**Class 19** – **Designed Experiments**

ChE310\_Sec1\_F2019 / 10.29.19

<http://www.reuelgroup.org/numerical-methods-che-310.html>

Announcements:

* Nov 12 Phase II of project is due. [Go over format!]
* Thursday – interactive class activity!
* No supplement instruction on Friday

**Warm Up Group Activity:** submit to slack by **2:20 pm**.

Fit the following data to the nonlinear model

y = ((x-b)\*x^c)/a

x = 1:10

y = [-0.08 0.20 2.42 6.81 19.76 41.31 71.88 99.11… 162.61 249.62];

Plot the data with the fit and 95% confidence intervals.

What is the coefficient of determination for the fit?

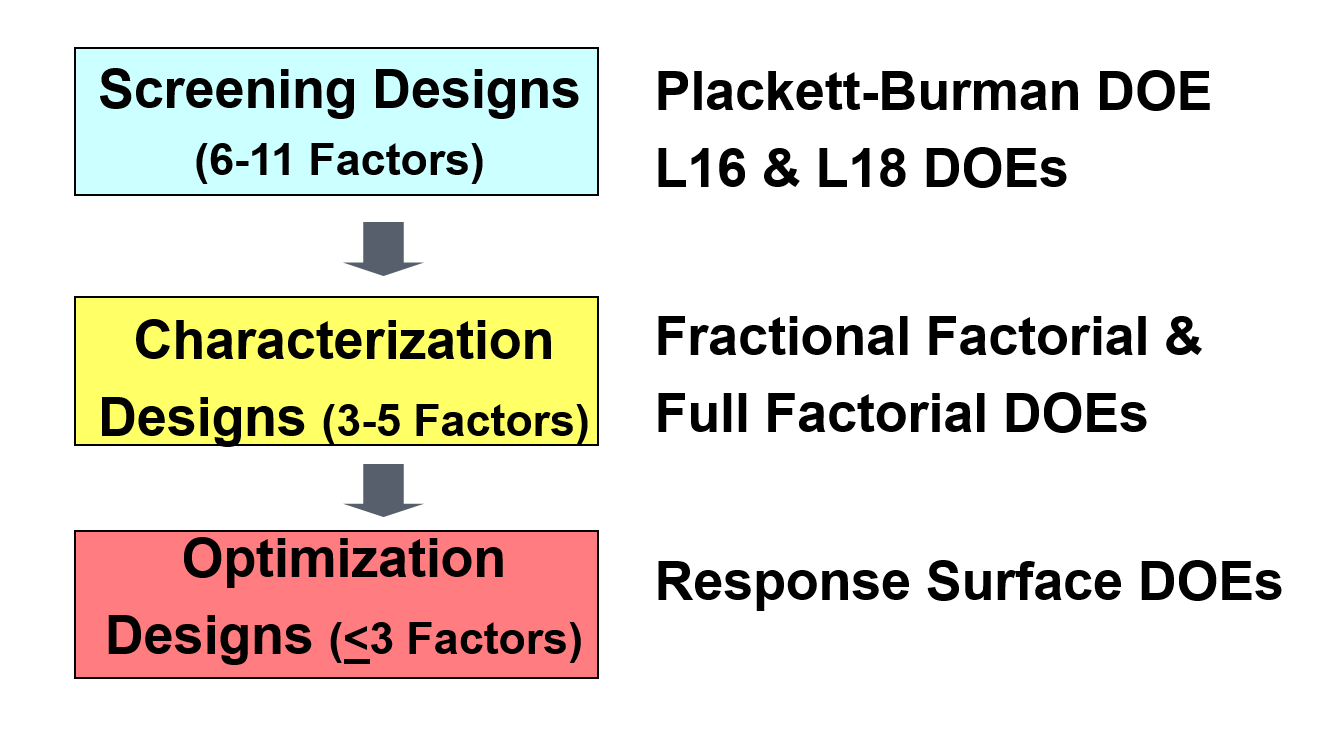
**Outline for Class 19 Lecture**

1. Real problem scenario:
   1. You’ve inherited a new reactor
   2. Pressures can range 10-200 PSI
   3. Temp can range from 300 to 450K
   4. Residence time range 1-5h
   5. You only have budget for 20 runs [$$$]
   6. Your boss wants to know optimal conditions ASAP!
   7. What do you do!?
2. Design of Experiments (DoE)

[most information for fewest number of runs]

* 1. Measured output is a result of multiple input variables
  2. Determine which input variable(s) is(are) significant
  3. Determine model for input variables (w/ interaction)
     1. NOTE: you would not see these effects if you did traditional testing of one variable at a time
  4. Use model to determine optimal set points of variables
  5. Do this in the LEAST number of runs while preserving statistical significance [save $$$]

1. DoE Roadmap



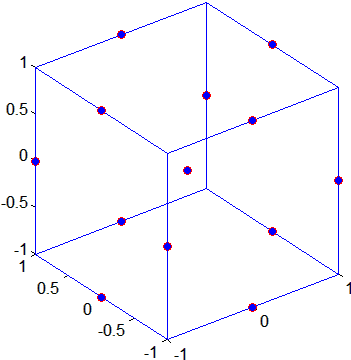
1. Screening Designs (not in this course)

* Measure only the main effects
* Plackett-Burman **hadamard**

1. Full Factorials

* Two or more factors
* Discrete high and low levels of each factor
* ALL combinations are tested
* # of Runs = 2^(factors)
* **ff2n** (2 level design, scalar for number of factors)
* **fullfact** (specify number of levels for each factor)

1. Fractional Factorials

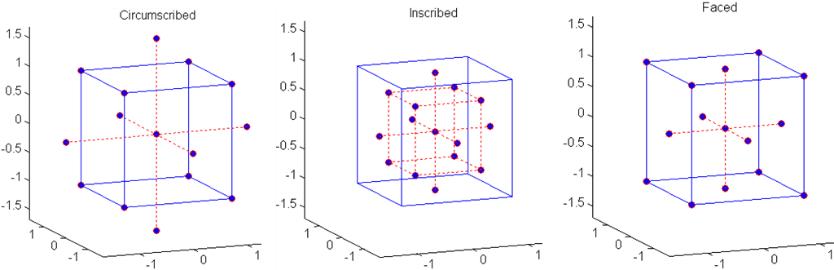
* Carefully chosen subset of the possible full fac. Runs
* ‘sparsity of effects’ principle
* # of Runs = 2^(factors-generators)
* Tabulated (see [Wikipedia](https://en.wikipedia.org/wiki/Fractional_factorial_design))
* **fracfactgen**
* **fracfact**

1. Response Surface Design

* Box-Behnken design (**bbdesign**) 🡪

\*Experiment [table](https://www.itl.nist.gov/div898/handbook/pri/section3/pri337.htm) (randomized)

* Central composite design (**ccdesign**)
  + Circumscribed (CCC – default), Inscribed (CCI), and Faced (CCF).



[Note: Run a response surface with least number of factors, typically 2-3, after you know which ones are most significant]

1. Fitting the results of a response surface

* Quadratic model is assumed (for three variables):

Y= β0 + β1X1 + β2X2 + β3X3 +

β12X1X2 + β13X1X3 + β23X2X3 + β123X1X2X3 + β11X21 + β22X22 + β33X23 + experimental error

* Main effects
* Interaction terms (two-way, three-way (typically not included on response surface), and quadratic terms
* DoE software also usually drops interaction terms with crossed (squared) factors as these are typically not realized in real systems.
* Plot response as a contour PLOT
* Optimization problems, try the **plotSlice** command

1. Example 1 – Radiator [together]

* **Significant Variables:**

Distance from radiator: 1 to 1.5 inches  
Pitch angle: 15 to 35 degrees   
Blade tip clearance: 1 to 2 inches

* We need at least 875 ft3 per minute
* bbdesign
* Measurements = [[837 864 829 856 880 879 872 874 834 833 860 859 874 876 875]

1. Example 2 – Reaction simulator – **rsmdemo** [teams]

* Hydrogen 100 to 470
* nPentane 80 to 300
* isoPentane 10 to 120
* Target reaction rate of 15

1. More reading on DoE

* NIST Process Improvement Handbook [LINK](https://www.itl.nist.gov/div898/handbook/pri/pri.htm)
* ISU Statistics 512 ‘Experimental Design’