Problem #1

N_2O_5 Decomposition

$$2N_2O_5 \longrightarrow 4NO_2 + O_2$$

Experimentally: $r = \frac{d[O_2]}{dt} = k[N_2O_5]$

$$N_2O_5 \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} NO_2 + NO_3$$

$$NO_2 + NO_3 \xrightarrow{k_2} NO_2 + O_2 + NO$$

$$NO + NO_3 \xrightarrow{k_3} 2NO_2$$

Need to solve for intermidiates: NO_3 and NO

$$\frac{d[NO_3]}{dt} = k_1[N_2O_5] - k_{-1}[NO_2][NO_3] - k_2[NO_2][NO_3] - k_3[NO][NO_3]$$

$$\frac{d[NO]}{dt} = k_2[NO_2][NO_3] - k_3[NO][NO_3]$$

Steady-State

$$\frac{d[NO]}{dt} = 0 \Rightarrow k_2[NO_2]\cancel{[NO_3]} = k_3[NO]\cancel{[NO_3]}$$

$$\boxed{[NO_2] = \frac{k_3}{k_2}[NO]}$$

Substitute $[NO_2]$ in $\frac{d[NO_3]}{dt} = 0$

$$0 = k_1[N_2O_5] - k_{-1}\frac{k_3}{k_2}[NO][NO_3] - \frac{\cancel{k_2}k_3}{\cancel{k_2}}[NO][NO_3] - k_3[NO][NO_3]$$

$$0 = k_1[N_2O_5] - [NO][NO_3]\left[\frac{k_{-1}k_3}{k_2} + 2k_3\right]$$

$$k_1[N_2O_5] = \left[\frac{k_{-1}k_3}{k_2} + 2k_3\right][NO][NO_3] \Rightarrow$$

→

$$\boxed{[NO_3] = \frac{k_1}{\left[\frac{k_{-1}k_3}{k_2} + 2k_3\right]} \frac{[N_2O_5]}{[NO]}}$$

$$\frac{d[O_2]}{dt} = k_2[NO_3][NO_2]$$

$$\frac{d[O_2]}{dt} = \cancel{k_2}\left(\frac{k_1}{\frac{k_{-1}k_3}{k_2} + 2k_3} \frac{[N_2O_5]}{\cancel{[NO]}}\right)\left(\frac{k_3}{\cancel{k_2}} \cancel{[NO]}\right) = \frac{k_1k_3}{\frac{k_{-1}k_3}{k_2} + 2k_3} [N_2O_5]$$

$$\frac{d[O_2]}{dt} = \frac{k_1\cancel{k_3}}{\cancel{k_3}\left(\frac{k_{-1}}{k_2} + 2\right)} [N_2O_5] = \frac{k_1}{\frac{k_{-1} + 2k_2}{k_2}} [N_2O_5]$$

$$\frac{d[O_2]}{dt} = \frac{k_1k_2}{k_{-1} + 2k_2} [N_2O_5]$$

$$K = \frac{k_1k_2}{k_{-1} + 2k_2}$$

$$\therefore \boxed{\frac{d[O_2]}{dt} = k[N_2O_5]}$$

Problem 2

Cp (mol/L)	Ca (mol/L)	rate (mmol/g*h)	rate (mol/g*h)	Estimated rate (mol/g*h)	Normalized error ^2
0.15	0.1	1.19	0.00119	0.001334666	0.014778865
0.15	0.2	1.74	0.00174	0.001657764	0.002233717
0.15	0.41	1.92	0.00192	0.001892409	0.000206511
0.15	0.6	1.97	0.00197	0.001976793	1.18909E-05
0.15	0.82	2.06	0.00206	0.002029178	0.000223863
0.15	1.04	2.09	0.00209	0.002060683	0.000196766
0.33	0.1	0.9	0.0009	0.00092271	0.000636694
0.33	0.11	1	0.001	0.00097514	0.000618024
0.33	0.2	1.29	0.00129	0.001310144	0.000243836
0.33	0.41	1.63	0.00163	0.00166911	0.000575692
0.33	0.6	1.88	0.00188	0.001819454	0.001037171
0.33	0.81	1.94	0.00194	0.001916007	0.000152953
0.33	1.01	1.97	0.00197	0.001975314	7.27504E-06
0.6	0.13	0.8	0.0008	0.000750162	0.003880994
0.6	0.13	0.79	0.00079	0.000750162	0.002542981
0.6	0.2	1.03	0.00103	0.000980812	0.00228058
0.6	0.42	1.45	0.00145	0.001399362	0.001219609
0.6	0.62	1.61	0.00161	0.001599532	4.22717E-05
0.6	0.83	1.74	0.00174	0.001731101	2.61558E-05
0.6	1.04	1.89	0.00189	0.001820365	0.001357463
0.72	0.14	0.73	0.00073	0.000697291	0.002007703
0.72	0.2	0.9	0.0009	0.000881236	0.000434689
0.72	0.41	1.27	0.00127	0.001286988	0.000178935
0.72	0.61	1.51	0.00151	0.001503094	2.09166E-05
0.72	0.82	1.56	0.00156	0.001648411	0.003211916
0.72	0.85	1.69	0.00169	0.001664913	0.000220355
0.72	1.06	1.75	0.00175	0.00176034	3.49121E-05
0.93	0.21	0.7	0.0007	0.000772731	0.010795461
0.93	0.42	1.16	0.00116	0.001156637	8.40442E-06
0.93	0.65	1.37	0.00137	0.00140334	0.000592232
0.93	0.93	1.51	0.00151	0.001589766	0.002790521
0.93	1.13	1.7	0.0017	0.001681549	0.000117799
				sum	0.052687154

rmax	0.002321
k1	0.000299
k2	0.009198
kpi	0.000665

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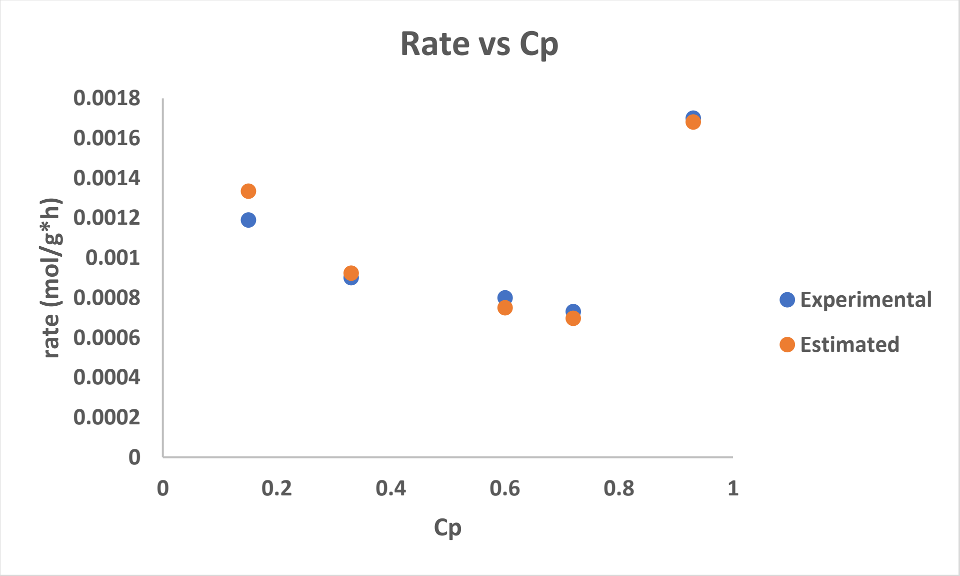

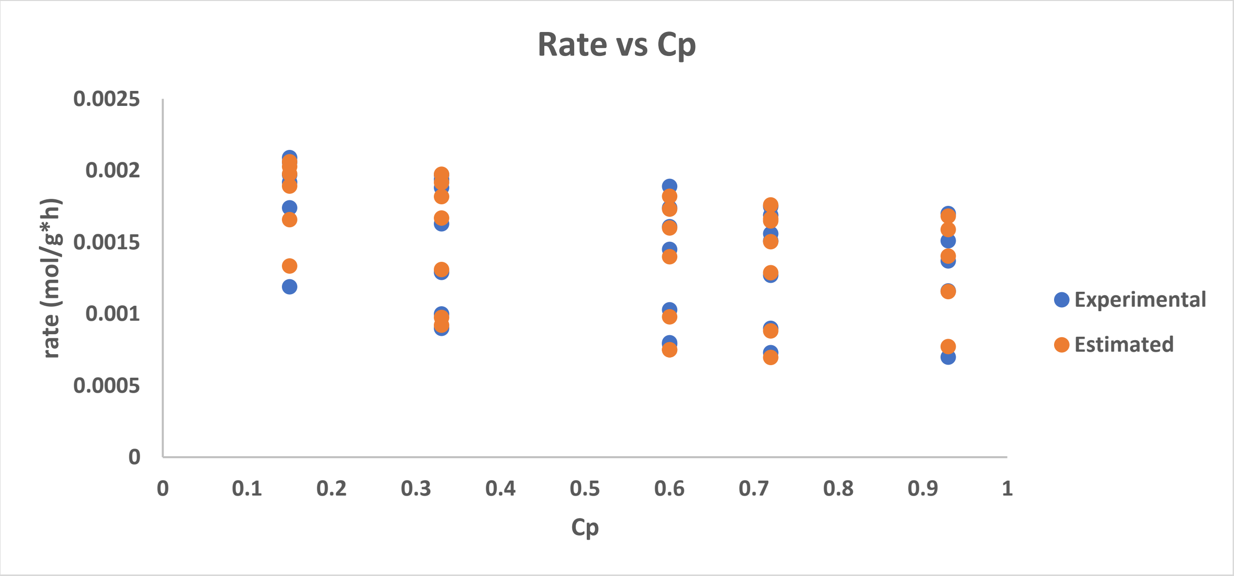

HW4 CH4 P4

(a) $E_z + S \overset{K_m}{\rightleftharpoons} E_zS \xrightarrow{k_2} E_z + P$

$$E_z + I \overset{K_i}{\rightleftharpoons} E_zI$$

$$r = k_2 C_{E_zS}$$

$$C_{E_z}^{0} = C_{E_zS} + C_{E_z} + C_{E_zI}$$

$\because$ Steady-State approximation

$$K_m = \frac{C_{E_z} C_S}{C_{E_zS}} \qquad K_i = \frac{C_{E_z} C_I}{C_{E_zI}}$$

$$C_{E_zS} = C_S C_{E_z} / K_m \qquad C_{E_zI} = C_I C_{E_z}$$

$$\therefore C_{E_z}^{0} = C_S C_{E_z}/K_m + C_I C_{E_z}/K_i + C_{E_z}$$

$$C_{E_z} = C_{E_z}^{0} / (1 + C_S/K_m + C_I/K_i)$$

$$\therefore C_{E_zS} = K_m C_S C_{E_z}^{0} / (1 + C_S/K_m + C_I/K_i)$$

$$r = k_2 C_{EzS}$$

$$= \frac{k_2 \quad C_S C_{Ez}^{0} / K_m}{1 + C_S/K_m + C_I/K_i}$$

$$= \frac{k_2 C_{Ez}^{0} \quad C_S}{K_m (1 + \frac{C_I}{K_i}) + C_S}$$

$$k_2 C_{Ez}^{0} = r_{max}$$

$$\therefore \; r = \frac{r_{max} C_S}{K_m (1 + \frac{C_I}{K_i}) + C_S}$$

(b) $E_z + S \underset{K_m}{\rightleftharpoons} E_zS \xrightarrow[k_2]{} E_z + P$

$$E_zS + I \underset{K_i}{\rightleftharpoons} E_zSI$$

$$r = k_2 C_{E_zS}$$

$$C_{E_z}^{o} = C_{E_z} + C_{E_zS} + C_{E_zSI}$$

∵ Steady-State Appx.

$$K_m = \frac{C_{E_z} C_S}{C_{E_zS}} \qquad K_i = \frac{C_{E_zS} C_I}{C_{E_zSI}}$$

$$\therefore C_{E_z} = \frac{K_m C_{E_zS}}{C_S} \qquad C_{E_zSI} = \frac{C_{E_zS} C_I}{K_i}$$

$$\therefore C_{E_z}^{o} = \frac{K_m}{C_S} C_{E_zS} + C_{E_zS} + \frac{C_I}{K_i} C_{E_zS}$$

$$C_{E_zS} = C_{E_z}^{o} \Big/ \left(1 + \frac{K_m}{C_S} + \frac{C_I}{K_i}\right)$$

$$\therefore r = k_2 C_{E_z}^{o} \Big/ \left(1 + \frac{K_m}{C_S} + \frac{C_I}{K_i}\right)$$

$$= \frac{r_{max} C_S}{\left(1 + \frac{C_i}{K_i}\right)} \Big/ \left[\frac{K_m}{\left(1 + \frac{C_i}{K_i}\right)} + C_S\right]$$