

$$T := 1000 \quad P_0 := 25 \cdot 101325 \quad v_0 := 0.42 \quad D := 0.5 \quad W := 500 \quad \eta := 2 \cdot 10^{-5} \quad \rho_b := 560$$

$$D_p := 0.01 \quad \phi := 0.30 \quad k_c := 5.6 \cdot 10^{-3} \quad R := 8.314 \quad F_{T0} := \frac{P_0 \cdot v_0}{R \cdot T} \quad a := \frac{4}{D} \quad A_c := \pi \cdot \frac{D^2}{4}$$

$$F_{C3H8} := F_{T0} \cdot 0.05 \quad F_{CO2} := .05 \cdot F_{T0} \quad F_{N2} := .01 \cdot F_{T0}$$

$$\begin{aligned} k_1 &:= 8.7 \cdot 10^{-6} & K_1 &:= 7.4 & k_2 &:= 0.092 & K_2 &:= 11.7 & k_3 &:= 0.056 & K_3 &:= 0.98 \\ k_4 &:= 12.5 \cdot 10^{-5} & K_4 &:= 3.6 \end{aligned}$$

$$r_1(F_{CH4}, F_{C2H4}, F_{H2}, v) := k_1 \cdot \left(\frac{F_{CH4}^2}{v^2} - \frac{F_{C2H4} \cdot F_{H2}^2}{K_1 \cdot v^3} \right)$$

$$r_2(F_{C2H4}, F_{H2}, F_{C6H6}, v) := \frac{k_2 \cdot \frac{F_{C2H4}}{v}}{1 + \frac{K_2}{v} \cdot (F_{C2H4} + F_{H2} + F_{C6H6})}$$

$$r_3(F_{C2H4}, F_{C6H6}, F_{H2}, F_{C10H8}, v) := \frac{k_3 \cdot F_{C2H4} \cdot F_{C6H6}}{v^2 \cdot \left(1 + \frac{K_3}{v^2} \cdot (F_{C2H4} + F_{H2} + F_{C6H6} + F_{C10H8})^2 \right)}$$

$$r_4(F_{C2H6}, F_{C2H4}, F_{H2}, v) := k_4 \cdot \left(\frac{F_{C2H6}}{v} - \frac{F_{C2H4} \cdot F_{H2}}{v^2 \cdot K_4} \right)$$

$$m := F_{T0} \cdot (.77 \cdot .016 + .12 \cdot .03 + .05 \cdot .044 + .05 \cdot .044 + .01 \cdot .028) \quad G := \frac{m}{A_c} \quad \rho_0 := \frac{m}{v_0}$$

$$\beta_0 := \frac{G \cdot (1 - \phi)}{\rho_0 \cdot D_p \cdot \phi^3} \cdot \left(\frac{150 \cdot (1 - \phi) \cdot \eta}{D_p} + 1.75 \cdot G \right) \quad \alpha := \frac{2 \cdot \beta_0}{A_c \cdot \rho_b \cdot (1 - \phi) \cdot P_0}$$

$$F_T(w) = F_{CH_4}(w) + F_{C_2H_6}(w) + F_{C_3H_8} + F_{CO_2} + F_{N_2} + F_{C_2H_4}(w) + F_{C_6H_6}(w) + F_{C_{10}H_8}(w) + F_{H_2}(w)$$

$$v(w) = \frac{P_0}{P(w)} \cdot \frac{F_T(w)}{F_{T0}}$$

$$\frac{d}{dw} F_{CH_4}(w) = -2 \cdot r_1(F_{CH_4}(w), F_{C_2H_4}(w), F_{H_2}(w), v(w))$$

$$\frac{d}{dw} F_{C_2H_6}(w) = -r_4(F_{C_2H_6}(w), F_{C_2H_4}(w), F_{H_2}(w), v(w))$$

$$\frac{d}{dw} F_{C_2H_4}(w) = r_1(F_{CH_4}(w), F_{C_2H_4}(w), F_{H_2}(w), v(w)) - 3 \cdot r_2(F_{C_2H_4}(w), F_{H_2}(w), F_{C_6H_6}(w), v(w)) - 2 \cdot r_3(F_{C_2H_4}(w), F_{C_6H_6}(w), F_{H_2}(w), F_{C_{10}H_8}(w), v(w)) +$$

$$\frac{d}{dw} F_{C_6H_6}(w) = r_2(F_{C_2H_4}(w), F_{H_2}(w), F_{C_6H_6}(w), v(w)) - r_3(F_{C_2H_4}(w), F_{C_6H_6}(w), F_{H_2}(w), F_{C_{10}H_8}(w), v(w))$$

$$\frac{d}{dw} F_{C_{10}H_8}(w) = r_3(F_{C_2H_4}(w), F_{C_6H_6}(w), F_{H_2}(w), F_{C_{10}H_8}(w), v(w))$$

$$\frac{d}{dw} F_{H_2}(w) = 2 \cdot r_1(F_{CH_4}(w), F_{C_2H_4}(w), F_{H_2}(w), v(w)) + 3 \cdot r_2(F_{C_2H_4}(w), F_{H_2}(w), F_{C_6H_6}(w), v(w)) + 3 \cdot r_3(F_{C_2H_4}(w), F_{C_6H_6}(w), F_{H_2}(w), F_{C_{10}H_8}(w), v(w)) +$$

$$\frac{d}{dw} P(w) = \frac{-\alpha}{2} \cdot \frac{P_0^2}{P(w)} \cdot \frac{F_T(w)}{F_{T0}}$$

$$F_{CH_4}(0) = .77 \cdot F_{T0}$$

$$F_{C_2H_6}(0) = .12 \cdot F_{T0}$$

$$F_{C_2H_4}(0) = 0$$

$$F_{C_6H_6}(0) = 0$$

$$F_{C_{10}H_8}(0) = 0$$

$$F_{H_2}(0) = 0$$

$$P(0) = P_0$$

$$F_T(0) = .77 \cdot F_{T0} + .12 \cdot F_{T0} + F_{C_3H_8} + F_{CO_2} + F_{N_2}$$

$$v(0) = \frac{.77 \cdot F_{T0} + .12 \cdot F_{T0} + F_{C_3H_8} + F_{CO_2} + F_{N_2}}{F_{T0}}$$

$$\begin{bmatrix} F_{CH_4} \\ F_{C_2H_6} \\ F_{C_2H_4} \\ F_{C_6H_6} \\ F_{C_{10}H_8} \\ F_{H_2} \\ P \\ F_T \\ v \end{bmatrix} := \text{odesolve} \left(\begin{bmatrix} F_{CH_4}(w) \\ F_{C_2H_6}(w) \\ F_{C_2H_4}(w) \\ F_{C_6H_6}(w) \\ F_{C_{10}H_8}(w) \\ F_{H_2}(w) \\ P(w) \\ F_T(w) \\ v(w) \end{bmatrix}, W \right)$$

