**NAME:** _____

> **Instructions:** The exam is closed book and closed notes. Write all answers on separate paper. Do not write any answers on the exam itself. Hand in your exam as well as your solution at the end. Make sure your name is on your solution and your exam.
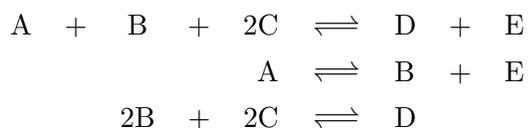
Exercise 1. Stoichiometry. 25 pts.

(a) What is the difference between a set of reactions that is linearly independent and a set of reactions that is linearly dependent?

(b) For the reaction

$$2NO + O_2 \rightleftharpoons 2NO_2$$
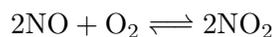
is it likely that this overall reaction would occur also as a molecular event? Why or why not?

(c) Consider the set of reactions

$$
\begin{array}{ccccccccc}
A & + & B & + & 2C & \rightleftharpoons & D & + & E \\
 & & & & A & \rightleftharpoons & B & + & E \\
2B & + & 2C & & & \rightleftharpoons & D & &
\end{array}
$$

1. Write out the species list and stoichiometric matrix. For ease of grading, please keep the species in alphabetical order in the species list.
2. By inspection, what is the rank of this matrix? Explain your answer.

Exercise 2. Equilibrium, friend or foe? 25 pts.

The following reaction takes place at low pressure in the gas phase

$$A + B \rightleftharpoons C$$

You charge a batch reactor with equal amounts of A and B and no C, run the reactor for a long time at a given temperature and pressure, and then open it up and find that you have converted about 50 percent of the starting materials.

But you need to reach 75 percent conversion for this process to be profitable. Your boss asks you to troubleshoot this process and make suggestions to save the project, which is about to be canceled. What do you tell your boss? Here are some options to consider. Feel free to choose one or more of these, or suggest your own options. The important point is to explain and justify your choice.

(a) Just run the reactor for a longer time. Eventually it will reach 75 percent conversion, guaranteed. You just have to be patient. State what other thermochemical data you require, if any, to justify this approach.

(b) Change the operating temperature. If you choose this option, what new temperature do you select? State what other thermochemical data you require, if any, to select the new temperature, and calculate the new temperature assuming whatever new data you require is available in your company's thermochemical database.

(c) Change the operating pressure. If you choose this option, what new pressure do you select? Again state what other thermochemical data, if any, you require to select the new pressure, and calculate the new pressure assuming whatever new data you require is available in your company's thermochemical database.

Exercise 3. Selectivity of competing first-order and second-order reactions. 50 pts.

The following two reactions take place in a constant-volume batch reactor

$$A + B \xrightarrow{k_1} C \qquad r_1 = k_1 c_A^2 c_B$$

$$A + B \xrightarrow{k_2} D \qquad r_2 = k_2 c_A c_B$$
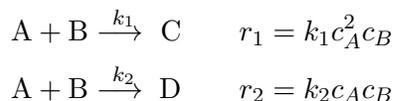
There is a large excess of reactant B initially, and therefore we can assume that c_B is approximately constant throughout the batch time. Note that, despite the stoichiometry, the first reaction is second-order in A, but the second reaction is first-order in A.

(a) Write out the component balance for species A in the reactor. How does it simplify when noting that B is in large excess?

(b) Solve the component balance for $c_A(t)$. Check that your solution satisfies the initial condition.

(c) Draw a sketch of $c_A(t)$ versus t.

(d) How would you define the *instantaneous* selectivity of product C, s_C (production of C relative to consumption of A). Explain in physical terms what this selectivity is measuring.

(e) How would you define the *overall* selectivity of product C, S_C as a function of the batch time, t. Explain in physical terms what this selectivity is measuring.

Are the two selectivities you have defined the same for this application? Why or why not?

(f) How would you define overall conversion of A for this reactor, x_A? Explain in physical terms what this conversion is measuring.

Hint: if you need to integrate something like

$$\int \frac{dx}{(x+a)(x+b)}$$

and, since WolframAlpha is unreachable, instead notice that you can express

$$\frac{1}{(x+a)(x+b)} = \frac{1}{b-a} \left[\frac{1}{x+a} - \frac{1}{x+b} \right]$$

and you know how to integrate both terms on the right-hand side. This is called a partial fraction expansion, and you will use it later in CBE 470.