

# A First Course on Kinetics and Reaction Engineering

## How To Generate a Rate Expression

1. Choose a reactor for the experiments
  - a. Generate design equations for that reactor
  - b. Validate the design equations
2. Gather experimental data
  - a. Use the widest possible range of environmental variables
  - b. At the minimum, span the range of environmental variables in which the rate expression is expected to be used
3. Pick a mathematical function to be tested as a rate expression either
  - a. Empirically or
  - b. Based on theory
4. Substitute the rate expression selected in step 3 into the design equation(s) from step 1 and fit the resulting equation(s) to the data from step 2 by
  - a. Calculating its average value if there is only one parameter in the rate expression or
  - b. Least-squares fitting if there are multiple parameters
5. Decide whether the fit of the design equation to the data is acceptable based upon
  - a. Correlation coefficient
  - b. Confidence intervals or standard deviation of the parameter(s)
  - c. Rectifying (parity) plot
  - d. Residuals plots
6. If the accuracy of the fit is **not** acceptable, go back to step 3 and repeat the process using a different mathematical function.
7. The mathematical function that yielded an acceptable fit may be used as the rate expression within the range of the experimental data used in the fitting
  - a. There may be other mathematical functions that are just as accurate
  - b. The rate expression may fail if extrapolated to values of the environmental variables outside the range used in the fitting