A First Course on Kinetics and Reaction Engineering

Unit 16. Numerical Data Analysis

Definitions

multiple response data - a kinetics data set where the value of two or more different quantities (response variables) were each experimentally measured in at least one experimental data point

complete multiple response data set - a multiple response data set, as defined above, where every response variable was measured in every experiment in the data set

Nomenclature

Φ objective function that characterizes the global error in a model's predicted responses relative to the experimentally measured responses

ε_{ij} error between the model-predicted response i and the experimentally measured response response i for experimental data point j

y_i response variable; the first subscript denotes which response variable and the second subscript (either "model" or "expt.") distinguishes the model-predicted response from the experimentally measured response

Equations

$$\Phi = \sum_{\substack{j=\text{ all}\\ \text{data}\\ \text{points}}} \left[\left(y_{1,\text{model}} - y_{1,\text{expt.}} \right)_j^2 + \left(y_{2,\text{model}} - y_{2,\text{expt.}} \right)_j^2 \right] \tag{16.1}$$

$$\Phi = \begin{vmatrix} \sum\limits_{\text{all j}} \left(\varepsilon_{1j}\right)^2 & \sum\limits_{\text{all j}} \varepsilon_{1j}\varepsilon_{2j} & \cdots & \sum\limits_{\text{all j}} \varepsilon_{1j}\varepsilon_{nj} \\ \sum\limits_{\text{all j}} \varepsilon_{1j}\varepsilon_{2j} & \sum\limits_{\text{all j}} \left(\varepsilon_{2j}\right)^2 & \cdots & \sum\limits_{\text{all j}} \varepsilon_{2j}\varepsilon_{nj} \\ \vdots & \vdots & \ddots & \vdots \\ \sum\limits_{\text{all j}} \varepsilon_{1j}\varepsilon_{nj} & \sum\limits_{\text{all j}} \varepsilon_{2j}\varepsilon_{nj} & \cdots & \sum\limits_{\text{all j}} \left(\varepsilon_{nj}\right)^2 \end{vmatrix} \tag{16.2}$$

$$\varepsilon_{ij} = \left(y_{i,\text{model}} - y_{i,\text{expt.}} \right)_j \tag{16.3}$$