A First Course on Kinetics and Reaction Engineering

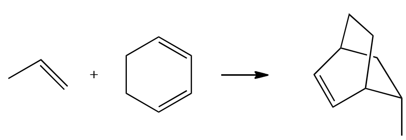
Activity 16.1

Problem Purpose

This problem will allow you to compare and contrast the integral and numerical methods of kinetics data analysis. The problem is the same as Example 15.2, which was solved using the integral method and linear least squares.

Problem Statement

Reaction (1) was studied at 600 K in a constant volume batch reactor. The initial charge to the reactor consisted of 150 Torr of A and 450 Torr of B. A spectrophotometer was used to record a signal from which the fractional conversion of A could be recorded versus time. Use the data given in the table below to test the validity of the rate expression, $r = k \cdot C_A \cdot C_B$, and find the "best" value for k. Use the integral method of data analysis.



$$A + B \rightarrow Z \qquad (1)$$

time (h)	***fractional conversion of A***
23.1	0.17
33.3	0.22
58.2	0.34
69.7	0.41
90.7	0.49
127.7	0.58
192.1	0.7
240.6	0.77
281.1	0.83

- Write mole balances for A, B and Z (to be solved numerically)
  - What must be provided to the software used to solve the set of ODEs?
    - For the code, what quantities will be known and what equations will used?
- Fit the model to the data using numerical least squares
  - What must be provided to the software used to perform the numerical least squares?
    - For the code, what quantities will be known and what equations will used?
- What is the result?