AFCoKaRE Practice Problem 4.5

Purpose: This problem allows you to practice converting between generalized and species-specific rate expressions and calculating pre-exponential factors and activation energies for the Arrehenius expression.

Problem Statement: A batch reaction engineering problem encountered later in the course might read as follows: An adiabatic batch reactor is filled with gas containing 67% A and 33% inert I at 300 K and 3 atm. It is necessary to convert 90 % of the A according to reaction (1). Reaction (1) is irreversible, and its rate expression is given by equation (2). The heat capacities, in cal mol^{-1} K^{-1}, of A, X, Y, and I are 7, 4, 4, and 8, respectively. The heat of reaction (1) is −30000 cal mol^{-1} at 298 K. The rate coefficient in equation (2) is equal to 0.12 h^{-1} at 298 K, and the activation energy is 25 kcal mol^{-1}. Calculate the time required and the final temperature.

$$2\,A \rightarrow X + Y \qquad (1)$$

$$r_1 = k_1 C_A \qquad (2)$$

In order to solve this problem, you would likely write mole balances and an energy balance. The mole balance on reagent A would include an expression for the rate of reaction (1) with respect to A, and in that rate expression, the rate coefficient k_1 would be written as an Arrhenius expression. Write the necessary rate expression, inserting the proper values for the pre-exponential factor and activation energy.