CHE384, From Data to Decisions: Measurement, Uncertainty, Analysis, and Modeling

Lecture 71
Response Surface Modeling

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Beyond Factorial Designs

- A two-level factorial (or fractional factorial) design looks for linear trends, possibly with interactions
  - Does the variable significantly impact the response? In what direction?
  - It helps to define the next experiment
- Response Surface Methodology (RSM) looks for quadratic or higher order trends
  - Assumes all variables are significant
  - A quadratic response always has a stationary point (minimum or maximum or saddle point)
  - Can be used to optimize a process

General Second Order Model

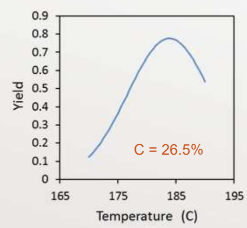
$$y_i = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{i<j}\sum \beta_{ij} x_i x_j + \varepsilon_i$$

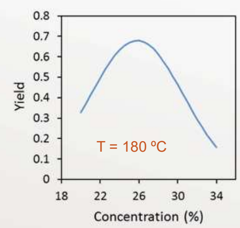
In matrix form: $\boldsymbol{Y} = \beta_0 + \boldsymbol{Xb} + \boldsymbol{XBX^T} + \boldsymbol{\varepsilon}$

$$\boldsymbol{Y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \quad \boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_n \end{bmatrix}, \quad \boldsymbol{b} = \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_k \end{bmatrix}, \quad \boldsymbol{X} = \begin{bmatrix} x_{11} & \cdots & x_{1,k} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{n,k} \end{bmatrix}$$

$$\boldsymbol{B} = \begin{bmatrix} \beta_{11} & \cdots & \beta_{1k}/2 \\ \vdots & \ddots & \vdots \\ \beta_{1k}/2 & \cdots & \beta_{k,k} \end{bmatrix}$$

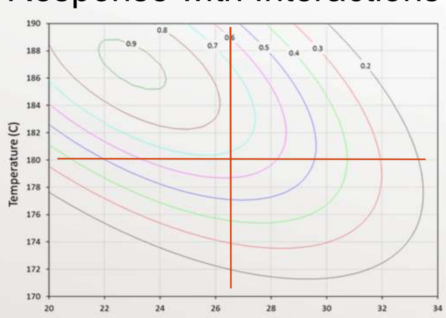
One at a Time Variables





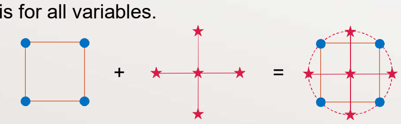
What are the optimum process conditions?

Response with Interactions



Central Composite Design

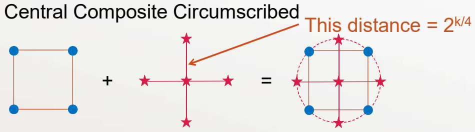
- Take the two-level factorial design and add:
  - A center point (the middle point between all of the factors), usually with repeats
  - Axial (star) points (the center point except with one variable changed to be at +/- an extreme value). Do this for all variables.



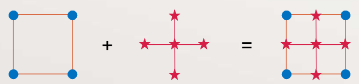
  - More efficient than a three-level factorial design

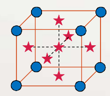
Central Composite Designs

- Central Composite Circumscribed



- Central Composite Face-centered



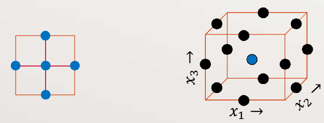


For k factors, $n = 2^k + 2k + 1$

(3 factors)

Box-Behnken Design

- Put a data point in the center, then one data point at the midpoints of each edge of the process space
  - Does not contain an embedded factorial design
  - No corner (extreme) points



Repeated Center Points

- Repeated center points are not randomized; they are run as the first and last data points, and evenly spread through the rest of data collection
  - A check against process instability
  - All other points should have randomized order
- The number of repeated center points can be set to create “uniform precision”
  - The variance of prediction is the same at the center as it is at the corners

RSM Properties

- Orthogonality: Are the factors correlated?
- Rotatability: A design is rotatable if the variance of the predicted response at any point x depends only on the distance of x from the design center point
  - All first-order orthogonal designs are rotatable
  - Composite face-centered design is not rotatable
- Uniformity: control the number of center points to achieve uniform precision
- Efficiency: how many experimental runs are required?

Notes on RSM

- Beware of extrapolation: is the stationary point (min or max) outside of the experimental space?
- Multiple responses: try overlapping the response contour plots
- Principle component analysis can be useful with RSM

Lecture 71: What have we learned?

- When is response surface modeling preferred over two-level factorial design?
- What is wrong with varying our factors one-at-a-time?
- Describe some of the RSM designs we have discussed
- Why are center points often repeated in RSM?
- What are the four properties we look for in RSM?