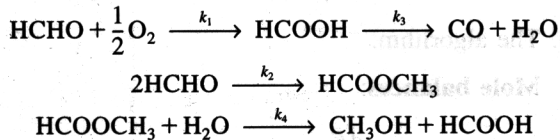


O.D.E. SOLVER ALGORITHM

MULTIPLE ELEMENTARY REACTIONS IN A PFR



Let A = HCHO, B = O₂, C = HCOOH, D = HCOOCH₃, E = CO, W = H₂O, G = CH₃OH

$$\frac{dF_A}{dV} = -k_1 C_{T0}^{3/2} \left(\frac{F_A}{F_T}\right) \left(\frac{F_B}{F_T}\right)^{1/2} - k_2 C_{T0}^2 \left(\frac{F_A}{F_T}\right)^2$$

$$\frac{dF_B}{dV} = -\frac{k_1}{2} C_{T0}^{3/2} \left(\frac{F_A}{F_T}\right) \left(\frac{F_B}{F_T}\right)^{1/2}$$

$$\frac{dF_C}{dV} = k_1 C_{T0}^{3/2} \left(\frac{F_A}{F_T}\right) \left(\frac{F_B}{F_T}\right)^{1/2} - k_3 C_{T0} \left(\frac{F_C}{F_T}\right) + k_4 C_{T0}^2 \left(\frac{F_W}{F_T}\right) \left(\frac{F_D}{F_T}\right)$$

$$\frac{dF_D}{dV} = \frac{k_2}{2} C_{T0}^2 \left(\frac{F_A}{F_T}\right)^2 - k_4 C_{T0}^2 \left(\frac{F_D}{F_T}\right) \left(\frac{F_W}{F_T}\right)$$

$$\frac{dF_E}{dV} = k_3 C_{T0} \left(\frac{F_C}{F_T}\right)$$

$$\frac{dF_W}{dV} = k_3 C_{T0} \left(\frac{F_C}{F_T}\right) - k_4 C_{T0}^2 \left(\frac{F_W}{F_T}\right) \left(\frac{F_D}{F_T}\right)$$

$$\frac{dF_G}{dV} = k_4 C_{T0}^2 \left(\frac{F_W}{F_T}\right) \left(\frac{F_D}{F_T}\right)$$

$$F_T = F_A + F_B + F_C + F_D + F_E + F_W + F_G$$

$$F_{A0} = 10, F_{B0} = 5, V_F = 1000, k_1 C_{T0}^{3/2} = 0.04, k_2 C_{T0}^2 = 0.007, k_3 C_{T0} = 0.014, k_4 C_{T0}^2 = 0.45$$