# Second Midterm Exam
# ChE 231
# Spring 2019

Problem 1 (40 pts). Consider the sequence of reactions 2A+B $\xrightarrow{v_1}$ C, A+B $\xrightarrow{v_2}$ D, 2A $\xrightarrow{v_3}$ E where $v_1$, $v_2$ and $v_3$ are the reaction rates. The reactants A and B are supplied at rates $v_A = 2$ and $v_B = 1$, respectively.

1. (10 pts) Show that mass balances on components A and B yield a linear system of equations $\mathbf{Av} = \mathbf{b}$ where:

$$\mathbf{A} = \begin{bmatrix} 2 & 1 & 2 \\ 1 & 1 & 0 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$$

   What is the rank of $\mathbf{A}$?

2. (15 pts) Compute the solution $\mathbf{v} = [v_1\ v_2\ v_3]^T$ using the least-squares method.

3. (10 pts) Let $v_2 = 0$. Formulate the linear system of equations $\tilde{\mathbf{A}}\tilde{\mathbf{v}} = \mathbf{b}$. What is the rank of $\tilde{\mathbf{A}}$? Compute the solution $\tilde{\mathbf{v}} = [v_1\ v_3]^T$.

4. (5 pts) Compute and compare the two norms of the solutions $\mathbf{v}$ from part 2 and $\tilde{\mathbf{v}}$ from part 3.

Problem 2 (45 pts). Consider the sequence of reactions 2A+B $\xrightarrow{v_1}$ C, A+B $\xrightarrow{v_2}$ D, 2A+C $\xrightarrow{v_3}$ E where $v_1$, $v_2$ and $v_3$ are the reaction rates. The reactants A and B are supplied at rates $v_A = 2$ and $v_B = 1$, respectively.

1. (10 pts) Show that mass balances on components A, B and C yield a linear system of equations $\mathbf{Av} = \mathbf{b}$ where:

$$\mathbf{A} = \begin{bmatrix} 2 & 1 & 2 \\ 1 & 1 & 0 \\ -1 & 0 & 1 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} 2 \\ 1 \\ 0 \end{bmatrix}$$

2. (15 pts) Perform Gauss-Jordan elimination to calculate $\mathbf{A}^{-1}$. Show all steps.

3. (5 pts) Use $\mathbf{A}^{-1}$ to calculate the solution $\mathbf{v} = [v_1\ v_2\ v_3]^T$ Show all steps.

4. (15 pts) Calculate the eigenvalues of $\mathbf{A}$. Show all steps.

Problem 3 (15 pts + extra credit). Consider the Peng-Robinson gas equation of state:

$$P = \frac{RT}{V-b} - \frac{a\alpha}{V^2 + 2bV - b^2} = f(V)$$

1. (15 pts) Formulate the Newton-Raphson equation for determining the roots $V$ of this equation. Show all steps

2. (10 pts; extra credit) Consider the conditions $T = 300$ K and $P = 10^6$ Pa, the gas constant $R = 8.314$ m$^3$·Pa/K/mol and the Peng-Robinson constants for propylene at this temperature $a = 0.906$ J·m$^3$/mol$^2$, $b = 5.07\times10^{-5}$ m$^3$/mol and $\alpha = 1.11$. Create an iteration table showing the iteration $n$, $V_n$, $f(V_n)$, $\frac{df}{dV}(V_n)$ and $V_{n+1}$ for the first four iterations with $V_0$ calculated from the ideal gas law.