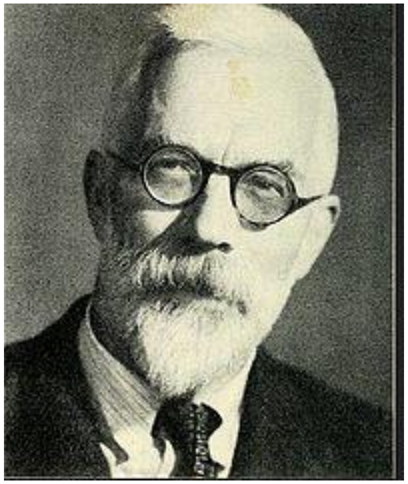
Experimental Design

- The experimental design problem
- Full factorial designs
- Reduced design methods
- In-class exercise

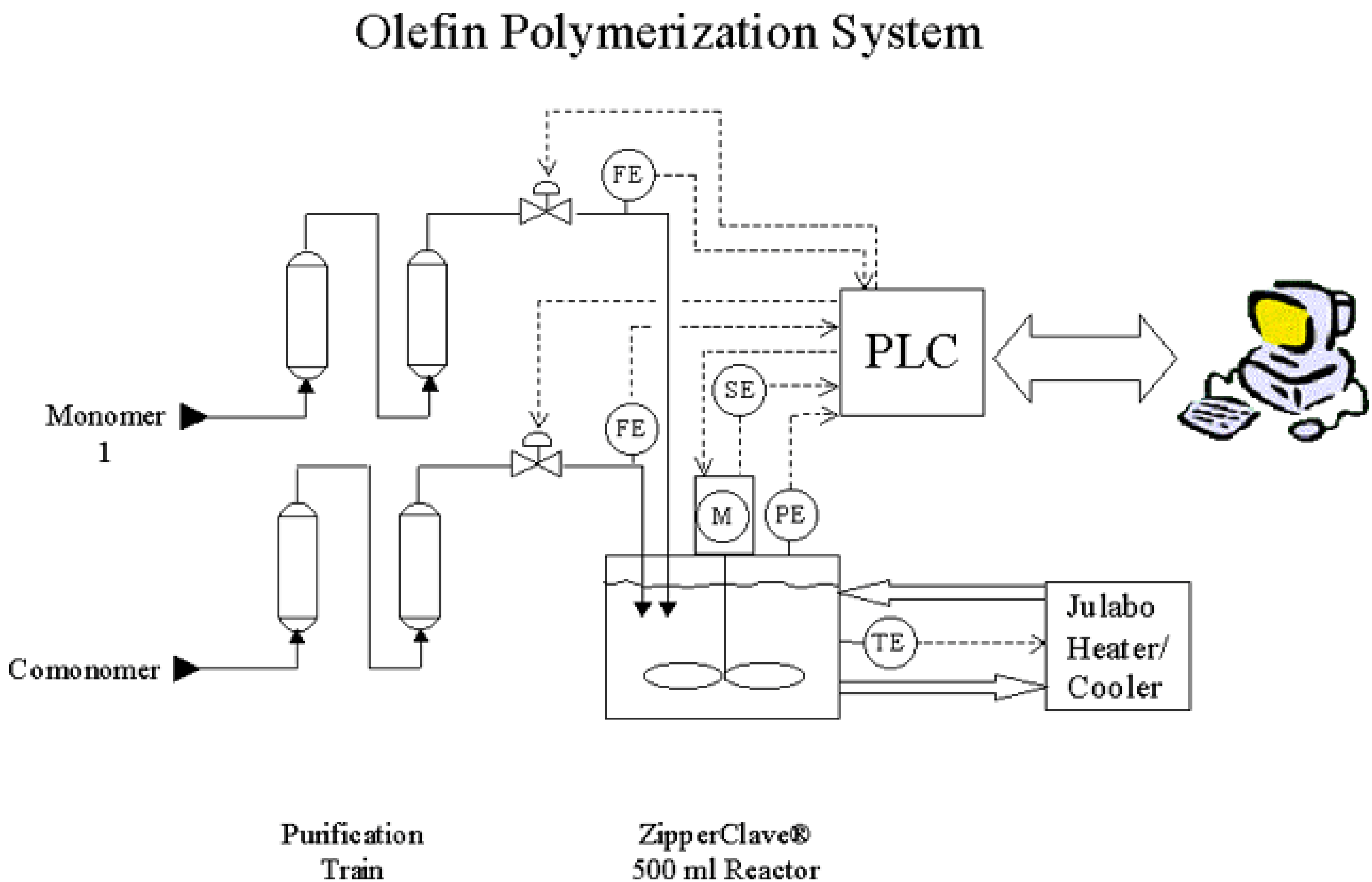
Experimental Design

The Experimental Design Problem



Ronald Fisher
1935

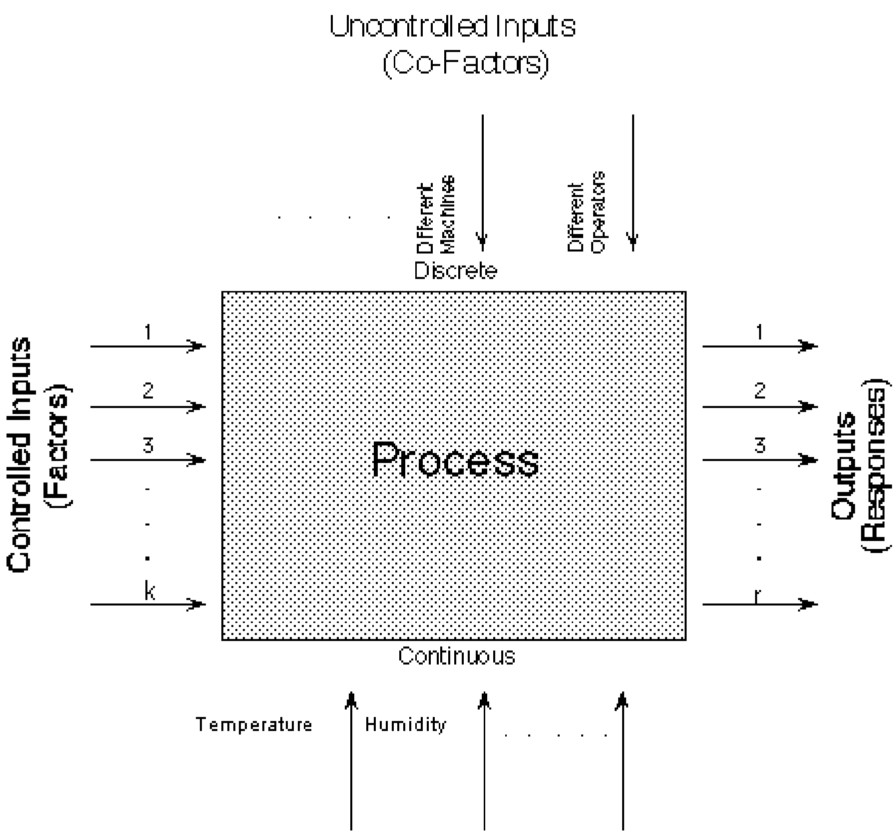
Polymerization Reactor Example



Experimental Design

- Operating objectives
  - » Maximize productivity
  - » Achieve target polymer properties
- Input variables
  - » Catalyst and co-catalyst concentrations
  - » Monomer and co-monomer concentrations
  - » Reactor temperature
- Output variables
  - » Polymer production
  - » Copolymer composition
  - » 2 molecular weight measures
- Experimental design problem
  - » Determine optimal input values
- Brute force approach
  - » Select values for the five inputs
  - » Conduct and analyze experiment
  - » Repeat until best inputs are found
- Statistical techniques
  - » Allow more efficient search of input space
  - » Handle nonlinear variable interactions
  - » Account for experimental error

The Experimental Design Problem



- Design objectives
  - » Information to be gained from experiments
- Input variables (factors)
  - » Independent variables
  - » Varied to explore process operating space
  - » Typically subject to known limits
- Output variables (responses)
  - » Dependent variables
  - » Chosen to reflect design objectives
  - » Must be measured
- Statistical design of experiments
  - » Maximize information with minimal experimental effort
  - » Experimental plan determined in advance

Alternative Design Approaches

- Comparative experiments
  - » Determine the best alternative out of various options
- Screening experiments
  - » Determine the most important factors
  - » Preliminary step for more detailed analysis
- Response surface modeling
  - » Achieve a specified output target
  - » Minimize or maximize a particular output
  - » Reduce output variability
  - » Determine predictive model over large operating regime

Input Levels

- Input level selection
  - » Low and high limits define operating regime
  - » Must be chosen carefully to ensure feasibility
- Two-level designs
  - » Two possible values for each input (low, high)
  - » Most efficient and economical
  - » Ideal for screening designs
- Three-level designs
  - » Three possible values for each input (low, nominal, high)
  - » Less efficient but yield more information
  - » Well suited for response surface designs

Response Surface Models

- Example
  - » Three factors (x_1, x_2, x_3) and one response (y)
- Linear model

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3$$

  - » Accounts for main effects
  - » Requires at least 4 experiments
- Linear model with interactions

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3$$

  - » Includes binary interactions
  - » Requires at least 7 experiments
- Quadratic model

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{33} x_3^2$$

  - » Accounts for response curvature
  - » Requires at least ten experiments
- Number of parameters per response variable

Factors	2	3	4	**5**	6
Linear	3	4	5	**6**	7
Interaction	4	7	11	**16**	22
Quadratic	6	10	15	**21**	28

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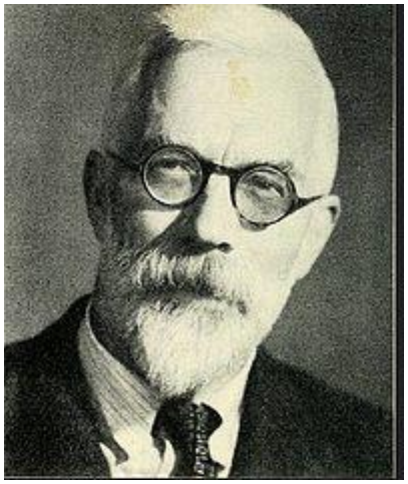
Experimental Design

Full Factorial Designs



Ronald Fisher
1935

General Design Procedure

1. Determine objectives
2. Select input variables and their levels
3. Select output variables
4. Perform experimental design
5. Execute designed experiments
6. Perform data consistency checks
7. Statistically analyze the data
8. Modify the design as necessary

Full Factorial Designs

- Basic features
  - » All permutations of factor levels considered
  - » L_i = number of levels for factor i
  - » k = number of factors
  - » n = number of repeated experiments
- Total number of experiments: $N = (L_1 L_2 \cdots L_k)n$
- No duplication, same number of levels: $N = L^k$

Factors	Two-Level	Three-Level
2	4	9
3	8	27
4	16	81
5	**32**	**243**
6	64	729
7	128	2187

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Full Factorial Design Examples

- Design for $k = 3$, $L = 2$, $n = 1$
  - » Input levels: -1 = minimum, +1 = maximum

Run	1	2	3	4	5	6	7	8
x_1	-1	+1	-1	+1	-1	+1	-1	+1
x_2	-1	-1	+1	+1	-1	-1	+1	+1
x_3	-1	-1	-1	-1	+1	+1	+1	+1

- Common extensions
  - » Repeat runs for improved statistics
  - » Add center points runs to capture nominal behavior

Run	1	2	3	4	5	6	7	8	9	10	11
x_1	-1	+1	-1	+1	-1	+1	-1	+1	0	0	0
x_2	-1	-1	+1	+1	-1	-1	+1	+1	0	0	0
x_3	-1	-1	-1	-1	+1	+1	+1	+1	0	0	0

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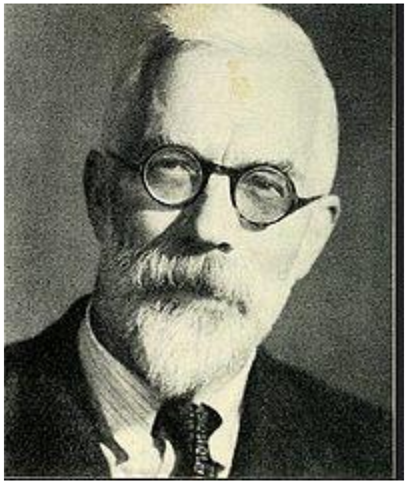
Experimental Design

Reduced Design Methods



Ronald Fisher
1935

George Box
1951

Fractional Factorial Designs

- Terminology
  - » Balanced design – all input level combinations have the same number of observations
  - » Orthogonal design – the effect of any factor sums to zero across the effect of the other factors

Run	1	2	3	4	Sum
x_1	-1	+1	+1	-1	0
x_2	-1	+1	-1	+1	0
x_3	-1	-1	+1	+1	0

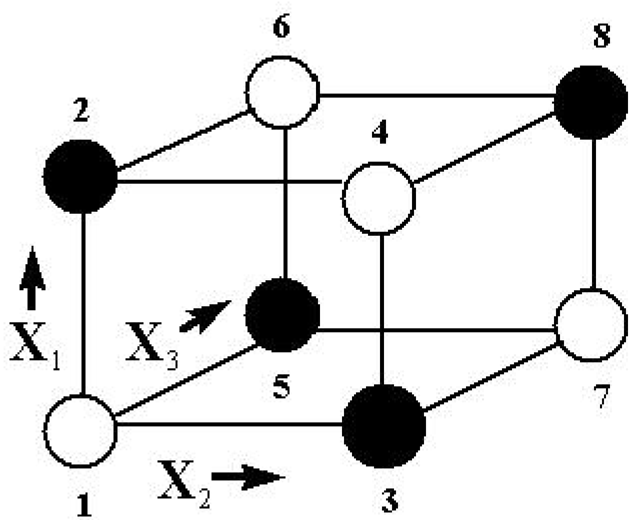
- Basic features
  - » Utilize a specified fraction of the full factorial design
  - » Both balanced and orthogonal
  - » Most useful for determining main effects
  - » Can determine interaction and/or quadratic effects

½-Fractional Factorial Designs

- Full factorial design: k = 3, L = 2, n = 1

Run	1	2	3	4	5	6	7	8
x_1	-1	+1	-1	+1	-1	+1	-1	+1
x_2	-1	-1	+1	+1	-1	-1	+1	+1
x_3	-1	-1	-1	-1	+1	+1	+1	+1

- Alternative ½-fractional factorial designs



Run	1	4	6	7
x_1	-1	+1	+1	-1
x_2	-1	+1	-1	+1
x_3	-1	-1	+1	+1
Run	2	3	5	8
x_1	+1	-1	-1	+1
x_2	-1	+1	-1	+1
x_3	-1	-1	+1	+1

Other Fractional Factorial Designs

- Two-level designs

Factors	3	4	**5**	6	7
Full	8	16	**32**	64	128
1/2	4	8	**16**	32	64
1/4	NA	4	**8**	16	32
1/8	NA	NA	**NA**	8	16

- Three-level designs

Factors	3	4	**5**	6	7
Full	27	81	**243**	729	2187
1/3	9	27	**81**	243	729
1/9	3	9	**27**	81	243
1/27	NA	NA	**9**	27	81

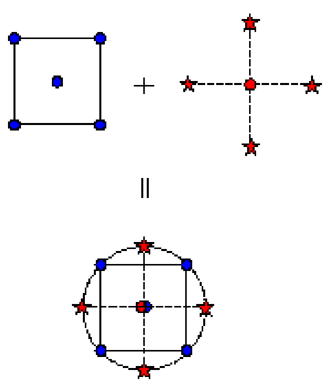
Fractional Factorial Design Example

- Polymer reactor: 5 inputs
- Full factorial design: $N = L^k = 2^5 = 32$
- ¼-fractional factorial design: $N = 8$

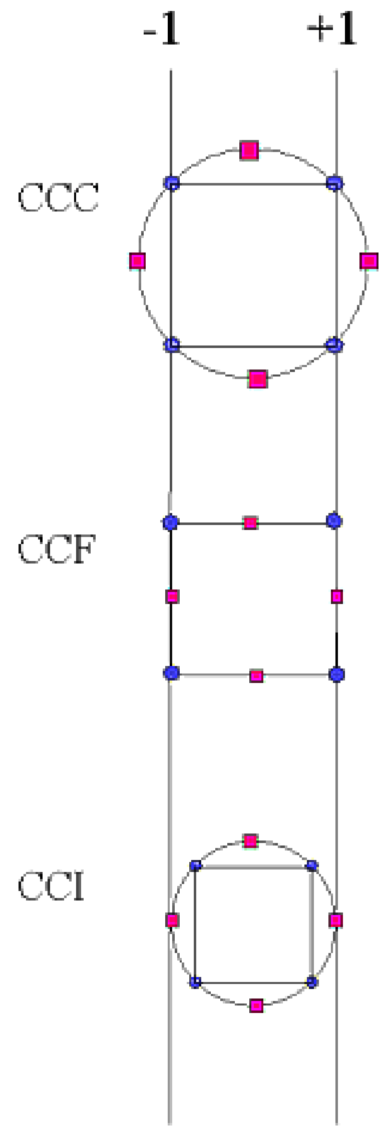
Run	1	2	3	4	5	6	7	8	Sum
x_1	-1	-1	-1	-1	+1	+1	+1	+1	0
x_2	-1	-1	+1	+1	-1	-1	+1	+1	0
x_3	-1	+1	-1	+1	-1	+1	-1	+1	0
x_4	-1	+1	+1	-1	+1	-1	-1	+1	0
x_5	+1	-1	-1	+1	+1	-1	-1	+1	0

Central Composite Designs

- Based on two-level full or fractional factorial design
- Star points
  - » Added to estimate response curvature
  - » Twice as many star points as factors
  - » Can represent new extreme factor values
- 10 point design
  - » Two-level design with center point
  - » 4 star points with center point



- Circumscribed (CCC)
  - » Require 5 levels
  - » New extreme values
  - » Rotatable
- Face Centered (CCF)
  - » Require 3 levels
  - » Old extremes retained
  - » Not rotatable
- Inscribed (CCI)
  - » Require 5 levels
  - » Old extremes retained
  - » Rotatable



Central Composite Design Example

- CCF design for 5 factors

-2	-2	-2	-2	2
-2	-2	-2	2	-2
-2	-2	2	-2	-2
-2	-2	2	2	2
-2	2	-2	-2	-2
-2	2	-2	2	2
-2	2	2	-2	2
-2	2	2	2	-2
2	-2	-2	-2	-2
2	-2	-2	2	2
2	-2	2	-2	2
2	-2	2	2	-2
2	2	-2	-2	2
2	2	-2	2	-2
2	2	2	-2	-2
2	2	2	2	2
-2	0	0	0	0
2	0	0	0	0
0	-2	0	0	0
0	2	0	0	0
0	0	-2	0	0
0	0	2	0	0
0	0	0	-2	0
0	0	0	2	0
0	0	0	0	-2
0	0	0	0	2
0	0	0	0	0

- This DOE is used for MATLAB homework #1

Experimental Design

In-class Exercise