1 Introduction to Engineering Calculation

- Base units

Dimension	SI	cgs	English
Length	m	cm	in, ft, mi
Mass	kg	g	lb_m
Time	s	s	s
Temperature	K	K	F
Current	A	A	
Light intensity	cd	cd	

- Derived units

Volume	liter	L	1000 cm^3
Force	Newton	N	1 kg m/s^2
	dyne		1 g cm/s^2
Energy/Work	Joule	J	1 N m = 1 kg m^2/s^2
	erg		1 dyne cm = 1 g cm^2/s^2
	calorie	cal	4.184 J
	Btu		1 Btu = 1055.05585 J
Power	Watt	W	1 J/s
	Horsepower	hp	1 hp = 745.7 W
Pressure	Pascal	Pa	1 N/m^2 = 1 J/m^3
	bar		10^5 Pa
	atmosphere	atm	1 atm = 1.01325 bar
	torr	torr	1/760 atm

- basic statistics

sample mean	*Sample variance*	*Standard deviation*
$\bar{X} = \sum_1^n X_i$	$s_X^2 = \frac{1}{N-1}\sum_1^n (X_i - \bar{X})^2$	$s_x = \sqrt{s_X^2}$

2 Processes and process variables

- Density

$$\rho = \frac{m}{V} = \frac{\dot{m}}{\dot{V}}$$

- Pressure

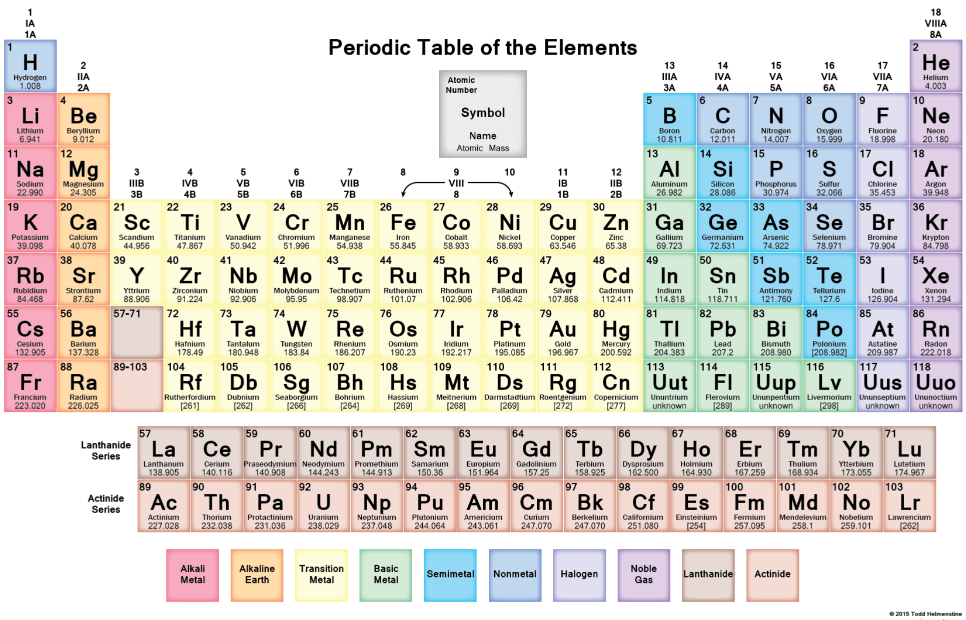
$$P = P_0 + \rho g h$$

$$P_{gauge} = P_{abs} - P_{atm}$$

- Temperature Scales

- Kelvin: absolute scale, $0 \to \infty$
- Celsius: $T(°C) = T(K) - 273.15)$
- Fahrenheit: $T(°F) = 1.8T(°C) + 32)$
- Rankine: absolute scale, $T(°R) = T(°F) + 459.67$

- Chemical composition



3 Material balances

- general balance

output = input + generation - consumption - accumulation

- Reaction progress

$$n_j = n_{j0} + \nu_j \xi$$

- *conversion*

$$X_j = \frac{n_{j0} - n_j}{n_{j0}} = -\frac{\nu_j \xi}{n_{j0}}$$

- Multiple reactions

$$n_j = n_{j0} + \sum_i \nu_{ij} \xi_i$$

- *yield* $= n_j / n_j^{\max}$
- *selectivity* (often) defined as amount of desired product over amount of undesired.

4 Properties of single-phase systems

- Ideal solution

$$v \text{ (l/mol)} = \sum_i x_i v_i$$

$$\frac{1}{\bar{\rho}} = \sum_i^n \frac{\omega_i}{\rho_i}$$

- Ideal gases

$$PV = nRT \text{ or } Pv = RT \text{ or } v = \frac{RT}{P}$$

R	8.314472 J / (K mol)	0.082057 atm l / (K mol)	1.3806504e-23 J / K

- Ideal gas mixture

$$V(N, T, P) = V_1(N_1, T, P) + V_2(N_2, T, P)$$

$$\frac{P_1}{P} = \frac{N_1 RT/V}{NRT/V} = y_1$$

- van der Waals model

$$P_{\mathrm{vdW}} = \frac{RT}{v - b} - \frac{a}{v^2}$$

$$b = v_c/3 \qquad a = \frac{9}{8} RT_c v_c$$

- reduced variables

$$T_r = T/T_c \quad P_r = P/P_c \quad v_r = v/v_c$$

- Soave-Redlich-Kwong (SRK) model

$$P_{\mathrm{SRK}} = \frac{RT}{v - b} - \frac{\alpha(T) a}{v(v + b)}$$

$$\begin{aligned} a &= 0.42747 \frac{(RT_c)^2}{P_c} \\ b &= 0.08664 \frac{RT_c}{P_c} \\ m &= 0.48508 + 1.55171\omega - 0.1561\omega^2 \\ \alpha &= 1 + m(1 - \sqrt{T_r}) \end{aligned}$$

2

- Pitzer "acentric" factor

$$\omega = -\log\left(\frac{P_{sat}}{P_c}\right)\Big|_{T_r=0.7} - 1$$

- Virial expansion

$$P = \frac{RT}{v}\left(1 + \frac{B_2(T)}{v} + \frac{B_3(T)}{v^2} + \cdots\right)$$

- *compressibility*

$$Z = \frac{P(v,T)v}{RT}$$

- Law of corresponding states

$$Z_c = 0.27$$

5 Two-phase systems

- Clapeyron equation

$$\frac{dP^*}{dT} = \frac{\Delta H_{\text{latent}}}{T(v_b - v_a)}$$

- Clausius-Clapeyron equation:

$$\ln\frac{P_2^*}{P_1^*} \approx -\frac{\Delta H_{\text{vap}}}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

- Antoine equation

$$\log_{10} P^* = A - \frac{B}{T + C}$$

- Gibbs phase rule

$$DOF = c - \Pi - r + 2$$

- Raoult's Law

$$x_A P_A^*(T) = P_A = y_A P$$

$$P_{\text{bubble}} = \sum x_i P_i^*$$

$$P_{\text{dew}} = \left(\sum_i \frac{y_i}{P_i^*}\right)^{-1}$$

- Relative humidity

$$RH(T) = P_{\mathrm{H_2O}}/P^*_{\mathrm{H_2O}}(T)$$

- Henry's Law

$$x_A H_A(T) = P_A = y_A P$$

- Colligative properties

$$\Delta T_b \approx \frac{RT_b^2}{\Delta H^*_{vap}} x$$

$$\Delta T_m \approx \frac{RT_m^2}{\Delta H^*_m} x$$

6 Energy balances

- Energy types

$$E_K = \frac{1}{2} m v^2 \qquad \dot{E}_K = \frac{1}{2} \dot{m} u^2$$

$$E_V = mgh \qquad \dot{E}_V = \dot{m} g z$$

$$U = U(T, P, x_i) \qquad H = U + PV$$

- Closed, constant volume system

$$\Delta U + \Delta E_K + \Delta E_V - q - w = 0$$

- Open system at steady-state

$$\Delta \dot{H} + \Delta \dot{E}_K + \Delta E_P = \dot{q} + \dot{W}_s$$

- Bernoulli equation:

$$\frac{1}{2} \Delta u^2 + g \Delta z + \frac{1}{\rho} \Delta P = 0$$

7 Energy balances on non-reactive systems

- heat capacity

$$C_v(T) = \left(\frac{\partial \hat{U}}{\partial T}\right)_v$$

$$C_p(T) = \left(\frac{\partial \hat{H}}{\partial T}\right)_p$$

- For liquids and solids, $C_p \approx C_v$
- For ideal gas, $C_p = C_v + R$

8 Energy balances on reactive systems

- Reaction energy

$$\Delta H_r^\circ = \sum_j \nu_j \Delta \hat{H}_{f,j}^\circ$$

- "Heat of reaction" method

$$\Delta \dot{H} = \xi \Delta \hat{H}_r^\circ + \sum_{out} \dot{n}_{out} \hat{H}_{out} - \sum_{in} \dot{n}_{in} \hat{H}_{in}$$

$$\Delta \dot{H} = \sum_i \xi_i \Delta \hat{H}_r^\circ + \sum_{out} \dot{n}_{out} \hat{H}_{out} - \sum_{in} \dot{n}_{in} \hat{H}_{in}$$

- "Heat of formation" method

$$\Delta \dot{H} = \sum_{out} \dot{n}_{out} \hat{H}_{out} - \sum_{in} \dot{n}_{in} \hat{H}_{in}$$

9 Transient processes

- General balance around any system or element of a system

$$\dot{F}_{out}(t) = \dot{F}_{in}(t) + r(t) - \frac{dF}{dt}$$