A First Course on Kinetics and Reaction Engineering

How To Use FitLinSR.m

1. Verify that FitLinSR.m is the appropriate script to use
   a. The data points must be of the form $\left(x_1, x_2, \cdots, x_{n_s}, \hat{y}\right)$
   b. The model being fit to those data must be of the form $y = m_1 x_1 + m_2 x_2 + \cdots + m_{n_s} x_{n_s} + b$
      i. If the model is missing the final parameter, b, convert it to the form above (see the informational reading for Supplemental Unit S3).
2. Make sure that FitLinSR.m is stored in the current MATLAB working directory or in a directory that is in the MATLAB search path
3. Create a matrix named `x` in the MATLAB workspace
   a. The first column of `x` should contain the values of x_1 for each of the data points, one per row; the second column should similarly contain the values of x_2, and so on through column n_s
   b. Column (n_s + 1) of `x` should contain the value 1.0 in every row
4. Create a column vector named `y_hat` in the MATLAB workspace; it should contain the values of $\hat{y}$ for each of the data points, one per row
5. Execute the script by typing the following at the MATLAB command prompt: `FitLinSR`
6. The following quantities will be listed in the MATLAB command window
   a. `r_squared` - the correlation coefficient for the fit
   b. `m` - a column vector containing the fitted slopes m_1 through m_{n_s}
   c. `m_u` - a column vector containing the ± 95% confidence limits for the fitted slopes
   d. `b` - the fitted intercept, b
   e. `b_u` - the ± 95% confidence limits for the fitted intercept
7. The following figures will be displayed
   a. A parity plot
   b. A set of residuals plots with each of the set variables as the abscissa