{-10} \text{ m}$$

$$= 10^{-8} \text{ cm}$$

$$= 1 \times 10^{-4} \text{ microns } (\mu)$$

Angle

$$1 \text{ rad} = 1/2\pi \text{ circle}$$

$$= 0.1592 \text{ rev}$$

$$= 0.637 \text{ quad}$$

$$= 57.3 \text{ deg}$$

$$= 3,438 \text{ min}$$

$$= 2.063 \times 10^5 \text{ s}$$

Mass

$$1 \text{ lb}_m = 0.4536 \text{ kg}$$

$$= 4.464 \times 10^{-4} \text{ long ton}$$

$$= 5 \times 10^{-4} \text{ short ton}$$

$$= 4.536 \times 10^{-4} \text{ metric ton}$$

$$= 0.4536 \text{ kg}$$

$$= 453.6 \text{ g}$$

$$= 0.0311 \text{ slug}$$

Pressure

$$1 \text{ lb}_f/\text{in}^2 \text{ abs} = 6.895 \times 10^3 \text{ N/m}^2$$

$$= 6.895 \times 10^3 \text{ Pascal}$$

$$\begin{aligned}
&= 0.06805 \text{ atm} \\
&= 0.07031 \text{ kg/cm}^2 \\
&= 2.036 \text{ in Hg @ } 32^\circ\text{F} \\
&= 2.307 \text{ ft H}_2\text{O @ } 39^\circ\text{F} \\
&= 70.307 \text{ g/cm}^2 \\
&= 51.72 \text{ mm Hg @ } 32^\circ\text{F} \\
&= 51.72 \text{ torr}
\end{aligned}$$

Power

$$\begin{aligned}
1 \text{ ft-lb/min.} &= 0.0226 \text{ W} \\
&= 2.26 \times 10^{-5} \text{ kW} \\
&= 3.03 \times 10^{-5} \text{ hp} \\
&= 3.24 \times 10^{-4} \text{ kg-cal/min} \\
&= 0.001285 \text{ Btu/min}
\end{aligned}$$

Temperature

$$\begin{aligned}
^\circ\text{F} &= 1.8(^\circ\text{C}) + 32 \\
^\circ\text{K} &= ^\circ\text{C} + 273 \\
^\circ\text{R} &= ^\circ\text{F} + 459
\end{aligned}$$

Time

$$1 \text{ nanosecond} = 1 \times 10^{-9} \text{ s}$$

Velocity

$$\begin{aligned}
1 \text{ ft/s} &= 0.3048 \text{ m/s} \\
&= 0.011364 \text{ mile/min} \\
&= 0.6818 \text{ mile/hr} \\
&= 1.0973 \text{ km./hr} \\
&= 18.29 \text{ m/min} \\
&= 30.48 \text{ cm/s} \\
1 \text{ rev/min} &= 0.1047 \text{ rad/s} \\
&= 6 \text{ deg/s}
\end{aligned}$$

Viscosity

$$\begin{aligned}1 \text{ centipoise} &= 0.001 \text{ Pa}\cdot\text{s} \\&= 0.001 \text{ N}\cdot\text{s}/\text{m}^2 \\&= 0.01 \text{ g}/\text{cm}\cdot\text{s} \\&= 6.72 \times 10^{-4} \text{ lb}_m/\text{ft}\cdot\text{s} \\&= 2.42 \text{ lb}_m/\text{ft}\cdot\text{hr}\end{aligned}$$

Volume

$$\begin{aligned}1 \text{ ft}^3 &= 0.02832 \text{ m}^3 \\&= 0.03704 \text{ yd}^3 \\&= 0.80357 \text{ bushel (U.S.)} \\&= 7.481 \text{ gal (U.S.)} \\&= 6.229 \text{ gal (British)} \\&= 25.714 \text{ qt (dry, U.S.)} \\&= 29.92 \text{ qt (liq., U.S.)} \\&= 1.728 \times 10^3 \text{ in}^3 \\&= 28.32 \text{ liters} \\&= 2.832 \times 10^4 \text{ cm}^3 \\&= 2.832 \times 10^4 \text{ ml} \\&= 59.8 \text{ pt (U.S. liq.)}\end{aligned}$$

Work and Energy

$$\begin{aligned}1 \text{ Btu} &= 1054 \text{ J} \\&= 2.93 \times 10^{-4} \text{ kW}\cdot\text{hr} \\&= 3.93 \times 10^{-4} \text{ hp}\cdot\text{hr} \\&= 0.252 \text{ kg cal} \\&= 0.293 \text{ W}\cdot\text{hr} \\&= 10.41 \text{ liter}\cdot\text{atm} \\&= 252 \text{ g cal} \\&= 778 \text{ ft}\cdot\text{lb}_f \\&= 0.3676 \text{ ft}^3\cdot\text{atm} \\&= 1.054 \times 10^{10} \text{ ergs}\end{aligned}$$

Mole fraction (x) to mass fraction (w)

$$w_A = \frac{x_A M_A}{x_A M_A + x_B M_B}$$

Mass fraction (w) to mole fraction (x)

$$x_A = \frac{w_A/M_A}{w_A/M_A + w_B/M_B}$$

where M_i = molecular weight of i

PHYSICAL CONSTANTS

Gas constants

$$\begin{aligned} R &= 0.0821 \text{ atm-liter/g-mole-K} \\ &= 1.987 \text{ g-cal/g-mole-K} \\ &= 1.987 \text{ Btu/lb}_m\text{-mole-}^\circ\text{R} \\ &= 8.314 \text{ joules/g-mole-K} \\ &= 1546 \text{ ft-lb}_f\text{/lb}_m\text{-mole-}^\circ\text{R} \\ &= 10.73 \text{ (psi)-ft}^3\text{/lb}_m\text{-mole-}^\circ\text{R} \\ &= 0.7302 \text{ atm-ft}^3\text{/lb}_m\text{-mole-}^\circ\text{R} \end{aligned}$$

Acceleration of gravity (standard)

$$g = 32.17 \text{ ft/s}^2 = 980.7 \text{ cm/s}^2$$

Avogadro's number

$$N = 6.023 \times 10^{23} \text{ molecules/g-mole}$$

Boltzmann's constant

$$K = 1.3805 \times 10^{-16} \text{ erg/molecule-K}$$

Newton's conversion constant

$$g_c = 32.17 \text{ lb}_m\text{-ft/lb}_f\text{-s}^2 = 1.000 \text{ kg-m/N-s}^2$$

Planck's constant

$$h = 6.624 \times 10^{-27} \text{ erg-s}$$

Stefan-Boltzmann constant

$$\begin{aligned}\sigma &= 1.355 \times 10^{-12} \text{ cal/s-cm}^2\text{-K}^4 \\ &= 1.712 \times 10^{-9} \text{ Btu/hr-sq ft-}^\circ\text{R}^4\end{aligned}$$

Velocity of light

$$c = 186,000 \text{ miles/s} = 3 \times 10^{10} \text{ cm/s}$$

Velocity of sound in dry air, 0°C and 1 atm

$$= 33,136 \text{ cm/s} = 1,089 \text{ ft/s}$$

Heat of fusion of water at 1 atm, 0°C

$$= 79.7 \text{ cal/g} = 144 \text{ Btu/lb}_m$$

Heat of vaporization of water at 1 atm, 100°C

$$= 540 \text{ cal/g} = 972 \text{ Btu/lb}_m$$

Ton of refrigeration = 12,000 Btu/hr

1 lb_m -mole of perfect gas occupies 359 ft^3 at standard conditions (32°F , 14.7 psi abs)

1 g-mole of perfect gas occupies 22.4 liters at 0°C and 760 mm Hg

Thermochemistry

$$F = 96,500 \text{ coulombs/gram equivalent}$$

$$\text{joules} = \text{volts} \times \text{coulombs}$$

$$\text{coulombs} = \text{amperes} \times \text{seconds}$$

Dimensionless Groups

Name	Symbol	Formula
Fanning friction factor	f	$-\Delta p g_c d / 2 L \rho V^2$
Heat transfer factor	j_H	$(h / c_p G)(C_p \mu / k)^{2/3}$
Mass transfer factor	j_M	$(k_c \rho / G)(\mu / \rho D)^{2/3}$
Froude number	N_{Fr}	$V^2 / g L$
Graetz number	N_{Gz}	$w c_p / k L$
Grashof number	N_{Gr}	$L^3 \rho^2 \beta_g \Delta T / \mu^2$
Nusselt number	N_{Nu}	$h d / k$
Peclet number	N_{Pe}	$L V \rho c_p / k$
Power number	N_{Po}	$P g_c / \rho n^3 d^5$
Prandtl number	N_{Pr}	$c_p \mu / k$
Reynolds number	N_{Re}	$L V \rho / \mu$
Schmidt number	N_{Sc}	$\mu / \rho D$
Sherwood number	N_{Sh}	$K_c L / D$

Notation

c_p = specific heat, Btu/lb_m-°F

D = molecular diffusivity, sq ft/hr

d = diameter, ft

G = mass velocity, lb_m/sq ft-hr

g = acceleration of gravity, 32.2 ft/s²

g_c = conversion factor = 32.2 ft-lb_m/(lb_f-s²)
= 1 m-kg/(N-s²)

h = heat transfer coefficient, Btu/sq ft-hr-°F

k = thermal conductivity, Btu/sq ft-(°F/ft)-hr

k_c = mass transfer coefficient, ft/hr

L = characteristic dimension, ft

n = rate of rotation, s⁻¹

P = power to agitator, ft-lb_f/s

p = pressure drop, lb_f/sq ft

T = temperature, °F

V = fluid velocity, ft/s

w = mass flow rate, lb_m/s

β = coefficient of bulk expansion, $^{\circ}\text{F}^{-1}$

ρ = density, lb_m/ft^3

μ = viscosity $\text{lb}_m/\text{ft}\cdot\text{hr}$

Abbreviations

atm = atmosphere

Btu = British thermal unit

cal = calorie

cm = centimeter

cu = cubic

ft = foot, feet

g = gram

hp = horsepower

hr = hour

in = inch

kg = kilogram

km = kilometer

kW = kilowatt

lb_m = pound-mass

lb_f = pound-force

m = meter

min = minute

ml = milliliter

pt = pint

qt = quart

quad = quadrant

$^{\circ}\text{R}$ = degrees Rankine

rad = radian

rev = revolution

s = second

yd = yard

μ = micron

GREEK ALPHABET

A, α	alpha	H, η	eta
B, β	beta	Θ, θ	theta
Γ, γ	gamma	I, ι	iota
Δ, δ	delta	K, κ	kappa
E, ϵ	epsilon	Λ, λ	lambda
Z, ζ	zeta	M, μ	mu
N, ν	nu	T, τ	tau
Ξ, ξ	xi	Υ, υ	upsilon
O, $\omicron$	omicron	Φ, ϕ	phi
Π, π	pi	X, χ	chi
P, ρ	rho	Ψ, ψ	psi
Σ, σ	sigma	Ω, ω	omega

MATHEMATICS

$$a^2 - b^2 = (a + b)(a - b)$$

$$a^3 + b^3 = (a + b)(a^2 - ab + b^2)$$

$$a^3 - b^3 = (a - b)(a^2 + ab + b^2)$$

$$ax^2 + bx + c = 0 \quad x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

$$\text{Area of circle} = \pi r^2$$

$$\text{Circumference of circle} = 2\pi r$$

$$\text{Surface of sphere} = 4\pi r^2$$

$$\text{Volume of sphere} = (4/3)\pi r^3$$

$$\text{Volume of cone or pyramid} = 1/3 (\text{base area})(\text{height})$$

$$dax = adx$$

$$dx^n = nx^{n-1}dx$$

$$d(u + v) = du + dv$$

$$d(uv) = u dv + v du$$

$$d\left[\frac{u}{v}\right] = \frac{v du - u dv}{v^2}$$

$$de^{ax} = ae^{ax} dx$$

$$da^x = a^x \log_e a dx$$

$$d \sin x = \cos x dx$$

$$d \cos x = -\sin x dx$$

$$d \tan x = \sec^2 x dx$$

$$\int (u + v) dx = \int u dx + \int v dx$$

$$\int u dv = uv - \int v du$$

$$\int x^n dx = x^{n+1}/(n+1) \text{ for } n \neq -1$$

$$\int \frac{dx}{x} = \log_e x = \ln x$$

$$\int e^{ax} dx = \frac{e^{ax}}{a}$$

Binomial series

$$(x + y)^n = x^n + nx^{n-1}y + \frac{n(n-1)}{2!}$$

$$x^{n-2}y^2 + \cdots (y^2 < x^2)$$

Taylor series

$$f(x) = f(a) + f'(a) \frac{x-a}{1!} + f''(a) \frac{(x-a)^2}{2!} + \cdots$$

MacLaurin series

$$f(x) = f(0) + f'(0) \frac{x}{1!} + f''(0) \frac{x^2}{2!} + \dots$$

Exponential series

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots$$

$$\pi = 3.1416, e = 2.71828, i = \sqrt{-1}, i^2 = -1, i^4 = 1$$

$$\log_{10} x = 0.4343 \ln x, \ln x = 2.303 \log_{10} x$$

Arithmetic mean

$$\frac{a + b}{2}$$

Geometric mean

$$\sqrt{ab}$$

Harmonic mean

$$\frac{2ab}{a + b}$$

Logarithmic mean

$$\frac{a - b}{\ln a/b}$$

Solution of

$$\frac{dy}{dx} + Py = Q$$

where P, Q are constants or functions of x

$$\text{Integrating factor} = e^{\int P dx} = IF$$

$$\text{Solution} = y \times IF = \int (IF \times Q) dx + C$$

CHEMICAL PROCESS SAFETY

Contributed by Joe Louvar

I. COMMON DEFINITIONS: GENERAL CONCEPTS

Chemical Process Safety—The application of technology and management practices a) to prevent accidents in plants, and/or b) to reduce the potential for accidents.

Process Safety Management—An OSHA regulation that emphasizes the management of safety within plants. This is an especially important and effective regulation that has 14 elements: 1) Employee Participation, 2) Process Safety Information, 3) Operating Procedures, 4) Process Hazards Analysis, 5) Mechanical Integrity, 6) Management of Change, 7) Incident Investigation, 8) Hot Work Permits, 9) Employee Training 10) Pre-Startup Review, 11) Emergency Planning, 12) Contractors, 13) Audits, and 14) Trade Secretes.

Safety Technology—Design features and control features to reduce the potential for accidents.

Safety Design Features—a) Inerting to control the concentration of a flammable gas to below the LFL, b) grounding and bonding to prevent static electricity charging and discharging (spark) and potential fire, c) installing relief valves to prevent vessel ruptures, d) installing double block and bleeds to prevent the backup of reactive chemicals into a monomer storage tank, e) installing an explosion suppression system to prevent dust explosions, f) installing containment systems to catch the release from relief valves, etc.

Safety Control Features—a) Monitoring the temperature and pressure to prevent abnormal conditions, b) adding reactor safeguards to prevent runaway reactions, c) adding redundant controls to decrease the frequency of accidents, d) adding more reliable instruments to reduce the frequency of plant accidents, etc.

II. COMMON DEFINITIONS: TERMS

Auto Ignition Temperature (AIT)—A fixed temperature above which a flammable mixture is capable of extracting enough energy from the environment to self-ignite.

Boiling Liquid Expanding Vapor Explosion (BLEVE)—A BLEVE occurs when a vessel ruptures which contains a liquid at a temperature above its atmospheric-pressure boiling point. It is the explosive vaporization of a large fraction of the vessel contents; possibly followed by the combustion or explosion of the vaporized cloud if it is combustible (similar to a rocket).

Deflagration—An explosion with a flame front moving in the unburned gas at a speed below the speed of sound (1250 ft/s).

Detonation—An explosion with a shock wave moving at a speed greater than the speed of sound in the unreacted medium.

Flash Point (FP)—The FP of a liquid is the lowest temperature at which it gives off enough vapor to form an ignitable mixture with air.

Flammability Limits (LFL and UFL)—A gas mixture will not burn when the composition is lower than the lower flammable limit (LFL). The mixture is also not combustible when the composition is above the upper flammability limit (UFL).

Flammability Limits of Mixtures—They are computed with the following equations:

$$LFL_{\text{MIXTURE}} = \frac{1}{\sum \left(\frac{y_i}{LFL_i} \right)}$$
$$UFL_{\text{MIXTURE}} = \frac{1}{\sum \left(\frac{y_i}{UFL_i} \right)}$$

Lower Flammability Limit in the Presence of Mists—

$$LFL_{\text{MISTS}} \approx 0.1 \times LFL_{\text{THEORETICAL}}$$

Mechanical Explosion—An explosion due to the sudden failure of a vessel containing a nonreactive gas at a high pressure.

Minimum Oxygen Concentration (MOC)—A mixture of gas will not burn if the oxygen concentration is below the minimum oxygen concentration.

Minimum Oxygen Concentration (MOC)—It is estimated using the following equation:

$$MOC = (LFL\%) \times \left(\frac{\text{Moles} \cdot \text{of} \cdot \text{Oxygen}}{\text{Moles} \cdot \text{of} \cdot \text{Fuel}} \right)$$

Overpressure—The pressure on an object as a result of an impacting shock wave.

Relief Valve—A device that relieves the pressure within a vessel when the pressure approaches the maximum allowable working pressure (MAWP). All vessels have reliefs.

Risk—This is the product of the frequency and the consequence of an accident scenario.

BIOCHEMICAL ENGINEERING

Contributed by David Murhammer

I. COMMON DEFINITIONS: GENERAL CONCEPTS

Aerobes—Organisms whose growth requires the presence of air or oxygen.

Anabolism—Metabolism involved with the biosynthesis of cellular components.

Anaerobes—Organisms that grow in the absence of air or oxygen.

Biochemical Engineering—The extension of chemical engineering principles to biological systems with the goal of producing useful products.

Bioreactor—A vessel used for biological processes. Examples include growing microorganisms and animal cells for the production of useful products.

Biotechnology—The use or development of methods of direct genetic manipulation for a socially desirable goal. Examples include the production of a particular chemical, production of better plants or seeds, and gene therapy.

Catabolism—Metabolism involved with the breakdown of materials for the production of intermediates and energy.

Enzyme—A catalytic protein (and in some cases RNA) produced by living cells.

Eukaryote—A cell or organism with a membrane-bound nucleus and well-developed organelles. Examples include yeast, animals, and plants.

Prokaryote—A cell lacking a true nucleus. Examples include bacteria and blue-green algae.

Virus—A noncellular entity that consists minimally of protein and DNA or RNA and that can replicate only after entry into specific types of living cells.

II. COMMON DEFINITIONS: TERMS

Antibiotics—Substances of microbial origin that in very small amounts have antimicrobial activity.

Antibodies—Glycoprotein molecules produced by B-lymphocytes in higher organisms in response to the introduction of a foreign material (antigen). These molecules react with antigens with great specificity.

Attachment Dependent—Cells whose growth requires attachment to a surface. Also referred to as Anchorage-Dependent.

Batch Culture—A culture that once supplied with raw materials is run to completion.

Chemostat—A bioreactor in which the continuous addition of fresh medium and removal of effluent results in constant nutrient, product, and cell concentrations when operated under steady state conditions.

Death Phase—The portion of the growth curve in culture in which there is a net decline in the number of viable (live) cells.

Exponential (Log) Growth Phase—A period of growth in a culture in which the number of cells or cell mass increases exponentially, i.e., the growth rate is proportional to the population density:

$$\frac{dX}{dt} = \mu X,$$

where X = cell number (cells/mL) or cell biomass (mg/mL), t is time, and μ is the specific growth rate (h^{-1}).

Fed-Batch Culture—A culture to which nutrients are periodically added during the operation of the culture.

Growth Yield—Yield of biomass based on substrate (e.g., glucose or oxygen) utilization:

$$Y_{X/S} = -\frac{dX}{dS},$$

where $Y_{X/S}$ is the yield coefficient of biomass (X) based on Substrate (S) and is usually given in terms of either (gm biomass/gm or mole substrate) or (cell number/gm or mole substrate).

$K_L a$ —Volumetric mass transfer coefficient usually measured in h^{-1} and often used to compare the efficiencies of bioreactors in supplying oxygen. The resulting oxygen transfer rate is then given by

$$\frac{dC_L}{dt} = K_L a (C^* - C_L),$$

where C_L is the dissolved oxygen concentration within the bioreactor, t in time, and C^* is the equilibrium dissolved oxygen concentration (i.e., solubility) under the specified conditions.

Lag Phase—The portion of the growth curve between inoculation and the beginning of cell growth.

Media Sterilization—Removal of undesired microorganisms from the media through filtration or heat to prevent their growth during the course of a bioreactor run.

Michaelis-Menton Kinetics—Common type of enzyme kinetics given by

$$v = \frac{v_{\max}[S]}{K_M + [S]},$$

where v is the reaction rate, $v_{\max}$ is the maximum reaction rate, K_M is the Michaelis Constant and is equal to the substrate concentration at $v = \frac{1}{2}v_{\max}$, and $[S]$ is the substrate concentration.

Perfusion Culture—A bioreactor in which cells are retained, medium is added continuously or semi-continuously, and spent medium containing toxic metabolites is removed.

Population Doubling Time (PDT)—The time required for the viable cell population to double. This term is commonly used for animal cell cultures, and is related to the specific growth rate (μ) by

$$PDT = \frac{\ln(2)}{\mu}.$$

Power Number (N_p)—A dimensionless number commonly used to determine the amount of power introduced to the bioreactor as a result of agitation. The

Power Number is given by

$$N_P = \frac{P}{\rho N^3 D^5},$$

where P is the power input, ρ is the density of the solution being agitated, N is the rotational speed of the impeller, and D is the impeller diameter.

Monod Equation—An equation commonly used to model the effect of the rate-limiting substrate concentration on the specific growth rate. This equation is given by

$$\mu = \frac{\mu_m [S]}{K_s + [S]},$$

where μ is the specific growth rate, μ_m is the maximum specific growth rate when $[S] \gg K_s$, $[S]$ is the substrate concentration, and K_s is the saturation constant or half-velocity constant and is equal to the substrate concentration when $\mu = \frac{1}{2}\mu_m$.

Stationary Phase—Phase in growth curve following the exponential growth phase in which there is no net growth. This phase is commonly associated with nutrient depletion.

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