Homework Assignment Number One
Assigned: Thursday, August 26, 1999
Due: Thursday, September 9, 1999 BEGINNING OF CLASS.

1. State which software platform you intend to use to solve the homework sets.

2. Kreyszig, page 330, Problem Set 6.3, Problem 16

3. Kreyszig, page 330, Problem Set 6.3, Problem 18

4. Given the reactions:

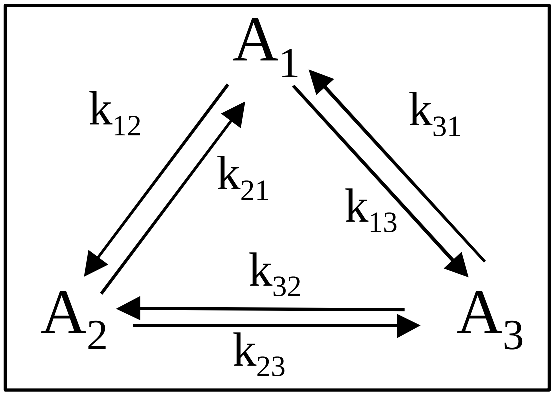
$$CH_4 + CH_4 \Leftrightarrow C_2H_6 + H_2$$
$$CH_4 + C_2H_6 \Leftrightarrow C_3H_8 + H_2$$
$$CH_4 + C_3H_8 \Leftrightarrow C_4H_{10} + H_2$$
$$C_2H_6 + C_2H_6 \Leftrightarrow C_4H_{10} + H_2$$
$$2CH_4 + 3O_2 \Leftrightarrow 2CO + 4H_2O$$
$$2C_2H_6 + 5O_2 \Leftrightarrow 4CO + 6H_2O$$
$$2C_3H_8 + 7O_2 \Leftrightarrow 6CO + 8H_2O$$
$$2C_4H_{10} + 9O_2 \Leftrightarrow 8CO + 10H_2O$$
$$2CO + O_2 \Leftrightarrow 2CO_2$$

(a) Write out the stoichiometric coefficient matrix
(b) Determine the number of independent reactions using the stoichiometric coefficient matrix
(c) Write a complete set of independent reactions
(d) Write out the atomic matrix
(e) Determine the number of independent reactions using the atomic matrix

5. Kreyszig, page 374, Problem Set 7.1, Problem 10

6. Find the eigenvalues and eigenvectors that describe the vibrational motion of acetylene, HCCH.

7. Consider that you have a three-component reactive mixture, all undergoing reversible reactions, as pictured below:



In this picture, the A's are concentrations of the three species and the k's are rate constants. An example of this system is the kinetic equilibrium between para-, meta-, and ortho-xylene.

(a) Find the eigenvalues and eigenvectors for the following rate constants in a batch reactor.

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k12 = 0.50;
k21 = 0.25;
k13 = 0.20;
k31 = 0.05;
k23 = 0.30;
k32 = 0.15;
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(b) Give a physical interpretation of these eigenvalues and eigenvectors.

(c) Find the steady-state composition.

(d) Additionally, allow for flow into and out of the reactor, making it a CSTR. Assume constant volume in the tank. Derive the model, (write the mass balances). Find the steady-state composition.

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F1_in = 0.1;
F2_in = 0.0;
F3_in = 0.05;
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