A First Course on Kinetics and Reaction Engineering

Activity 16.2

Problem Purpose

This example illustrates the analysis of kinetics data from a CSTR using numerical least squares The problem is the same as Example 13.3 which was solved using linear least squares.

Problem Statement

A new enzyme has been found for the dehydration reaction given in equation (1). A series of experiments were performed using a CSTR operating at steady-state and isothermally. The inlet flow rate was fixed at 5 mL per min and the reactor fluid volume was constant at 50 mL in all experiments. The inlet concentration of substrate, S, was changed for each experiment and the data given below for the product, P, concentration were recorded. Determine whether Michaelis-Menten kinetics adequately describe the rate of reaction, and if they do, determine the best values for the two kinetic parameters in the Michaelis-Menten rate equation.

$$S \rightarrow P + H_2O \qquad (1)$$

Inlet S Concentration (mmol/L)	*Outlet P Concentration (mmol/L)*
12.6	1.01
11.2	0.98
9.0	0.92
8.1	0.90
6.3	0.83
5.6	0.79
4.3	0.71
3.6	0.65
2.3	0.52
1.0	0.29

- 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 algebraic equations?
    - 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?