Homework No 3 (Chemical Kinetics)

1. Consider the overall oxidation reason of propane:

$$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$$

The following global mechanism has been proposed for this reaction

Reaction rate=$8.6 \cdot 10^{11} \exp\left(-\frac{30}{R_0 T}\right)[C_3H_8]^{0.1}[O_2]^{1.65}$,

Where CGS units (cm, s, gmol (1 gmol=0.001 kmol), kcal, K) are employed

A. Identify the order to the reaction with respect to propane;
B. Identify the order to the reaction with respect to O2;
C. What is the overall order of the global reaction?
D. Identify the activation energy for the reaction.

2. Consider the following elementary reaction mechanism where both the forward and reverse reactions are important.

$$CO + O_2 \overset{1}{\Leftrightarrow} CO_2 + O$$
$$O + H_2O \overset{2}{\Leftrightarrow} OH + OH$$
$$CO + OH \overset{3}{\Leftrightarrow} CO_2 + H$$
$$H + O_2 \overset{4}{\Leftrightarrow} OH + O$$

Using the compact notation, write down the species and reactions and the stoichiometric coefficient matrices.

3. Consider the CO oxidation reaction:

$$CO + OH \overset{k_1}{\rightarrow} CO_2 + H$$

$k_1\left(\frac{cm^3}{gmol-s}\right) = 1.17 \cdot 10^7 T(K)^{1.35} \exp\left[+\frac{3000}{R_0 T(K)}\right]$. Calculate the characteristic time for this reaction at T=2000 K and p=1 bar. The CO mole fraction is 0.011 and OH mole fraction is 3.68 x 10^{-3}.