A First Course on Kinetics and Reaction Engineering

How To Test a Rate Expression Using CSTR Kinetics Data*

1. Write the CSTR mole balance design equation for any one reactant or product, substituting the mathematical function to be tested as a rate expression
2. If necessary, linearize the equation from step 1
   a. The slope(s) and intercept in the linearized equation should only depend upon quantities that have the same value for every experimental data point
3. For each data point, calculate the value of the dependent variable and the independent variable(s) in the linearized form of the design equation.
4. Fit the equation from step 1 or step 2 to the experimental data using linear least squares
   a. obtain best values for each slope and, if present, the intercept
   b. obtain estimates for the uncertainty in the slope(s) and, if present, the intercept
   c. obtain a correlation coefficient
   d. obtain or generate a model plot or a parity plot and residuals plots
5. Decide whether the function is sufficiently accurate in representing the data
   a. based on a correlation coefficient value close to 1.0
   b. based upon small deviations of the experimental data from the model prediction in the model plot or from the diagonal of the parity plot
   c. based upon random, non-systematic deviations of the experimental data from the model prediction in the model plot or the residuals plots
6. If the fit is sufficiently accurate, use the resulting slope(s) and intercept, and their uncertainties, to calculate the best values of the parameters that appear in the rate expression being tested, along with their uncertainties
7. If the fit is not sufficiently accurate, guess a different function and repeat from step 1

* Assuming only one reaction is taking place and the reactor model can be written in the form of a linear equation