REB, The Course
Class 5 Practice Assignment Calculations

Equation numbers correspond to Class 5 Practice Assignment Solution

Rate expression for the non-elementary reaction:

$$r_{j_{non}} = r_{j_{rds}} = k_{j_{rds},f} \prod_{i_r} [i_r]^{-\nu_{i_r,j_{rds}}} - k_{j_{rds},r} \prod_{i_p} [i_p]^{\nu_{i_p,j_{rds}}}$$

$$r_1 = k_{3,f} \left[NO_2\right] \left[NO_3\right] - k_{3,r} \left[NO_2\right] \left[O_2\right] \left[NO\right] \tag{6}$$

Quasi-equilibrium expressions:

$$K_{j_{nrd}} = \prod_i [i]^{\nu_{i,j_{nrd}}}$$

$$K_2 = \frac{\left[NO_2\right] \left[NO_3\right]}{\left[N_2O_5\right]} \tag{7}$$

$$K_4 = \frac{\left[NO_2\right] \left[N_2O_4\right]}{\left[NO\right] \left[N_2O_5\right]} \tag{8}$$

$$K_5 = \frac{\left[N_2O_4\right]}{\left[NO_2\right]^2} \tag{9}$$

Start by solving equations (7) through (9) to generate expressions for $\left[NO_2\right]$, $\left[NO_3\right]$, and $\left[NO\right]$. Equation (9) can be solved for the concentration of NO_2.

$$\left[NO_2\right] = \sqrt{\frac{\left[N_2O_4\right]}{K_5}} \tag{10}$$

After substitution of equation (10) into equation (8), it can be solved for the concentration of NO.

$$K_4 = \frac{\sqrt{\frac{[N_2O_4]}{K_5}}\,[N_2O_4]}{[NO]\,[N_2O_5]}$$

$$[NO] = \frac{[N_2O_4]^{\frac{3}{2}}}{K_4\sqrt{K_5}\,[N_2O_5]} \tag{11}$$

After substitution of equation (10) into equation (7), it can be solved for the concentration of NO_3.

$$K_2 = \frac{\sqrt{\frac{[N_2O_4]}{K_5}}\,[NO_3]}{[N_2O_5]}$$

$$[NO_3] = \frac{K_2\sqrt{K_5}\,[N_2O_5]}{\sqrt{[N_2O_4]}} \tag{12}$$

Substitution of equations (10) - (12) into equation (6) yields the rate expression.

$$r_1 = k_{3,f}[NO_2]\,[NO_3] - k_{3,r}[NO_2]\,[O_2]\,[NO]$$

$$r_1 = k_{3,f}\sqrt{\frac{[N_2O_4]}{K_5}}\frac{K_2\sqrt{K_5}\,[N_2O_5]}{\sqrt{[N_2O_4]}} - k_{3,r}\sqrt{\frac{[N_2O_4]}{K_5}}\,[O_2]\,\frac{[N_2O_4]^{\frac{3}{2}}}{K_4\sqrt{K_5}\,[N_2O_5]}$$

$$r_1 = k_{3,f}K_2\,[N_2O_5] - \frac{k_{3,r}}{K_4K_5}\frac{[N_2O_4]^2\,[O_2]}{[N_2O_5]} \tag{13}$$

Step 3. The rate coefficients and equilibrium constants can be grouped as shown in equations (14) and (15). Substitution into equation (13) yields the rate expression in terms of apparent rate coefficients, equation (16).

$$k_f = k_{3,f} K_2 \tag{14}$$

$$k_r = \frac{k_{3,r}}{K_4 K_5} \tag{15}$$

$$r_1 = k_f \left[N_2O_5\right] - k_r \frac{\left[N_2O_4\right]^2 \left[O_2\right]}{\left[N_2O_5\right]} \tag{16}$$