# Response Surface Methodology: Alternative Designs

BIOE 498/598 PJ

Spring 2021

# Why alternatives to the CCD?

- The CCD is excellent (and in many ways optimal) for RSM.
- Many alternatives have been developed to address one of two CCD shortcomings:
    1. The CCD requires 5 levels for each factor.
    2. The CCD requires a lot of runs.

# Box-Behnken Designs (BBD)

- 3-level design with performance close to a CCD.
- Similar number of runs to a CCD.
- Built from $2^2$ factorials for each pair of factors.

Note that in the bottom row $\mathbf{0}$ is a vector, i.e. a set of repeated center points.

# Box-Behnken Designs (BBD)

- 3-level design with performance close to a CCD.
- Similar number of runs to a CCD.
- Built from $2^2$ factorials for each pair of factors.

| $x_1$ | $x_2$ | $x_3$ |
|---|---|---|
| $-1$ | $-1$ | $0$ |
| $-1$ | $1$ | $0$ |
| $1$ | $-1$ | $0$ |
| $1$ | $1$ | $0$ |
| $-1$ | $0$ | $-1$ |
| $-1$ | $0$ | $1$ |
| $1$ | $0$ | $-1$ |
| $1$ | $0$ | $1$ |
| $0$ | $-1$ | $-1$ |
| $0$ | $-1$ | $1$ |
| $0$ | $1$ | $-1$ |
| $0$ | $1$ | $1$ |
| $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{0}$ |

Note that in the bottom row $\mathbf{0}$ is a vector, i.e. a set of repeated center points.

# Box-Behnken Designs (BBD)

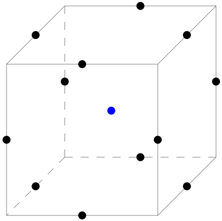
- 3-level design with performance close to a CCD.
- Similar number of runs to a CCD.
- Built from $2^2$ factorials for each pair of factors.
- Nearly rotatable (rotatable for $k = 4$ or 7).
- 3–5 center runs are recommended. (At least one center run is required for $k = 4$ or 7).

| $x_1$ | $x_2$ | $x_3$ |
|---|---|---|
| $-1$ | $-1$ | $0$ |
| $-1$ | $1$ | $0$ |
| $1$ | $-1$ | $0$ |
| $1$ | $1$ | $0$ |
| $-1$ | $0$ | $-1$ |
| $-1$ | $0$ | $1$ |
| $1$ | $0$ | $-1$ |
| $1$ | $0$ | $1$ |
| $0$ | $-1$ | $-1$ |
| $0$ | $-1$ | $1$ |
| $0$ | $1$ | $-1$ |
| $0$ | $1$ | $1$ |
| $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{0}$ |

Note that in the bottom row $\mathbf{0}$ is a vector, i.e. a set of repeated center points.

## The BBD is a spherical design

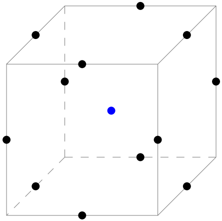
- All points in a BBD are on the edges, not the corners, of the design space.
- For $k = 3$, all points are $\sqrt{2}$ away from the design center.



BBD with $k = 3$.
Center point is in blue.

# The BBD is a spherical design

- All points in a BBD are on the edges, not the corners, of the design space.
- For $k = 3$, all points are $\sqrt{2}$ away from the design center.
- The BBD is not good at predicting responses near the corners (*extremes*) of the design space.
- Since the BBD is spherical and rotatable, "ample" center points should be used (Myers 2009).



BBD with $k = 3$.
Center point is in blue.

# Hoke Designs

- Hoke (1974) developed smaller, 3-level designs for $k = 3$ – 6 factors.
- For each $k$ there are seven variants, $\mathbf{D}_1 \ldots \mathbf{D}_7$. Design $\mathbf{D}_1$ – $\mathbf{D}_3$ are saturated, and the other are near-saturated.
- The most popular designs are $\mathbf{D}_2$ and $\mathbf{D}_6$. For $k = 3$ factors:

$\mathbf{D}_2 =$

| $x_1$ | $x_2$ | $x_3$ |
|---|---|---|
| −1 | −1 | −1 |
| 1 | 1 | −1 |
| 1 | −1 | 1 |
| −1 | 1 | 1 |
| 1 | −1 | −1 |
| −1 | 1 | −1 |
| −1 | −1 | 1 |
| −1 | 0 | 0 |
| 0 | −1 | 0 |
| 0 | 0 | −1 |

$\mathbf{D}_6 =$

| $x_1$ | $x_2$ | $x_3$ |
|---|---|---|
| −1 | −1 | −1 |
| 1 | 1 | −1 |
| 1 | −1 | 1 |
| −1 | 1 | 1 |
| 1 | −1 | −1 |
| −1 | 1 | −1 |
| −1 | −1 | 1 |
| −1 | 0 | 0 |
| 0 | −1 | 0 |
| 0 | 0 | −1 |
| 1 | 1 | 0 |
| 1 | 0 | 1 |
| 0 | 1 | 1 |

# Koshal Designs

- Koshal (1933) developed saturated $d$-level designs for modeling a response surface of order $d$.
- Koshal designs are augmented OFAT designs. They should be reserved for small numbers of factors.

First-order design
$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2$

| $x_1$ | $x_2$ | $x_3$ |
|---|---|---|
| $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{0}$ |
| 1 | 0 | 0 |
| 0 | 1 | 0 |
| 0 | 0 | 1 |

FO+TWI design
$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2$

| $x_1$ | $x_2$ | $x_3$ |
|---|---|---|
| $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{0}$ |
| 1 | 0 | 0 |
| 0 | 1 | 0 |
| 0 | 0 | 1 |
| 1 | 1 | 0 |
| 1 | 0 | 1 |
| 0 | 1 | 1 |

Second-order design
$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2$

| $x_1$ | $x_2$ | $x_3$ |
|---|---|---|
| $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{0}$ |
| 1 | 0 | 0 |
| 0 | 1 | 0 |
| 0 | 0 | 1 |
| 1 | 1 | 0 |
| 1 | 0 | 1 |
| 0 | 1 | 1 |
| $-1$ | 0 | 0 |
| 0 | $-1$ | 0 |
| 0 | 0 | $-1$ |

Note that in the top row $\mathbf{0}$ is a vector, i.e. a set of repeated center points.

# Roquemore Hybrid Designs

- Roquemore (1976) defined a series of **hybrid designs** for $k = 3$, 4, 6, & 7.
- The designs are near-rotatable and saturated or near-saturated.

$\mathbf{D}_{310}$ (saturated)

| $x_1$ | $x_2$ | $x_3$ |
|---|---|---|
| 0 | 0 | 1.2906 |
| 0 | 0 | $-0.1360$ |
| $-1$ | $-1$ | 0.6386 |
| 1 | $-1$ | 0.6386 |
| $-1$ | 1 | 0.6386 |
| 1 | 1 | 0.6386 |
| 1.736 | 0 | $-0.9273$ |
| $-1.736$ | 0 | $-0.9273$ |
| 0 | 1.736 | $-0.9273$ |
| 0 | $-1.736$ | $-0.9273$ |

$\mathbf{D}_{311\mathrm{A}}$ (near-saturated)

| $x_1$ | $x_2$ | $x_3$ |
|---|---|---|
| 0 | 0 | $\sqrt{2}$ |
| 0 | 0 | $-\sqrt{2}$ |
| $-1$ | $-1$ | $1/\sqrt{2}$ |
| 1 | $-1$ | $1/\sqrt{2}$ |
| $-1$ | 1 | $1/\sqrt{2}$ |
| 1 | 1 | $1/\sqrt{2}$ |
| $\sqrt{2}$ | 0 | $-1/\sqrt{2}$ |
| $-\sqrt{2}$ | 0 | $-1/\sqrt{2}$ |
| 0 | $\sqrt{2}$ | $-1/\sqrt{2}$ |
| 0 | $\sqrt{2}$ | $-1/\sqrt{2}$ |
| $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{0}$ |

Note that in $\mathbf{D}_{311\mathrm{A}}$ the bottom row $\mathbf{0}$ is a vector, i.e. a set of repeated center points.

## Small Composite Design (SCD)

- A CCD uses a full or Resolution V factorial core.
- One alternative is to replace the core with a Resolution III$^*$ design — a Resolution III with no 4-letter word in the defining relation.

| $x_1$ | $x_2$ | $x_3$ |
|---|---|---|
| $-1$ | $-1$ | $-1$ |
| $1$ | $1$ | $-1$ |
| $1$ | $-1$ | $1$ |
| $-1$ | $1$ | $1$ |
| $-\alpha$ | $0$ | $0$ |
| $\alpha$ | $0$ | $0$ |
| $0$ | $-\alpha$ | $0$ |
| $0$ | $\alpha$ | $0$ |
| $0$ | $0$ | $-\alpha$ |
| $0$ | $0$ | $\alpha$ |
| $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{0}$ |

# Small Composite Design (SCD)

- A CCD uses a full or Resolution V factorial core.
- One alternative is to replace the core with a Resolution III$^*$ design — a Resolution III with no 4-letter word in the defining relation.
- Unfortunately, the SCD has high variance for main effects and TWI terms.
- However, a Resolution III$^*$ design from steepest ascent can be converted into an SCD by adding axial points and center points.

| $x_1$ | $x_2$ | $x_3$ |
|---|---|---|
| $-1$ | $-1$ | $-1$ |
| $1$ | $1$ | $-1$ |
| $1$ | $-1$ | $1$ |
| $-1$ | $1$ | $1$ |
| $-\alpha$ | $0$ | $0$ |
| $\alpha$ | $0$ | $0$ |
| $0$ | $-\alpha$ | $0$ |
| $0$ | $\alpha$ | $0$ |
| $0$ | $0$ | $-\alpha$ |
| $0$ | $0$ | $\alpha$ |
| **0** | **0** | **0** |

# Final recommendations

Many designs can be used for RSM. Here are our recommendations in descending order of preference.

1. The **CCD** is the best overall choice for RSM.
2. A **BBD** is a close second, but only preferable to a CCD when 3-level factors are more convenient than 5-level factors.
3. **Hoke** or **Hybrid** designs are the preferred designs when your run budget is too small for a CCD or BBD.
4. The **SCD** should only be used when a tight budget demands immediate follow-up from steepest ascent. In this case, you need to use a Resolution III$^*$ screening design for steepest ascent.
5. **Koshal** designs are obsolete; we include them only for a historical perspective.