

REB, The Book

Example 4.8.5 Calculations

Equation numbers correspond to the Example 4.8.5 Solution

Apparent Rate of the Non-Elementary Reaction

$$r_1 = r_4 = k_{4,f} \theta_A \theta_B - k_{4,r} \theta_Y \theta_Z \quad (7)$$

Quasi-Equilibrium Expressions

$$K_2 = \frac{\theta_A}{[A] \theta_v} \quad (8)$$

$$K_3 = \frac{\theta_B}{[B] \theta_v} \quad (9)$$

$$K_5 = \frac{[Y] \theta_v}{\theta_Y} \quad (10)$$

$$K_6 = \frac{[Z] \theta_v}{\theta_Z} \quad (11)$$

Site Conservation Equation

$$1 = \theta_v + \theta_A + \theta_B + \theta_Y + \theta_Z \quad (12)$$

Solve equations (8) through (11) for the coverages of A, B, Y, and Z, respectively.

$$\theta_A = K_2 [A] \theta_v \quad (A)$$

$$\theta_B = K_3 [B] \theta_v \quad (B)$$

$$\theta_Y = \frac{[Y]}{K_5} \theta_v \quad (C)$$

$$\theta_Z = \frac{[Z]}{K_6} \theta_v \quad (D)$$

Substitute (A) through (D) into equation (12) and solve for the vacant site coverage.

$$1 = \theta_v + \theta_A + \theta_B + \theta_Y + \theta_Z$$

$$1 = \theta_v + K_2 [A] \theta_v + K_3 [B] \theta_v + \frac{[Y]}{K_5} \theta_v + \frac{[Z]}{K_6} \theta_v$$

$$\theta_v = \frac{1}{1 + K_2 [A] + K_3 [B] + \frac{1}{K_5} [Y] + \frac{1}{K_6} [Z]} \quad (E)$$

Substitute equation (E) into equations (A) through (D).

$$\theta_A = \frac{K_2 [A]}{1 + K_2 [A] + K_3 [B] + \frac{1}{K_5} [Y] + \frac{1}{K_6} [Z]} \quad (14)$$

$$\theta_B = \frac{K_3 [B]}{1 + K_2 [A] + K_3 [B] + \frac{1}{K_5} [Y] + \frac{1}{K_6} [Z]} \quad (15)$$

$$\theta_Y = \frac{\frac{1}{K_5} [C]}{1 + K_2 [A] + K_3 [B] + \frac{1}{K_5} [Y] + \frac{1}{K_6} [Z]} \quad (16)$$

$$\theta_Z = \frac{\frac{1}{K_6} [D]}{1 + K_2 [A] + K_3 [B] + \frac{1}{K_5} [Y] + \frac{1}{K_6} [Z]} \quad (17)$$

Substitute equations (14) through (17) into equation (7)

$$r_1 = \frac{k_{4,f} K_2 K_3 [A] [B] - \frac{k_{4,r}}{K_5 K_6} [Y] [Z]}{\left(1 + K_2 [A] + K_3 [B] + \frac{1}{K_5} [Y] + \frac{1}{K_6} [Z] \right)^2} \quad (18)$$