A First Course on Kinetics and Reaction Engineering

How To Test a Rate Expression Using Integral Data Analysis*

1. Write the design equation for the type of reactor used in the experiments (batch or pfr)
2. Substitute the mathematical function to be tested as a rate expression into equation the design equation
3. Identify all quantities appearing in the resulting design equation that vary with time (batch) or axial position (pfr)
   a. Re-express any such quantities other than the dependent and independent variable in terms of the dependent and independent variable
4. Integrate the resulting differential equation to obtain an algebraic model equation
5. If necessary, linearize the algebraic model equation so that the slope(s) and intercept (optional)
   a. Each include at least one unknown parameter from the rate expression in a unique combination
   b. Additionally only include quantities that have the same value for the entire data set (known constants)
6. For each data point, calculate the value of the dependent variable and the independent variable(s) in the linearized form of the algebraic model equation
7. Fit the linearized algebraic model equation to the experimental data
   a. obtain estimates for the slope(s) and (if present) intercept of the linearized model
   b. obtain estimates for the uncertainty in the values of those parameters
   c. obtain a correlation coefficient
   d. obtain or generate a model plot or a parity plot and residuals plots
8. 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
9. If the fit is sufficiently accurate, calculate the best values and the corresponding uncertainties of the kinetics parameters from the best values and uncertainties of the slope(s) and intercept.
10. If the fit is not sufficiently accurate, guess another function and repeat from step 2

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