1 Selected Constants, Conversions, & Definitions

$\rho_{\text{water}} = \dfrac{62.43\text{lb}_\text{m}}{\text{ft}^3} = \dfrac{1000\text{ kg}}{\text{m}^3} = \dfrac{1\text{ g}}{\text{cm}^3}$

$g = 32.174\dfrac{\text{ft}}{\text{s}^2} = 9.8066\dfrac{\text{m}}{\text{s}^2}$

$1\text{ lb}_\text{f} = \dfrac{32.174\text{ lb}_\text{m}\cdot\text{ft}}{\text{s}^2}$

$1\text{ gallon} = 3.785\,\text{L} = 3.785\text{E}{-3}\,\text{m}^3 = 231\text{ in}^3$

$1\text{ lbmol} = 453.59\,\text{mol}$

$1\text{ W} = \dfrac{1\text{ kg}\cdot\text{m}^2}{\text{s}^3} = 1.34\times10^{-3}\text{ hp}$

$T[\text{K}] = T[^\circ\text{C}] + 273.15$

$T[^\circ\text{R}] = T[^\circ\text{F}] + 459.67 = 1.8(T[\text{K}])$

$T[^\circ\text{F}] = 1.8(T[^\circ\text{C}]) + 32$

$\Delta T = 1\text{K} = 1^\circ\text{C} = 1.8^\circ\text{F} = 1.8^\circ\text{R}$

$\hat{x} \equiv \dfrac{x}{m} \qquad \check{x} \equiv \dfrac{x}{n} \qquad$ for any quantity x

$m = V\rho \qquad \dot{m} = \dot{V}\rho = \vec{v}A_\sigma\rho$

$\rho = \sum_i \rho_i \qquad \rho_{\text{R},A} \equiv \dfrac{\rho_A}{\rho^{\ominus}}$

$n_i = \dfrac{m_i}{\check{m}_i} \qquad \dfrac{n_2}{n_1} = \dfrac{x_2}{x_1}$

$x_i = \dfrac{n_i}{n_\text{T}} = w_i\dfrac{\langle\check{m}\rangle}{\check{m}_i} \qquad w_i = \dfrac{m_i}{m_\text{T}} = \dfrac{\rho_i}{\rho}$

$\langle\check{m}\rangle = \dfrac{m_{\text{T,mix}}}{n_{\text{T,mix}}} = \sum_i x_i\check{m}_i = \left(\sum_i \dfrac{w_i}{\check{m}_i}\right)^{-1}$

$c_i = \dfrac{n_i}{V} = \dfrac{\rho_i}{\check{m}_i} \qquad c_i = x_i c \qquad c = \dfrac{\rho}{\langle\check{m}\rangle}$

1.1 Scaling & Linear Interpolation

$f_\text{s} = \frac{\text{original basis}}{\text{new basis}}$

$y = f(x) : \dfrac{y_\text{high} - y}{y_\text{high} - y_\text{low}} = \dfrac{x_\text{high} - x}{x_\text{high} - x_\text{low}}$

$\Delta\% = \frac{y_2 - y_1}{y_1} \times 100$

2 Ideal Gases

$PV = nRT \qquad P\dot{V} = \dot{n}RT \qquad p_iV = n_iRT \qquad \rho = \dfrac{P\langle\check{m}\rangle}{RT}$

$p_i = y_iP \qquad P = \sum_i p_i \qquad V_i = y_iV \qquad V = \sum_i V_i$

3 Material Balances

Input + Generation = Output + Accumulation + Consumption

$f_{\text{excess},A} = \dfrac{n_{A,\text{fed}} - n_{A,\text{stoich}}}{n_{A,\text{stoich}}}$

$f_{\text{conversion},A} = \dfrac{n_{A,\text{reacted}}}{n_{A,\text{fed}}}$

$f_{\text{yield},P} = \dfrac{n_{P,\text{formed}}}{n_{P,\text{theoretical}}} \qquad P$: desired product

$f_{\text{selectivity},P/Q} = \dfrac{n_P}{n_Q} \qquad P$: desired prd. $\quad Q$: undesired prd.

$n_i = n_{i0} + \nu_i\xi = n_{i0} - n_{i,\text{reacted}} \qquad n_i = n_{i0} + \sum_j \nu_{ij}\xi_j$

$\xi = \dfrac{n_i - n_{i0}}{\nu_i} = \dfrac{n_{i,\text{reacted}}}{\nu_i}$

$\dot{\xi} = \dfrac{\dot{n}_i - \dot{n}_{i0}}{\nu_i}$

4 Phase Equilibrium

Gibbs phase rule: $\nu = 2 + N_\text{species} - N_\text{phases}$

4.1 Vapour Pressure

Clausius-Clapeyron:

$\ln\dfrac{p_1^\star}{p_2^\star} = \left[\dfrac{-\Delta_\text{vap}\check{H}}{R}\right]\left[\dfrac{1}{T_1} - \dfrac{1}{T_2}\right]$

$\ln\, p_1^\star = \left[\dfrac{-\Delta_\text{vap}\check{H}}{R}\right]\left[\dfrac{1}{T_1}\right] + \left[\ln\, p_1^\star + \dfrac{\Delta_\text{vap}\check{H}}{RT_1}\right] \qquad [y = mx + b]$

Antoine: $\log p_i^\star = A - \dfrac{B}{T + C}$

4.2 Ideal Solution Vapour-Liquid Equilibrium

Raoult's law $\{x_i \approx 1\} : p_i = y_iP = x_ip_i^\star(T)$

Henry's law $\{x_i \approx 0\} : p_i = y_iP = x_i\mathcal{H}_i(T)$

$\{T = T_\text{bp}\} : y_i = \dfrac{p_i}{P_\text{bp}} \qquad p_i = x_ip_i^\star(T_\text{bp}) \qquad P = \sum_i x_ip_i^\star(T_\text{bp})$

$\{T = T_\text{dp}\} : x_i = \dfrac{y_iP}{p_i^\star(T_\text{dp})} \qquad P_\text{dp} = \left(\sum_i \frac{y_i}{p_i^\star(T)}\right)^{-1}$

Saturated vapour: $p_i = p_i^\star$

Superheated vapour: $y_iP < p_i^\star(T) \qquad {}^\circ$superheat $\equiv T_{(\text{g})} - T_\text{dp}$

$\{T_\text{sh} \to T_\text{dp}\} : p_i = y_iP = p_i^\star(T_\text{dp})$

4.3 Saturation and Humidity

$\underset{\cdot}{S} = \dfrac{p_i\check{m}_i}{(P - p_i)\check{m}_\text{dry}}\left[\frac{\text{kg vapour}}{\text{kg dry gas}}\right]$

$\underset{\cdot}{S}_\text{M} = \dfrac{p_i}{P - p_i}\left[\frac{\text{mol vapour}}{\text{mol dry gas}}\right]$

$\underset{\cdot}{S}_\text{P} = \dfrac{p_i/(P - p_i)}{p_i^\star/(P - p_i^\star)}$

$\underset{\cdot}{S}_\text{R} = \dfrac{p_i}{p_i^\star(T)}$

$\underset{\cdot}{H}_\text{X} :\quad$ gas $\to$ air $\quad$ vapour $\to$ $H_2O\,(\text{v})$

5 Energy Balance

$\leftarrow (-)Q(+) \rightarrow \boxed{\text{System}} \leftarrow (-)W(+) \rightarrow$

$E_\text{k} = \dfrac{m\vec{v}^2}{2} \qquad E_\text{p} = mgz$

5.1 Closed System

$\Delta U + \Delta E_\text{k} + \Delta E_\text{p} = Q_\text{in} - W_\text{s, by}$

$\Delta U = \sum\limits_\text{out} m_i\hat{U}_i - \sum\limits_\text{in} m_i\hat{U}_i = \sum\limits_\text{final} n_i\check{U}_i - \sum\limits_\text{initial} n_i\check{U}_i$

5.2 Open System at Steady State

$\Delta\dot{H} + \Delta\dot{E}_\text{k} + \Delta\dot{E}_\text{p} = \dot{Q}_\text{in} - \dot{W}_\text{s, by}$

$\dot{W} = \dot{W}_\text{s} + \dot{W}_\text{fl}$

$\dot{W}_\text{fl} = \sum\limits_\text{out} P_\text{out}\dot{V}_\text{out} - \sum\limits_\text{in} P_\text{in}\dot{V}_\text{in}$

$\Delta\dot{E}_\text{k} = \sum\limits_\text{out}\dfrac{\dot{m}_i\vec{v}_i^2}{2} - \sum\limits_\text{in}\dfrac{\dot{m}_iv_i^2}{2}$

$\Delta\dot{E}_\text{p} = \sum\limits_\text{out}\dot{m}_igz_i - \sum\limits_\text{in}\dot{m}_igz_i$

$H = U + PV$

$\Delta\dot{H} = \sum\limits_\text{out}\dot{m}_i\hat{H}_i - \sum\limits_\text{in}\dot{m}_i\hat{H}_i = \sum\limits_\text{out}\dot{n}_i\check{H}_i - \sum\limits_\text{in}\dot{n}_i\check{H}_i$

$\{\dot{m}_\text{out} = \dot{m}_\text{in}\} : \Delta\dot{H} = \dot{m}(\hat{H}_\text{out} - \hat{H}_\text{in}) = \dot{m}\Delta\hat{H}$

5.3 Mechanical System

$\dfrac{\Delta P}{\rho} + \dfrac{\Delta(\vec{v}^2)}{2} + g\Delta z + \sum\hat{F} = \dfrac{\dot{W}_\text{s, by}}{\dot{m}} \qquad \hat{F} = \Delta\hat{U} - \dfrac{\dot{Q}}{\dot{m}}$

6 Energy Balance on Nonreactive Processes

Liquid, solid: $\Delta H = V\Delta P + \int\limits_{T_1}^{T_2} C_P(T)\,dT$

6.1 Isothermal: $\{\Delta T = 0, \Delta P \neq 0\}$

Liquid, solid: $\Delta U = 0 \qquad \Delta H = V\Delta P$
Ideal gas: $\Delta U = 0 \qquad \Delta H = 0$

6.2 Isobaric: $\{\Delta P = 0, \Delta T \neq 0\}$

Ideal gas, liquid, solid: $\Delta U = \int_{T_1}^{T_2} C_V(T)\,dT$

Ideal gas: $\Delta H = \int_{T_1}^{T_2} C_P(T)\,dT$

6.3 Heat Capacity Estimation

Liquid, solid: $C_P \approx C_V \qquad$ Ideal gas: $\check{C}_P = \check{C}_V + R$
$\check{C}_{P,\text{mix}}(T) = \sum_i x_i \check{C}_{P,i}(T) \qquad \hat{C}_{P,\text{mix}} = \sum_i w_i \hat{C}_{P,i}$

$\Delta H = \int_{T_1}^{T_2} C_{P,\text{mix}}(T)\,dT$

6.4 Phase Change Operations

Example: $1 \xrightarrow{\Delta T} 2 \xrightarrow{\Delta\text{phase}} 3 \xrightarrow{\Delta T} 4$

$$\Delta H = \int_{T^\ominus}^{T_{\text{trs}}} C_P^\alpha\,dT \pm \Delta_{\text{trs}}H + \int_{T_{\text{trs}}}^{T_{\text{final}}} C_P^\beta\,dT$$

Trouton: $\Delta_{\text{vap}}\check{H} = 88\frac{\text{J}}{\text{mol K}}T_{\text{bp}}$ [nonpolar liquids]

Chen: $\Delta_{\text{vap}}\check{H} = RT_{\text{bp}}\dfrac{3.978(T_{\text{bp}}/T_{\text{c}}) - 3.958 + 1.555\ln P_{\text{c}}}{1.07 - T_{\text{bp}}/T_{\text{c}}}$

Watson: $\Delta_{\text{vap}}\check{H}(T_2) = \Delta_{\text{vap}}\check{H}(T_1)\left(\frac{T_{\text{c}}-T_2}{T_{\text{c}}-T_1}\right)^{0.38}$

Psychrometry: $\dot{m}_{\text{water(v)}} = \dfrac{H\dot{V}_{\text{air}}}{V_H}$

7 Energy Balance on Reactive Processes

7.1 Heat of Reaction

$$\Delta H = \frac{\Delta_{\text{r}}\check{H}(T^\ominus, P^\ominus)}{|\nu_i|}n_{i,\text{reacted}} = \xi\Delta_{\text{r}}\check{H}(T^\ominus, P^\ominus)$$

$\Delta_{\text{r}}\check{H} = \check{H}_{\text{prd}} - \check{H}_{\text{rct}} \qquad (+)$: endo $\quad (-)$: exo
Reference states: substance, phase, T, P

$$\Delta\dot{H} = \sum_{\text{reactions}} \dot{\xi}_j^\ominus \Delta_{\text{r}}\check{H}_j^\ominus + \sum_{\text{out}} \dot{n}_i\check{H}_i - \sum_{\text{in}} \dot{n}_i\check{H}_i$$

$$\check{H}_i = (\pm \text{ phase change } \check{H}) + \int_{T^\ominus}^{T_{\text{final}}} \check{C}_{P,i}\,dT$$

Closed: $\Delta_{\text{r}}\check{U}(T) = \Delta_{\text{r}}\check{H}(T) - RT\left(\sum_{\substack{\text{product}\\\text{ideal gas}}}|\nu_i| - \sum_{\substack{\text{reactant}\\\text{ideal gas}}}|\nu_i|\right)$

Hess's law: $\Delta_{\text{r}}\check{H}_3^\ominus = \Delta_{\text{r}}\check{H}_1^\ominus - \Delta_{\text{r}}\check{H}_2^\ominus$

7.2 Heat of Formation

$\Delta_{\text{r}}\check{H}^\ominus = \sum_i \nu_i\Delta_{\text{f}}\check{H}_i^\ominus$
$\check{H}^\ominus$: element in most stable form; T, P for $\Delta_{\text{f}}\check{H}^\ominus$; T, P uniform

$$\Delta\dot{H} = \sum_{\text{out}} \dot{n}_i\check{H}_i - \sum_{\text{in}} \dot{n}_i\check{H}_i \qquad \check{H}_i = \Delta_{\text{f}}\check{H}_i^\ominus + \int_{T_{\text{ref}}}^{T_2} \check{C}_{P,i}\,dT$$

7.3 Heat of Combustion

$\Delta_{\text{r}}\check{H}^\ominus = -\sum_i \nu_i\Delta_{\text{c}}\check{H}_i^\ominus$

7.4 Fuels

$\hat{H}_{\text{H}} = -\Delta_{\text{c}}\hat{H}^\ominus$ (when H_2O(l) produced)
$\hat{H}_{\text{L}} = -\Delta_{\text{c}}\hat{H}^\ominus$ (when H_2O(g) produced)
$\hat{H}_{\text{H}} = \hat{H}_{\text{L}} + n_{\text{out,water}}\Delta_{\text{vap}}\check{H}_{\text{water}}(25\,^\circ\text{C})$
$\check{H}_{\text{H}\vee\text{L,mix}} = \sum_i x_i\check{H}_{\text{H}\vee\text{L},i} \qquad \hat{H}_{\text{H}\vee\text{L,mix}} = \sum_i w_i\hat{H}_{\text{H}\vee\text{L},i}$

8 Balances on Transient Processes

$\frac{dm}{dt} = \dot{m}_{\text{in}} - \dot{m}_{\text{out}} + \dot{r}_{\text{gen}} - \dot{r}_{\text{cons}}$

Example: storage tank with increasing $\dot{m}_{\text{out}}$

$\frac{dm}{dt} = \dot{m}_{\text{in}} - \dot{m}_{\text{out}}$

$$\dot{m}_{\text{out}}(t) = \frac{\dot{m}_{\text{out},f} - \dot{m}_{\text{out},i}}{t_f - t_i}t + \dot{m}_{\text{out},i}$$

$$\int_{m_i}^{m} dm = \int_{t_0}^{t}(\dot{m}_{\text{in}} - \dot{m}_{\text{out}})\,dt \to \boxed{m(t) - m_i = \int_{t_0}^{t}(\dot{m}_{\text{in}} - \dot{m}_{\text{out}})\,dt}$$

References

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