A First Course on Kinetics and Reaction Engineering

How To Test a Single Parameter 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. Re-arrange the algebraic model equation in the form of an expression for calculation of the single kinetic parameter
6. Use each data point to calculate a value of the single kinetic parameter
7. Find the average and the standard deviation of the single kinetic parameters from step 6
8. Decide whether the function is sufficiently accurate in representing the data
    a. based on a standard deviation that is a small fraction of the average value
    b. based upon random, non-systematic deviations of the single kinetic parameters calculated in step 6 from their average, calculated in step 7
9. If the fit is not sufficiently accurate, guess another function and repeat from step 2

* Assuming only one reaction is taking place and an algebraic model equation (after integration) that cannot be linearized for linear least squares fitting