1 Thermodynamics

1.1 Heat Capacities

- Equation can either be in the form: $c_p = A + BT + CT^2 + DT^3 + ET^{-2}$ or $c_p/R = A + BT + CT^2 + DT^3 + ET^{-2}$
- Reference sources for preset compounds:
    - Elementary Principles of Chemical Processes 3rd ed - R. Felder, R. Rousseau (Wiley, 2005)
    - Introduction to Chemical Engineering Thermodynamics 7th Ed. - J. M. Smith, H. C. van Ness, M. M. Abbott (McGraw-Hill)
- Possible calculation mode(s):

Inputs	Outputs
Eqn mode (c_p or c_p/R)	ΔH
Preset chemical compound	ΔU
Parameter A [optional]	ΔS ($= \int c_p/T \ dT$)
Parameter B [optional]	
Parameter C [optional]	
Parameter D [optional]	
Parameter E [optional]	
Initial temperature T1	
Final temperature T2	

- Units for presets: T in K, ΔH & ΔU in J/mol and ΔS in J/(mol.K)

1.2 Antoine Equation

- Equation can either be in the form: $\ln(p^*) = A - \frac{B}{C+T}$ or $\lg(p^*) = A - \frac{B}{C+T}$
- Units for presets: Vapour pressure p* in kPa, T in $^\circ$C
- Possible calculation mode(s):

Inputs	Outputs
Logarithm base used (log 10 or natural log) [mandatory] Temperature T [mandatory] Antoine parameter A [mandatory] Antoine parameter B [mandatory] Antoine parameter C [mandatory] Preset chemical compound [optional]	Vapour pressure P
Logarithm base used (log 10 or natural log) [mandatory] Vapour pressure P [mandatory] Antoine parameter A [mandatory] Antoine parameter B [mandatory] Antoine parameter C [mandatory] Preset chemical compound (optional)	Temperature T
Logarithm base used (log 10 or natural log) [mandatory] Vapour pressure P [mandatory] Temperature T [mandatory] Antoine parameter B [mandatory] Antoine parameter C [mandatory] Preset chemical compound (optional)	Antoine parameter A
Logarithm base used (log 10 or natural log) [mandatory] Vapour pressure P [mandatory]	Antoine parameter B

Temperature T [mandatory] Antoine parameter A [mandatory] Antoine parameter C [mandatory] Preset chemical compound (optional)	
Logarithm base used (log 10 or natural log) [mandatory] Vapour pressure P [mandatory] Temperature T [mandatory] Antoine parameter A [mandatory] Antoine parameter B [mandatory] Preset chemical compound (optional)	Antoine parameter C

- Reference sources for preset compounds:
  - Elementary Principles of Chemical Processes 3rd ed - R. Felder, R. Rousseau (Wiley, 2005)
  - Introduction to Chemical Engineering Thermodynamics 7th Ed. - J. M. Smith, H. C. van Ness, M. M. Abbott (McGraw-Hill)

1.3 2nd Virial Equation of State

- Units: All temperatures in Kelvins and all pressures in bar
- Calculation scheme using Pitzer correlations:
  - $T_r \equiv \frac{T}{T_c}$ and $P_r \equiv \frac{P}{P_c}$
  - $B^0 = 0.083 - \frac{0.422}{T_r^{1.6}}$ and $B^1 = 0.139 - \frac{0.172}{T_r^{4.2}}$
  - $\hat{B} = B^0 + \omega B^1$ and $B = \hat{B}\frac{RT_c}{P_c}$
  - $\frac{dB^0}{dT_r} = \frac{0.675}{T_r^{2.6}}$ and $\frac{dB^1}{dT_r} = \frac{0.722}{T_r^{5.2}}$
  - $H^R = RT_c P_r \left(B^0 - T_r \frac{dB^0}{dT_r} + \omega \left(B^1 - T_r \frac{dB^1}{dT_r} \right) \right)$ and $S^R = -RP_r \left(\frac{dB^0}{dT_r} + \omega \frac{dB^1}{dT_r} \right)$
  - $\frac{dB}{dT_r} = \frac{S^R}{P}$
  - $Z = 1 + \hat{B}\frac{P_r}{T_r}$
  - $V = Z\frac{RT}{P}$
- Possible calculation mode(s):

Inputs	Outputs
Preset chemical compound System temperature T Critical temperature T$_c$ System pressure P Critical pressure P$_c$ Acentric factor ω	Reduced temperature T$_r$ Reduced pressure P$_r$ Pitzer coefficient B^0, B^1, $\hat{B}$, B Pitzer derivatives $\frac{dB^0}{dT_r}, \frac{dB^1}{dT_r}, \frac{dB}{dT_r}$ Residual enthalpy H^R Residual entropy S^R Molar volume V Compressibility factor Z

1.4 van der Waals Equation of State

- Units: All temperatures in Kelvins and all pressures in bar
- Calculation scheme:
  - $T_r \equiv \frac{T}{T_c}$ and $P_r \equiv \frac{P}{P_c}$

- $a = \frac{27}{64}\frac{R^2 T_c^2}{P_c}$ and $b = \frac{RT_c}{8P_c}$
- V is solved from: $P = \frac{RT}{V-b} - \frac{a}{V^2}$ (iterative calculation using Newton-Raphson method)
- $H^R = RT\left(\frac{\rho b}{1-\rho b} - \frac{2\rho a}{RT}\right)$ and $S^R = R\ln\left(1 - \frac{\rho a}{RT} + \frac{\rho^2 ab}{RT}\right)$
- $Z = \frac{1}{1-\rho b} - \frac{\rho a}{RT}$ where $\rho = \frac{1}{V}$

- Possible calculation mode(s):

Inputs	Outputs
Preset chemical compound	Reduced temperature T_r
System temperature T	Reduced pressure P_r
Critical temperature T_c	Van der Waals EoS parameters *a, b*
System pressure P	Residual enthalpy H^R
Critical pressure P_c	Residual entropy S^R
	Molar volume V
	Compressibility factor Z

1.5 Fugacity

- Units: All temperatures in Kelvins, all pressures in bar, all fugacities in bar and all volumes in cm³/mol
- Calculation scheme:
  - $T_r \equiv \frac{T}{T_c}$ and $P_r \equiv \frac{P}{P_c}$
  - $B^0 = 0.083 - \frac{0.422}{T_r^{1.6}}$ and $B^1 = 0.139 - \frac{0.172}{T_r^{4.2}}$
  - $\hat{B} = B^0 + \omega B^1$
  - $V^{sat} = V_c Z_c^{(1-T_r)^{2/7}}$ (Rackett equation)
  - $\phi = \exp\left(\hat{B}\frac{P_r}{T_r}\right)$ and $\phi^{sat} = \exp\left(\hat{B}\frac{P_r}{T_r}\right)$
  - Three possibilities for physical state:
    - P < P^{sat}: $f = \phi P$ (vapour)
    - P > P^{sat}: $f = \phi^{sat} P^{sat} \times \exp\left(\frac{V^L}{RT}(P - P^{sat})\right)$ (liquid, Poynting correction factor)
    - P = P^{sat}: $f = \phi P$ (vapour-liquid equilibrium)
- Possible calculation mode(s):

Inputs	Outputs
Preset chemical compound	Physical state (this determines if the system is in liquid or vapour phase)
System temperature T	
Critical temperature T_c	Reduced temperature T_r
System pressure P	Reduced pressure P_r
Critical pressure P_c	Pitzer coefficient B^0, B^1, $\hat{B}$
Acentric factor ω	Molar volume at saturation V_{sat}
Critical molar volume V_c	Poynting correction factor PCR
Critical compressibility factor Z_c	Fugacity coefficient Φ
	Fugacity coefficient at saturation Φ_{sat}
	Fugacity *f*

1.6 Cross-Virial Binary Vapour Mixture Calculations

- Units: All temperatures in Kelvins, all pressures in bar, all fugacities in bar and all volumes in cm³/mol

- $\omega_{ij} = \frac{1}{2}(\omega_i + \omega_j)$, $(T_c)_{ij} = \sqrt{(T_c)_i (T_c)_j}$, $(Z_c)_{ij} = \frac{1}{2}((Z_c)_i + (Z_c)_j)$

- $(V_c)_{ij} = \left(\frac{1}{2}\left((V_c)_i^{\frac{1}{3}} + (V_c)_j^{\frac{1}{3}}\right)\right)^3$, $(P_c)_{ij} = \frac{(Z_c)_{ij} R (T_c)_{ij}}{(V_c)_{ij}}$

- $(T_r)_{ii} = \frac{T}{(T_c)_{ii}}$, $(T_r)_{jj} = \frac{T}{(T_c)_{jj}}$, $(T_r)_{ij} = \frac{T}{(T_c)_{ij}}$

- $(P_r)_{ii} = \frac{P}{(P_c)_{ii}}$, $(P_r)_{jj} = \frac{P}{(P_c)_{jj}}$, $(P_r)_{ij} = \frac{P}{(P_c)_{ij}}$

- $B_{ii}^0 = 0.083 - \frac{0.422}{T_{r,ii}^{1.6}}$, $B_{ii}^0 = 0.083 - \frac{0.422}{T_{r,jj}^{1.6}}$, $B_{ij}^0 = 0.083 - \frac{0.422}{T_{r,ij}^{1.6}}$

- $B_{ii}^1 = 0.139 - \frac{0.172}{T_{r,ii}^{4.2}}$, $B_{jj}^1 = 0.139 - \frac{0.172}{T_{r,jj}^{4.2}}$, $B_{ij}^1 = 0.139 - \frac{0.172}{T_{r,ij}^{4.2}}$

- $\widehat{B_{ii}} = B_{ii}^0 + \omega_{ii} B_{ii}^1$, $\widehat{B_{JJ}} = B_{jj}^0 + \omega_{jj} B_{jj}^1$, $\widehat{B_{ij}} = B_{ij}^0 + \omega_{ij} B_{ij}^1$

- $B_{ii} = \frac{\widehat{B_{ii}} R (T_c)_{ii}}{(P_c)_{ii}}$, $B_{jj} = \frac{\widehat{B_{JJ}} R (T_c)_{jj}}{(P_c)_{jj}}$, $B_{ij} = \frac{\widehat{B_{ij}} R (T_c)_{ij}}{(P_c)_{ij}}$

- $\delta_{ij} = 2B_{ij} - B_{ii} - B_{jj}$

- $\widehat{\phi_i} = \exp\left(\frac{P}{RT}\left(B_{ii} + y_j^2 \delta_{ij}\right)\right)$ and $\widehat{\phi_j} = \exp\left(\frac{P}{RT}\left(B_{jj} + y_i^2 \delta_{ji}\right)\right)$

- $f_{ii} = \widehat{\phi_i} y_i P$ and $f_{jj} = \widehat{\phi_j} y_j P$

- $B_{mix} = \sum \sum y_i y_j B_{ij} = y_1^2 B_{11} + 2 y_1 y_2 B_{12} + y_2^2 B_{22}$

- $Z_{mix} = 1 + \frac{B_{mix} P}{RT}$

1.7 Bubble, Dew & Flash Calculations

- For ideal and non-ideal systems
- Equations used:
    - Margules for non-ideal liquid phase
    - Pitzer and cross-virial for non-ideal vapour phase
- Supported types of systems: ideal gas + ideal solution (up to 4 components), ideal gas + non-ideal solution (up to 3 components), non-ideal gas + non-ideal solution (up to 2 components)

	2 components	3 components	4 components
Ideal vapour phase + ideal liquid phase	✓	✓	✓
Ideal vapour phase + non-ideal liquid phase	✓	✓	
Non-ideal vapour phase + non-ideal liquid phase	✓		

Ideal vapour phase + ideal liquid phase	$y_i P = x_i P_i^{sat}$ Compute P_{bbp} at constant T (we know x_i): $$\boldsymbol{P_{bbp}} = \sum y_i P = \sum x_i P_i^{sat}(T)$$

	Compute T_{bbp} at constant P (we know x_i): [iteration using Newton-Raphson] $$P = \sum y_i P = \sum x_i P_i^{sat}(\boldsymbol{T_{bbp}})$$ Compute T_{dp} at constant P (we know y_i): [iteration using Newton-Raphson] $$1 = \sum x_i = \sum \frac{y_i P}{P_i^{sat}(\boldsymbol{T_{dp}})}$$ Compute P_{dp} at constant T (we know y_i): $$1 = \sum x_i = (\boldsymbol{P_{dp}})\left(\sum \frac{y_i}{P_i^{sat}(T)}\right)$$ Flash calculations: [iteration using Newton-Raphson] $$z_i F = \boldsymbol{x_i} L + y_i V = y_i \frac{P}{P_i^{sat}(T)}(F - V) + y_i V$$ $$\sum \boldsymbol{y_i} = \sum \frac{z_i F}{\dfrac{P}{P_i^{sat}(T)}(F - V) + V} = 1$$
Ideal vapour phase + non-ideal liquid phase	$$\boldsymbol{y_i P = x_i \gamma_i(x_i, x_j, \dots) P_i^{sat}}$$ Compute P_{bbp} at constant T (we know x_i): $$\boldsymbol{P_{bbp}} = \sum \boldsymbol{y_i} P = \sum x_i \gamma_i(x_i) P_i^{sat}(T)$$ Compute T_{bbp} at constant P (we know x_i): [iteration using Newton-Raphson] $$P = \sum \boldsymbol{y_i} P = \sum x_i \gamma_i(x_i) P_i^{sat}(\boldsymbol{T_{bbp}})$$ Compute T_{dp} at constant P (we know y_i): [iteration using Newton-Raphson] $$1 = \sum \boldsymbol{x_i} = \sum \frac{y_i P}{\gamma_i(\boldsymbol{x_i}) P_i^{sat}(\boldsymbol{T_{dp}})}$$ Compute P_{dp} at constant T (we know y_i): [iteration using Newton-Raphson] $$1 = \sum \boldsymbol{x_i} = (\boldsymbol{P_{dp}})\left(\sum \frac{y_i}{\gamma_i(\boldsymbol{x_i}) P_i^{sat}(T)}\right)$$ Flash calculations: [iteration using Newton-Raphson] $$z_i F = \boldsymbol{x_i} L + y_i V = y_i \frac{P}{\gamma_i(\boldsymbol{x_i}) P_i^{sat}(T)}(F - V) + y_i V$$ $$\sum \boldsymbol{y_i} = \sum \frac{z_i F}{\dfrac{P}{\gamma_i(\boldsymbol{x_i}) P_i^{sat}(T)}(F - V) + V}$$
Non-ideal vapour phase + non-ideal liquid phase	$$\boldsymbol{y_i \widehat{\phi_i}(T, P, y_{j \neq i}, \dots) P}$$ $$= \boldsymbol{\gamma_i(x_i, x_j, \dots) x_i}$$ $$\times \boldsymbol{P_i^{sat} \phi_i^{sat} \exp\left(\frac{V^L}{RT}(P - P_i^{sat})\right)}$$ Compute P_{bbp} at constant T (we know x_i): [iteration using Newton-Raphson] $$\boldsymbol{P_{bbp}} = \sum \boldsymbol{y_i P_{bbp}} = \sum \frac{x_i \gamma_i(x_i) P_i^{sat}(T)}{\widehat{\phi_i}(T, \boldsymbol{P_{bbp}, y_j})}$$

Compute T_{bbp} at constant P (we know x_i): [iteration using Newton-Raphson]

$$P = \sum y_i P = \sum \frac{x_i \gamma_i(x_i) P_i^{sat}(T_{bbp})}{\hat{\phi}_i(T_{bbp}, P, y_j)}$$

Compute T_{dp} at constant P (we know y_i): [iteration using Newton-Raphson]

$$1 = \sum x_i = \sum \frac{y_i \hat{\phi}_i(T_{dp}, P, y_j) P}{\gamma_i(x_i) P_i^{sat}(T_{dp})}$$

Compute P_{dp} at constant T (we know y_i): [iteration using Newton-Raphson]

$$1 = \sum x_i = (P_{dp}) \left(\sum \frac{y_i \hat{\phi}_i(T, P_{dp}, y_j)}{\gamma_i(x_i) P_i^{sat}(T)} \right)$$

Flash calculations: [iteration using Newton-Raphson]

$$z_i F = x_i L + y_i V = y_i \frac{P}{\gamma_i(x_i) P_i^{sat}(T)} (F - V) + y_i V$$

$$\Sigma y_i = \sum \frac{z_i F}{\frac{P \hat{\phi}_i(T, P, y_j)}{\gamma_i(x_i) P_i^{sat}(T)} (F - V) + V}$$

- For each calculation mode key in all editable fields. Please ensure all input compositions add up to unity
- For Antoine presets, pressure is in kPa (using natural logarithm) and temperature is in ˚C
- For non-ideal liquid phase binary mixtures, use
  - $A_{12}=A_{21}$ and C=0 for 1-parameter Margules, and
  - C=0 for 2-parameter Margules
- For non-ideal liquid phase ternary mixtures, use
  - $A_{ij}=A_{ji}$ and C=0 for 1-parameter Margules, and
  - C=0 for 2-parameter Margules

1.8 Steam Calculations
- Using linear interpolation of IAPWS-IF97 reference tables.
- Saturated properties and superheated/subcooled properties are both supported

2 Fluid Mechanics

2.1 Standard Atmosphere Calculations
- Calculation mode: The only input required is altitude z in metres.

- Troposphere (0-11km) [adiabatic conditions, B≠0]: $T = T_0 - Bz \rightarrow \frac{P}{P_0} = \left(\frac{T_0 - Bz}{T_0} \right)^{\frac{M_r g}{RB}}$
  - surface temperature $T_0 = 288.15$ K, lapse rate $B = 0.00650$ K/m
- Stratosphere (11-20km) [isothermal conditions, B=0]: $T = T_c \rightarrow P = P_c \exp\left(\frac{M_r g(z_c - z)}{RT_C} \right)$
  - stratosphere base temperature $T_c = 216.65$ K, $P_c = 22.6$ kPa, $z_c = 11$ km

2.2 Friction Factor Calculations
- Dimensionless variables as inputs/outputs: Fanning friction factor φ, Reynolds number Re, relative roughness e/D

- Calculation modes:

Laminar flows	Re → e/D e/D → Re	$$\varphi = \frac{16}{Re}$$
Turbulent flows, smooth pipe	Re → φ	$$\frac{1}{\sqrt{\varphi}} = 4.03\lg\left(\frac{Re}{1/\sqrt{\varphi}}\right) - 0.50$$ (Iterate using Newton-Raphson)
	φ → Re	$$Re = 1.33067\left(1/\sqrt{\varphi}\right)e^{0.571361\left(1/\sqrt{\varphi}\right)}$$
Turbulent flows, Blasius (smooth pipe)	Re → φ	$$\varphi = 0.079Re^{-0.25}$$
	φ → Re	$$Re = \left(\frac{0.079}{\varphi}\right)^4$$
Turbulent flows, rough pipe	e/D → φ	$$\frac{1}{\sqrt{\varphi}} = 4.0\lg\left(\frac{D}{e}\right) + 2.2765$$
	φ → e/D	$$\frac{e}{D} = 10^{-0.25\left(\frac{1}{\sqrt{\varphi}}\right)+0.569125}$$
Colebrook	e/D & Re → φ	$$\frac{1}{\sqrt{\varphi}} = -4\lg\left(\frac{e}{3.715D} + \frac{1.255}{Re\sqrt{\varphi}}\right)$$ (Iterate using Newton-Raphson)
	φ & Re → e/D	$$\frac{e}{D} = -0.018575e^{-0.57565\left(\frac{1}{\sqrt{\varphi}}\right)}$$ $$\times \frac{\left(251\times10^{0.25\left(1/\sqrt{\varphi}\right)}\left(1/\sqrt{\varphi}\right) - 200Re\right)}{Re}$$
	φ & e/D → Re	$$Re = -\frac{186493\times 2^{\left(\frac{\left(1/\sqrt{\varphi}\right)}{4}-3\right)}5^{\left(\frac{\left(1/\sqrt{\varphi}\right)}{4}-2\right)}\left(1/\sqrt{\varphi}\right)}{2^{\left(\frac{\left(1/\sqrt{\varphi}\right)}{4}+3\right)}5^{\left(\frac{\left(1/\sqrt{\varphi}\right)}{4}+2\right)}(e/D) - 743}$$
Chen	e/D & Re → φ	$$\frac{1}{\sqrt{\varphi}} = -4\lg\left(\frac{\left(\frac{e}{D}\right)}{3.7065} - \frac{5.0452}{Re}\lg\left(\frac{\left(\frac{e}{D}\right)^{1.1098}}{2.8257} + \left(\frac{7.149}{Re}\right)^{0.8981}\right)\right)$$
	φ & Re → e/D	Iterate using binary search with $10^{-9} < \frac{e}{D} < 10^{-1}$ • If iterated φ is too high, reduce e/D • If iterated φ is too low, increase e/D
	φ & e/D → Re	Iterate using binary search with $10^{3} < Re < 10^{10}$ • If iterated φ is too high, reduce Re • If iterated φ is too low, increase Re

3 Reaction Kinetics

3.1 Kinetic Data Analysis

3.2 Single Reactor Performance Calculator

- For batch reactor, plug flow reactor (PFR) and continuous stirred-tank reactor (CSTR)
- If the fractional change in system volume ε_a is left blank, its value is assumed to be zero.

- Reference source for reactor sizing equations: Table 5.2 Performance Equations for nth-order Kinetics, in Chemical Reaction Engineering 3rd Ed., Octave Levenspiel (John Wiley & Sons)
- Possible calculation mode(s):

Inputs	Outputs
Reaction order n [mandatory – default value is 0th order] Reaction rate constant k [mandatory] Fraction change in system volume ε_a [optional, assumed zero if left blank] Initial concentration c_{A0} [mandatory] Final concentration c_A	Conversion X Space/reactor time t or τ
Reaction order n [mandatory – default value is 0th order] Reaction rate constant k [mandatory] Fraction change in system volume ε_a [optional, assumed zero if left blank] Initial concentration c_{A0} [mandatory] Conversion X	Final concentration c_A Space/reactor time t or τ
Reaction order n [mandatory – default value is 0th order] Reaction rate constant k [mandatory] Fraction change in system volume ε_a [optional, assumed zero if left blank] Initial concentration c_{A0} [mandatory] Space/reactor time t or τ	Conversion X Final concentration c_A

3.3 CSTRs in Series

4 Heat & Mass Transfer

4.1 Convective Heat Transfer

4.2 Transient Heat Transfer

4.3 Heat Exchanger

4.4 Mass Diffusivity Coefficients

4.5 Convective Mass Transfer

5 Fluid-Solid Systems

5.1 Single Particle Motion Properties

- For all single particle settling regimes (Stokes, Intermediate, Newton). Assumes perfectly spherical particle.
- Calculation scheme:
  - First assumes Stokes' Law applies:
    - $U_T = \frac{x^2(\rho_p - \rho_f)g}{18\mu}$
    - $C_D = \frac{4}{3}\frac{gx}{U_T^2}\left(\frac{\rho_p - \rho_f}{\rho_f}\right)$

- $Re_p = \frac{xU_T\rho_f}{\mu}$
  - If calculated $Re_p > 0.3$, assume Newton Law instead:
    - $U_T = 1.74\sqrt{\frac{xg(\rho_p-\rho_f)}{\rho_f}}$
    - $C_D = 0.44$
    - $Re_p = \frac{xU_T\rho_f}{\mu}$
  - If calculated $Re_p < 500$, assume intermediate region:
    - Iterate C_D via binary search to solve $C_D = \frac{1}{Re_p^2}\frac{4}{3}\frac{x^3\rho_f(\rho_p-\rho_f)g}{\mu^2}$ and $C_D = \frac{24}{Re_p}\left(1+0.15Re_p^{0.687}\right)$ simultaneously
    - Then as usual $Re_p = \frac{xU_T\rho_f}{\mu}$

5.2 Packed & Fluidised Bed Calculations

5.3 Pneumatic Transport

- Calculation scheme:
  - $A = \frac{\pi D^2}{4}$, $G_p = \frac{M_p}{A}$
  - $U_{SALT} = \left[\frac{M_p}{\rho_f A} \times 10^{(1440x+1.96)} \times \left(\sqrt{gD}\right)^{(1100x+2.5)}\right]^{\left(\frac{1}{1100x+3.5}\right)}$ (Rizk)
  - $U_{fs} = \left(1 + \frac{m}{100}\right) \times \max(U_{SALT}, U_{CH})$
  - $U_{pH} = U_{fs}\left(1 - 0.0638x^{0.3}\rho_p^{0.5}\right)$ (Hinkle)
  - $\varepsilon_H = 1 - \frac{G_p}{\rho_p U_{pH}}$ and $U_{fH} = \frac{U_{fs}}{\varepsilon_H}$
  - $Re_p = \frac{\rho_f(U_{fH}-U_{pH})x}{\mu}$
  - $C_D = \frac{24}{Re_p}\left(1 + 0.1806Re_p^{0.6459}\right) + \left(\frac{0.4251}{1+\frac{6880.95}{Re_p}}\right)$
  - $U_T = \sqrt{\frac{4}{3}\frac{gx}{C_D}\left(\frac{\rho_p-\rho_f}{\rho_f}\right)}$
  - $\frac{\rho_f^{0.77}}{2250D}\left(\frac{G_p}{\rho_P}\right)^2 = (\varepsilon_{CH}^{-4.7} - 1)(1 - \varepsilon_{CH})^2 \rightarrow$ Iterate for ε_{CH} using Newton-Raphson
  - $U_{CH} = \varepsilon_{CH}\left(U_T + \frac{G_p}{\rho_P(1-\varepsilon_{CH})}\right)$ (Punwani et. al.) $\rightarrow$ Check that $U_{CH} < U_{SALT}$, otherwise recalculate again up till C_D
  - $f_p = \frac{3\rho_f D}{8\rho_p x}C_D\left(\frac{U_{fH}-U_{pH}}{U_{pH}}\right)^2$ and $F_{pwH} = \frac{2f_p G_p U_{pH}}{D}$
  - $Re_f = \frac{\rho_f U_{fs}D}{\mu}$
  - $\frac{1}{\sqrt{f_f}} = -4\lg\left(\frac{\left(\frac{e}{D}\right)}{3.7065} - \frac{5.0452}{Re}\lg\left(\frac{\left(\frac{e}{D}\right)^{1.1098}}{2.8257} + \left(\frac{7.149}{Re}\right)^{0.8981}\right)\right)$ (Chen)
  - $F_{fw} = \frac{2f_f\rho_f U_{fs}^2}{D}$
  - $U_T\varepsilon_V^2 - \left(U_T + U_{fs} + \frac{G_p}{\rho_p}\right)\varepsilon_V + U_{fs} = 0 \rightarrow$ solve using quadratic formula
  - $U_{fV} = \frac{U_{fs}}{\varepsilon_V}$ and $U_{pV} = \frac{G_p}{\rho_p(1-\varepsilon_V)}$

- $F_{pwV} = 0.057 G_p \sqrt{\frac{g}{D}}$ (Konno & Saito)

- Pressure drop terms:

$$P_1 - P_2 = \underbrace{\frac{1}{2}\varepsilon\rho_f U_f^2}_{(1)} + \underbrace{\frac{1}{2}(1-\varepsilon)\rho_p U_p^2}_{(2)} + \underbrace{F_{fw}L}_{(3)} + \underbrace{F_{pw}L}_{(4)} + \underbrace{\rho_p L(1-\varepsilon)g\sin\theta}_{(5)} + \underbrace{\rho_f L\varepsilon g\sin\theta}_{(6)}$$

(1) pressure drop due to <u>initial</u> gas acceleration <u>(decide what is the starting direction)</u>
(2) pressure drop due to <u>initial</u> particle acceleration <u>(decide what is the starting direction)</u>
(3) pressure drop due to gas-to-wall friction
(4) pressure drop related to solids-to-wall friction
(5) pressure drop due to the static head of solids (<u>=0 for horizontal</u>)
(6) pressure drop due to the static head of gas (<u>=0 for horizontal</u>)

- Equivalent length approach: ΔP across one 90° bend = ΔP across 7.5m vertical pipe

6 Process Control
6.1 Laplace Transforms
6.2 2nd Order Dynamics

- For all step response types of second order transfer functions (overdamped, critically damped, underdamped): $G(s) = \dfrac{constant}{\tau^2 s^2 + 2\zeta\tau s + 1} = \dfrac{1}{As^2 + Bs + C}$
- Inputs: Parameters A, B and C
- Calculation scheme:
  - <u>Time of first peak</u>: $t_p = \dfrac{\pi\tau}{\sqrt{1-\zeta^2}}$
  - <u>Overshoot</u>: $OS = \dfrac{a}{b} = \exp\left(-\dfrac{\pi\zeta}{\sqrt{1-\zeta^2}}\right)$
  - <u>Decay ratio</u> (successive maxima): $DR = \dfrac{c}{b} = \exp\left(-\dfrac{2\pi\zeta}{\sqrt{1-\zeta^2}}\right) = \dfrac{a^2}{b^2} = (OS)^2$
  - <u>Period of oscillation</u>: $p = \dfrac{2\pi t}{\sqrt{1-\zeta^2}}$
  - <u>Cyclical freq</u>: $f = \dfrac{1}{p}$
  - <u>Radian freq</u>: $\omega = 2\pi f$
  - <u>Settling time</u> $t_s = -\dfrac{\ln\left(0.05\sqrt{1-\zeta^2}\right)}{\zeta\omega_n}$: time needed for response to come within specified % (e.g. 5%) of its final value
  - <u>Rise time</u> t_r: time needed for response to reach its final value for the first time. Characterizes speed of response. Iterated using binary search using the time-domain step response function

$$y(t) = KM\left(1 - e^{-\frac{\zeta t}{\tau}}\left(\cos\sqrt{1-\zeta^2}\,\frac{t}{\tau} + \frac{\zeta}{\sqrt{1-\zeta^2}}\sin\sqrt{1-\zeta^2}\,\frac{t}{\tau}\right)\right)$$

  - <u>Natural period of oscillations</u> (special case signifying 'frictionless' or 'no damping' situation): $\omega_n = \omega|_{\zeta=0} = \dfrac{1}{\tau}$

7 Process Safety & Health

7.1 Probit Calculations

- Probit correlation used: $Y = k_1 + k_2 \ln V$ (parameter values k_1, k_2 from Chemical Process Safety, Fundamentals with Applications, by Daniel A. Crowl & Joseph F. Louvar (Prentice Hall))
- Probit variable vs. probability conversion: $P = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{Y-5} \exp\left(-\frac{u^2}{2}\right) du = \frac{1}{2} \operatorname{erf}\left(\frac{Y-5}{\sqrt{2}}\right) + \frac{1}{2}$
- Units of causative variable V are dependent on user input, unless preset is chosen
- Please fill in: both k_1 and k_2, and only one of V, P or Y

7.2 Flammability Calculations

7.3 Source Term Calculations

7.4 Pasquill-Gifford Model

- Models supported: Puff (instantaneous release), Plume (continuous release, steady-state)
- Pasquill stability class correlations are utilised in dispersion coefficient calculations (Reference source: Chemical Process Safety, Fundamentals with Applications, 3rd ed, Prentice Hall by Daniel A. Crowl & Joseph F. Louvar)

Puff	$\langle C \rangle(x,y,z,t) = \dfrac{Q_m^*}{\sqrt{2}\pi^{3/2}\sigma_x\sigma_y\sigma_z} \exp\left[-\frac{1}{2}\left(\left(\frac{x-u_x t}{\sigma_x}\right)^2 + \left(\frac{y}{\sigma_y}\right)^2 + \left(\frac{z}{\sigma_z}\right)^2\right)\right]$
	$\langle C \rangle(u_x t,0,0,t) = \dfrac{Q_m^*}{\sqrt{2}\pi^{3/2}\sigma_x\sigma_y\sigma_z}$
	$\langle C \rangle(x,0,0,t) = \dfrac{Q_m^*}{\sqrt{2}\pi^{3/2}\sigma_x\sigma_y\sigma_z} \exp\left[-\frac{1}{2}\left(\left(\frac{x-u_x t}{\sigma_x}\right)^2\right)\right]$
Plume	$\langle C \rangle(x,y,z) = \dfrac{Q_m}{\pi\sigma_y\sigma_z u_x} \exp\left[-\frac{1}{2}\left(\left(\frac{y}{\sigma_y}\right)^2 + \left(\frac{z}{\sigma_z}\right)^2\right)\right]$
	$\langle C \rangle(x,0,0) = \dfrac{Q_m}{\pi\sigma_y\sigma_z u_x}$