Selection of 'Best'
Model

Objectives

- Define 'best' model
- Consider factors associated with output plots;
- Consider parameter variability; and
- Consider statistical parameters such as AIC and F-test
  – in the selection of a 'best' model

Best Model

- Empirical or Physical
- Can Theory provide model and parameters
- Smallest model given the data available and proposed use
- Can the parameters be determined (Identifiable)
- What will the model be used for
- Is the model too small?
- Is the model too big?

Calculated versus Observed Plots

- Look for Systematic Deviations
- Subjectively Evaluate Alternate Models
  - Distribution Phase
  - Straight Line Elimination on Semi-log Plots
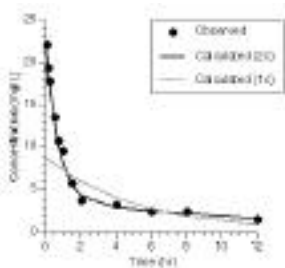 - Plasma and Urine Date to be Included in Model

Calculated versus Observed Plot

Weighted Residual Plot

- Look for Patterns which may Suggest Alternate Models
- Definite Pattern may Indicate a More Complex Model is Required

Weighted Residual Plots
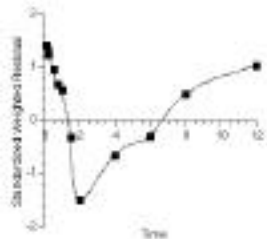

Parameter Variability

- High Values for Coefficient of Variation
  - Large Values for Standard Deviations

↑

Model Too Large
Not Enough Data
Too Much Error in the Data

Statistical Parameters
- AIC, Akaike's Information Criterion

$$AIC = N \cdot \ln(WSS) + 2 \cdot M$$

N = number of data points (non-zero wt)
M = number of parameters (adjustable)

Used to Help Select 'Correct' Model
Lower Number is Better
- MUST Use the Same Weighting Scheme

AIC

	M	N	WSS	AIC Value
One Compartment Model	2	12	2.02	12.4
Two Compartment Model	4	12	0.0769	-22.8
Three Compartment Model	6	12	0.0769	-18.8

F-Test

$$F = \frac{WSS_j - WSS_k}{WSS_k} \times \frac{df_k}{df_j - df_k}$$

WSS = weighted sum of squares
df = degrees of freedom (N-M)
**j, k are two fit results (same weighting
scheme), k with more parameters**

Compare Calculated Value with Tabled Value

F-Test

	Calculated	Tabled	n,m
1 vs 2	101	4.46	2, 8
2 vs 3	0	5.14	2, 6

n = df_j - df_k
m = df_k
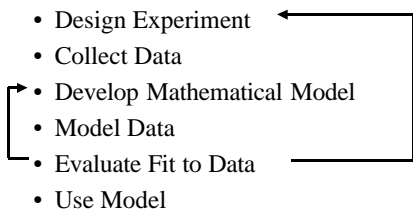
General Method

- Design Experiment
- Collect Data
- Develop Mathematical Model
- Model Data
- Evaluate Fit to Data
- Use Model

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