A First Course on Kinetics and Reaction Engineering

Problem 14.1

Problem Purpose

This problem will help you determine whether you have mastered the learning objectives for this unit. The solution will also provide you with some additional insight related to the use of forward and backward differences.

Problem Statement

The data in the table to the right represent the conversion versus time behavior for reaction (1) taking place in a 5 L batch reactor with an initial composition that was 1 M in A, 1.5 M in B and contained no Y or Z. Actually, the data in the table were calculated using an ideal batch reactor model with the rate expression given in equation (2) and with k_{1f} = 0.0947 L mol^{-1} min^{-1} and k_{1r} = 0.0369 L mol^{-1} min^{-1}. As such, these data do not contain any experimental noise. Perform a differential data analysis to find the values and uncertainties of the two rate coefficients using forward differences. Then repeat the analysis only using backward differences. Comment upon any differences among the actual values and the values obtained using the two different analysis methods.

t (min)	C_A (M)
0	1
0.5	0.933
1	0.8732
1.5	0.8197
2	0.7717
2.5	0.7284
3	0.6894
3.5	0.6542
4	0.6222
4.5	0.5932
5	0.5668
5.5	0.5427
6	0.5208
6.5	0.5008
7	0.4825
7.5	0.4657
8	0.4503
8.5	0.4362
9	0.4233
9.5	0.4114
10	0.4005

$$A + B \rightleftarrows Y + Z \qquad (1)$$

$$r_1 = k_{1f}C_AC_B - k_{1r}C_YC_Z \qquad (2)$$