Chemical Engineering Mathematics 06-262
Homework 1
Due: Thursday January 25, 2001
Note: Do these by hand and show all work, do **not** use MathCAD.

Matrix Manipulations

1. **(15 points)** Compute the products **AB** and **BA** and the sum **A** + **B** where possible. Specify any products or sums that are not defined, and explain why.

a) $\mathbf{A} = \begin{bmatrix} -6 & 2 & -12 \\ 2 & 5 & 1 \\ 1 & 6 & 0 \end{bmatrix}$ $\qquad \mathbf{B} = \begin{bmatrix} 1 & -8 & 6 \\ -5 & 0 & 3 \\ 2 & 6 & 8 \end{bmatrix}$

b) $\mathbf{A} = \begin{bmatrix} -6 & 2 \\ -12 & 2 \\ 5 & 1 \\ 1 & 6 \end{bmatrix}$ $\qquad \mathbf{B} = \begin{bmatrix} 1 & -8 \\ 6 & -5 \\ 0 & 3 \\ 2 & 6 \end{bmatrix}$

c) $\mathbf{A} = \begin{bmatrix} 2 & -1 \\ 4 & 0 \end{bmatrix}$ $\qquad \mathbf{B} = \begin{bmatrix} -3 & 8 & 0 & 5 \\ 3 & -4 & 1 & 2 \end{bmatrix}$

d) Using the matrices in (c), calculate $(\mathbf{AB})^{\mathbf{T}} + \mathbf{B}^{\mathbf{T}}\mathbf{A}$ or show that it is not defined.

e) Using the matrices in (c), calculate $(\mathbf{AB})^{\mathbf{T}} + \mathbf{A}^{\mathbf{T}}\mathbf{B}$ or show that it is not defined.

2. **(15 points)** Any square matrix can be written as the sum of a symmetric matrix **S** and a skew-symmetric matrix **T**. Determine the elements in the matrices **S** and **T** that can be used to express **B** = **S** + **T** for the following **B** matrix:

$$\mathbf{B} = \begin{bmatrix} 1 & 3 & 2 & -1 \\ 0 & 2 & 4 & 1 \\ 1 & 0 & 0 & 5 \\ 2 & 7 & -2 & 1 \end{bmatrix}$$

3. **(15 points)** Matrix multiplication is a form of linear transformation. You can say that **A** acts to transform the vector **x** into vector **y** in the expression **y** = **A x**. Given the matrix **A** and vector **x**:

$$\mathbf{A} = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix} \quad \text{and} \quad \mathbf{x} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

   a) Calculate the vector **y** where **y** = **A x**.
   b) Consider vectors to be representations of lines in a Cartesian coordinate frame. Think of **x** as representing a line that goes through the points (0,0) and (1,1). Sketch the lines represented by **y** for the cases $\theta = \pi/4$ and $\theta = 3\,\pi/2$.
   c) Explain why the matrix **A** in this problem is called a rotation matrix.

<u>Linear Dependence of a System of Equations and Gauss Elimination</u>

4. **(15 points)** To perform balances on reactive systems, you must know how many independent reactions occur in the process. Matrix algebra is an easy way to verify the number of independent reactions in a system. For example, the following six combustion reactions are not necessarily independent:

$$CH_4 + 3/2\ O_2 \rightarrow CO + 2\ H_2O$$
$$CH_4 + 5\ CO_2 \rightarrow O_2 + 6\ CO + 2\ H_2O$$
$$CO \rightarrow CO_2 + 1/2\ O_2$$
$$CH_4 + 3\ CO_2 \rightarrow 4\ CO + 2\ H_2O$$
$$O_2 + CO_2 + CH_4 \rightarrow 2\ H_2O + 2CO$$
$$2\ O_2 + CH_4 \rightarrow CO + 2\ H_20$$

a) Write the stoichiometry in the form **A x** = **0**. Let **x** be a vector of the components (i.e., $\mathbf{x}^T=(CH_4,O_2,CO,CO_2,H_2O)$) and **A** be a matrix of the stoiciometry.
b) Use Gauss elimination to determine the minimum number of independent rows of the matrix **A**.
c) Write out a set of independent chemical reactions.

5. **(15 points)** The following sets of linear algebraic equations might arise from doing mass or energy balances on a system. Even though each appears to have the same number of unknowns as equations, the equations may not all be linearly independent.

   For each set of equations, write the set of equations in matrix form (**A x** = **b**), solve for the unknown vector, **x**, using Gauss Elimination, check your answer by calculating the product **Ax**. If Gauss Elimination fails, explain why it fails.

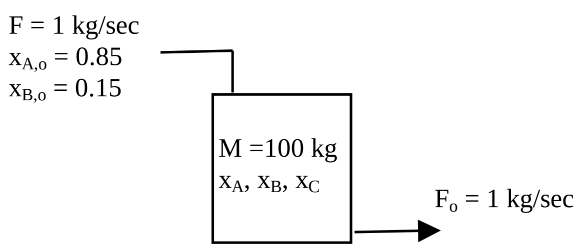
a) $x_1 + 3\,x_3 = 4$
$2\,x_2 + 4\,x_3 + 6\,x_4 = 2$
$3\,x_1 + 5\,x_3 + x_4 = 0$
$2\,x_1 + 3\,x_2 + x_4 = 9$

b) $3\,x_1 + x_2 + 4\,x_3 = -1$
$5\,x_2 + 8\,x_3 = 3$
$x_1 + 2\,x_2 + 4\,x_3 = 4$

c) $x_3 + x_4 + x_5 = 10$
$x_2 - 1.4\,x_3 + x_5 = 2$
$x_1 - 2\,x_4 + 2\,x_5 = 3$
$2\,x_2 + 3\,x_4 = 4$
$x_5 = 2$

<u>Gauss Elimination</u>

6. **(15 points)** A well-mixed batch reactor is used to generate the infamous product C which arises from the simple irreversible reaction A → B → C. The reactor is fed at a constant rate F with a mixture of A and B while product stream is pulled off at a constant rate of F_o.



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

$k_1 = 0.1\ \text{sec}^{-1}$
$k_2 = 0.05\ \text{sec}^{-1}$

The total mass of material in the reactor is constant at M = 100 kg and the concentrations are in terms of mass fractions (i.e., x_A [=] gm A/gm total). The reactions are first order such that mass consumed = k $x_{reactant}$.

a) Perform mass balances on each component to find three equations describing the <u>steady state</u> values of the mass fractions in the reactor. Begin with the conservation equation *Acc = In – Out + Gen – Cons* and state all assumptions.
b) Convert this set of three equations into a matrix equation containing the unknown vector $\mathbf{x} = [\ x_A\ \ x_B\ \ x_C\ ]^T$. Show the elements of all matrices in terms of the variables in the problem statement.
c) Solve for **x**. Explain which technique you used.
d) Check your solution for **x** by solving multiplying **A x**. Does the solution make sense physically?