ChE-403 Problem Set 1.1

Week 1

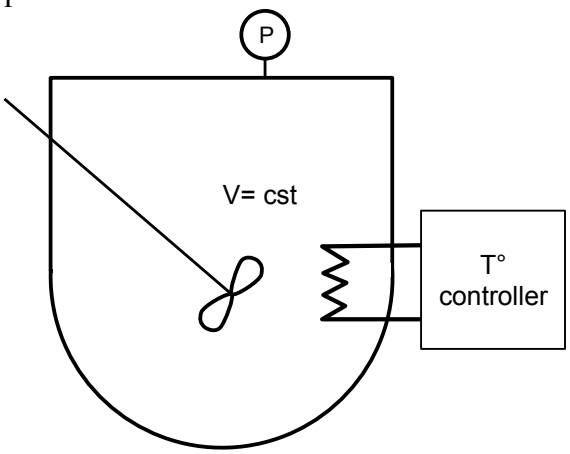
Problem 1

Take the following gas phase decomposition reaction:

$$2N_2O_5 \Rightarrow 2N_2O_4 + O_2$$

The reaction is first order in N_2O_5 and the kinetics are not affected by pressure. You can work at low pressures (<5 bars) where the ideal gas law is valid.

Can you suggest an approach for measuring the activation energy E_a with just some chemicals and this setup?

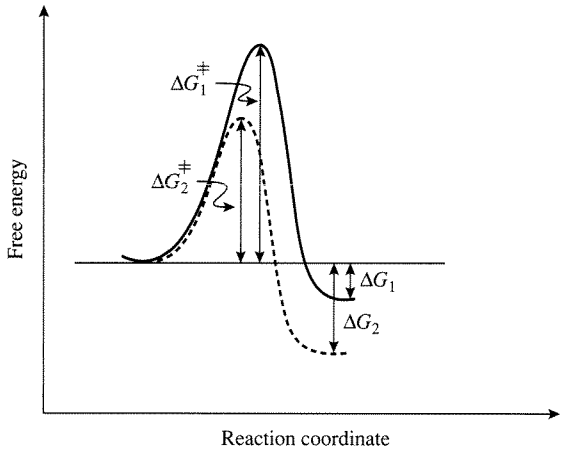


Problem 2

For similar reactions, trends in equilibrium constants can often be similar to trends in rate constants and thus can be used to predict each other. One approximation that can often be made for similar reactions is that the difference in transition state free energies is proportional to the difference in free energies of reaction:

$$\Delta G_{0,1}^{\ddagger} - \Delta G_{0,2}^{\ddagger} = \alpha\left(\Delta G_{0,1} - \Delta G_{0,2}\right)$$

For two similar reactions (for example, same reactants with different products):



Can you find a way to express the rate constants as a function of the equilibrium constants (and α) $f(k_1, k_2) = g(K_1, K_2)$?

Problem 3

For the following reaction in series in a batch reactor at constant T, V and P:

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

Find the concentration of C as a function of time with $C_A(0) = C_{A,0}$ and $C_B(0) = C_C(0) = 0$.