Assignment - 2

Combustion Explosion and Detonation (AS 5640)

Department of aerospace Engineering, IIT Madras

Due date: **12/02/2019**

Assignment is to be submitted latest by 4pm on the above due date

1. One of the mechanisms of atom and radical combinations, called the energy-transfer mechanism, is described by the following chemical steps:

$$2R \underset{k_2}{\overset{k_1}{\leftrightarrow}} R_2^*$$

$$R_2^* + X \overset{k_3}{\rightarrow} R_2 + X$$

Where *R* represents a radical or an atom and *X* is a third body. Use the steady-state treatment for R_2^* to determine the rate of consumption of *R*. What is the order of recombination reaction when the concentration of *X* is sufficiently large such that $k_3 C_X \gg k_2$? What is the order of the recombination reaction at very low pressures?

2. At low pressure, assuming no wall reaction, the H_2-O_2 reaction may be accounted for by the mechanism

$H_2 + O_2 \overset{k_1}{\rightarrow} 2OH$	$k_1 = 10^{12} e^{-\left(\frac{39.0}{TR_u}\right)}\ cm^3/mole\ sec$
$OH + H_2 \overset{k_2}{\rightarrow} H_2O + H$	$k_2 = 10^{13.8} e^{-\left(\frac{5.9}{TR_u}\right)}\ cm^3/mole\ sec$
$H + O_2 \overset{k_3}{\rightarrow} OH + O$	$k_3 = 2.2 \times 10^{14} e^{-\left(\frac{16.5}{TR_u}\right)}\ cm^3/mole\ sec$
$O + H_2 \overset{k_4}{\rightarrow} OH + H$	$k_4 = 1.1 \times 10^{13} e^{-\left(\frac{9.4}{TR_u}\right)}\ cm^3/mole\ sec$
$H + OH + M \overset{k_5}{\rightarrow} H_2O + M$	$k_5 = 10^{17}\ cm^6/mole^2 sec \quad E_a = 0\ kcal/mole$

Using the steady state hypothesis, derive the differential equations expressing rate of formation of water (dC_{H_2O}/dt) in terms of C_{H2} and C_{O2}.