Equations to use in Polymath

Isothermal Operation

$$\frac{df_{1B}}{dX} = \Re_{1B}$$

$$\frac{df_{2B}}{dX} = \Re_{2B}$$

$$\frac{df_{M}}{dX} = \Re_{M}$$

$$\frac{df_{T}}{dX} = \Re_{T}$$

$$\Re_{1B} = alfa \times \frac{k_1\, K_M\, K_{1B}\, x_M\, x_{1B}\left(\frac{1}{Keq_1}\frac{x_T}{x_M\, x_{1B}} - 1\right)}{\left(1 + K_{1B}\, x_{1B} + K_{2B}\, x_{2B} + K_M\, x_M + K_T\, x_T\right)^2} + \frac{k_3\, K_{1B}\, x_{1B}\left(\frac{1}{Keq_3}\frac{x_{2B}}{x_{1B}} - 1\right)}{\left(1 + K_{1B}\, x_{1B} + K_{2B}\, x_{2B} + K_M\, x_M + K_T\, x_T\right)}$$

$$\Re_{2B} = alfa \times \frac{k_2\, K_M\, K_{2B}\, x_M\, x_{1B}\left(\frac{1}{Keq_2}\frac{x_T}{x_M\, x_{2B}} - 1\right)}{\left(1 + K_{1B}\, x_{1B} + K_{2B}\, x_{2B} + K_M\, x_M + K_T\, x_T\right)^2} - \frac{k_3\, K_{1B}\, x_{1B}\left(\frac{1}{Keq_3}\frac{x_{2B}}{x_{1B}} - 1\right)}{\left(1 + K_{1B}\, x_{1B} + K_{2B}\, x_{2B} + K_M\, x_M + K_T\, x_T\right)}$$

$$\Re_M = \Re_{1B} + \Re_{2B}$$

$$\Re_T = -\Re_M$$

$$x_{1B} = \frac{f_{1B}}{f_{1B} + f_{2B} + f_M + f_T}$$

$$x_{2B} = \frac{f_{2B}}{f_{1B} + f_{2B} + f_M + f_T}$$

$$x_M = \frac{f_M}{f_{1B} + f_{2B} + f_M + f_T}$$

$$x_T = \frac{f_T}{f_{1B} + f_{2B} + f_M + f_T}$$

$$Keq_1 = \exp\left(\frac{5.0166 \times 10^3}{T} - 10.839\right)$$

$$Keq_2 = \exp\left(\frac{3.7264 \times 10^3}{T} - 9.6367\right)$$

$$Keq_3 = \frac{Keq_1}{Keq_2}$$

$$k_1 = 3.2870\times10^{10}\ \exp\left(-\frac{76.8\times10^3}{R\,T}\right)$$

$$k_2 = 3.9682\times10^{13}\ \exp\left(-\frac{99.7\times10^3}{R\,T}\right)$$

$$k_3 = 7.4767\times10^{10}\ \exp\left(-\frac{81.7\times10^3}{R\,T}\right)$$

$$K_{1B} = \exp\left(\frac{4.6825\times10^3}{T} - 10.157\right)$$

$$K_{2B} = \exp\left(\frac{3.4420\times10^3}{T} - 6.5849\right)$$

$$K_M = \exp\left(\frac{1.0014\times10^3}{T} + 4.7496\right)$$

$$K_T = \exp\left(\frac{2.3934\times10^3}{T} - 3.5736\right)$$

$$alfa = \frac{\rho_b}{\varepsilon\, C_{total}^{IN}}$$

Initial values: $X_0 = 0.0$, $f_{1B} = \frac{C_{1B}^{IN}}{C_{total}^{IN}}$, $f_{2B} = \frac{C_{2B}^{IN}}{C_{total}^{IN}}$, $f_M = \frac{C_M^{IN}}{C_{total}^{IN}}$, $f_T = \frac{C_T^{IN}}{C_{total}^{IN}}$

Final value: $X_f = 1.0$

Non-Isothermal Operation
$$\frac{df_{1B}}{dX} = \Re_{1B}$$

$$\frac{df_{2B}}{dX} = \Re_{2B}$$

$$\frac{df_{M}}{dX} = \Re_{M}$$

$$\frac{df_{T}}{dX} = \Re_{T}$$

$$\frac{dT}{dX} = \frac{1}{\varepsilon}\left[\frac{\rho_b\,\tau}{\rho\,Cp}\sum_{j=1}^{M\ reactions}\left(\Delta H_j^R\ r_j\right) - NTU\left(T - T_w\right)\right]$$

$$\Re_{1B} = alfa \times \frac{k_1\,K_M\ K_{1B}\ x_M\ x_{1B}\left(\frac{1}{Keq_1}\frac{x_T}{x_M\ x_{1B}} - 1\right)}{\left(1 + K_{1B}\ x_{1B} + K_{2B}\ x_{2B} + K_M\ x_M + K_T\ x_T\right)^2} + \frac{k_3\ K_{1B}\ x_{1B}\left(\frac{1}{Keq_3}\frac{x_{2B}}{x_{1B}} - 1\right)}{\left(1 + K_{1B}\ x_{1B} + K_{2B}\ x_{2B} + K_M\ x_M + K_T\ x_T\right)}$$

$$\Re_{2B} = alfa \times \frac{k_2\,K_M\ K_{2B}\ x_M\ x_{1B}\left(\frac{1}{Keq_2}\frac{x_T}{x_M\ x_{2B}} - 1\right)}{\left(1 + K_{1B}\ x_{1B} + K_{2B}\ x_{2B} + K_M\ x_M + K_T\ x_T\right)^2} - \frac{k_3\ K_{1B}\ x_{1B}\left(\frac{1}{Keq_3}\frac{x_{2B}}{x_{1B}} - 1\right)}{\left(1 + K_{1B}\ x_{1B} + K_{2B}\ x_{2B} + K_M\ x_M + K_T\ x_T\right)}$$

$$\Re_M = \Re_{1B} + \Re_{2B}$$

$$\Re_T = -\,\Re_M$$

$$r_1 = \frac{k_1\,K_M\ K_{1B}\ x_M\ a_{1B}\left(\frac{1}{Keq_1}\frac{x_T}{x_M\ x_{1B}} - 1\right)}{\left(1 + K_{1B}\ x_{1B} + K_{2B}\ x_{2B} + K_M\ x_M + K_T\ x_T\right)^2}$$

$$r_2 = \frac{k_2\,K_M\ K_{2B}\ x_M\ x_{1B}\left(\frac{1}{Keq_2}\frac{x_T}{x_M\ x_{2B}} - 1\right)}{\left(1 + K_{1B}\ x_{1B} + K_{2B}\ x_{2B} + K_M\ x_M + K_T\ x_T\right)^2}$$

$$r_3 = \frac{k_3\ K_{1B}\ x_{1B}\left(\frac{1}{Keq_3}\frac{x_{2B}}{x_{1B}} - 1\right)}{1 + K_{1B}\ x_{1B} + K_{2B}\ x_{2B} + K_M\ x_M + K_T\ x_T}$$

$$x_{1B} = \frac{f_{1B}}{f_{1B} + f_{2B} + f_M + f_T}$$

$$x_{2B} = \frac{f_{2B}}{f_{1B} + f_{2B} + f_M + f_T}$$

$$x_M = \frac{f_M}{f_{1B} + f_{2B} + f_M + f_T}$$

$$x_T = \frac{f_T}{f_{1B} + f_{2B} + f_M + f_T}$$

$$Keq_1 = \exp\left(\frac{5.0166\times10^3}{T} - 10.839\right)$$

$$Keq_2 = \exp\left(\frac{3.7264\times10^3}{T} - 9.6367\right)$$

$$Keq_3 = \frac{Keq_1}{Keq_2}$$

$$k_1 = 3.2870\times10^{10}\ \exp\left(-\frac{76.8\times10^3}{R\,T}\right)$$

$$k_2 = 3.9682\times10^{13}\ \exp\left(-\frac{99.7\times10^3}{R\,T}\right)$$

$$k_3 = 7.4767\times10^{10}\ \exp\left(-\frac{81.7\times10^3}{R\,T}\right)$$

$$K_{1B} = \exp\left(\frac{4.6825\times10^3}{T} - 10.157\right)$$

$$K_{2B} = \exp\left(\frac{3.4420\times10^3}{T} - 6.5849\right)$$

$$K_M = \exp\left(\frac{1.0014\times10^3}{T} + 4.7496\right)$$

$$K_T = \exp\left(\frac{2.3934\times10^3}{T} - 3.5736\right)$$

$$alfa = \frac{\rho_b}{\varepsilon\, C_{total}^{IN}}$$

$$NTU = \frac{2U\,\tau}{\rho\, Cp\, R_0}$$

$$\Delta H_1^R = -41.708 \times 10^3$$

$$\Delta H_2^R = -30.981 \times 10^3$$

$$\Delta H_3^R = -10.727 \times 10^3$$

Initial values: $X_0 = 0.0$, $f_{1B} = \frac{C_{1B}^{IN}}{C_{total}^{IN}}$, $f_{2B} = \frac{C_{2B}^{IN}}{C_{total}^{IN}}$, $f_M = \frac{C_M^{IN}}{C_{total}^{IN}}$, $f_T = \frac{C_T^{IN}}{C_{total}^{IN}}$; $T = T_0$

Final value: $X_f = 1.0$

$$C_{total}^{IN} = \sum_i C_i^{IN}$$