A First Course on Kinetics and Reaction Engineering

Activity 14.1

Problem Statement

A rate expression is needed for the reaction A $\rightarrow$ Y + Z, which takes place in the liquid phase. It doesn't need to be highly accurate, but it is needed quickly. Only one experimental run has been made, that using an isothermal batch reactor. The reactor volume was 750 mL and the reaction was run at 70 °C. The initial concentration of A was 1M, and the concentration was measured at several times after the reaction began; the data are listed below.

t (min)	***C_A(M)***
1	0.874
2	0.837
3	0.800
4	0.750
5	0.572
6	0.626
7	0.404
8	0.458
9	0.339
10	0.431
12	0.249
15	0.172
20	0.185

(a) Plot the data, fit a 2nd, 3rd, 4th and 5th order polynomial to the data and plot the polynomials. Choose the best polynomial and use it to estimate $\frac{dC_A}{dt}$ for each experimental data point.

(b) Use forward, backward and central differences to estimate $\frac{dC_A}{dt}$ for each experimental data point. When using central differences, use a forward difference for the first data point and a backward difference for the last data point.

(c) Find the best value for a first order rate coefficient using the differential method of analysis and each of the estimates of $\frac{dC_A}{dt}$ from parts (a) and (b). Comment upon the results.