StatEase
statistics made easy
Make the most from every experiment!

A Crash Course in Mixture Design of Experiments

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Making the most of this learning opportunity

Hide the Control Panel
Mute your line

To prevent audio disruptions, all attendees will be muted.

Questions can be posted in the **Question** area. If they are not addressed during the webinar, I will reply via email afterwards.

Questions may also be sent to stathelp@statease.com. Please provide your company name and, if you are using Design-Expert, the serial number (found under Help, About).

Note: The slides and a recording of this webinar will be posted on the Webinars page of the Stat-Ease website within a few days.

Stat-Ease Latest News

Just Released **December 2022!**

Preview at the end of this crash course.

Live Web Mixture DOE Workshop

March 20-23, 2023

Mixture Design for Optimal Formulations (DL)

Find the sweet spot and optimize your formulations by mastering mixture designs in this 1-week (4 half-day sessions) instructor-led online course. 10:00am - 1:30pm (USA Central Time)

Agenda

- **What is a Mixture Experiment?**
- Types of Mixture Designs
- Tips and Tricks
- Conclusion
- Preview of Stat-Ease® 360

What is a Mixture Experiment?

- A typical non-mixture experiment looks something like this:
  - Suppose we are baking a cake
  - We can vary (1) **time** and (2) **temperature** in the oven:

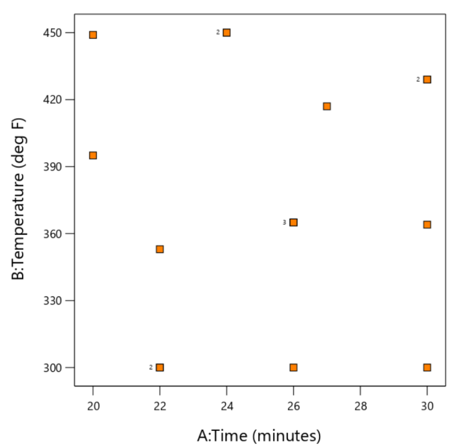
    time: 20 to 30 minutes

    temperature: 300°F to 450°F
  - The **response** we are measuring is moisture content of the cake.
  - In this experiment, both of our factors can be set independently. That is, if we set time to 25 minutes, temperature can take any value between 300F and 450F.
  - This is a typical **response surface method** experiment (RSM).

What is a Mixture Experiment?

An example response surface DOE would look something like this:

Run	Factor 1 A:Time minutes	Factor 2 B:Temperature deg F	Response 1 Moisture
1	20	395	
2	27	417	
3	24	450	
4	26	365	
5	30	364	
6	30	429	
7	30	429	
8	24	450	
9	26	365	
10	26	300	
11	22	300	
12	20	449	
13	22	300	
14	26	365	
15	22	353	
16	30	300	



What is a Mixture Experiment?

- Now consider this experiment:
  - Suppose we are deciding what cheese to put on a pizza.
  - We can blend three cheeses to make up the blend (A) **mozzarella** (B) **provolone** and (C) **white cheddar**.
  - We try various combinations of the three cheeses. Each pizza that we cook will be topped with a total of 6 ounces of cheese.

mozzarella:	0 to 6 ounces
provolone:	0 to 6 ounces
white cheddar:	0 to 6 ounces

  - **Notice: mozzarella + provolone + white cheddar** = 6 ounces

What is a Mixture Experiment?

- The responses we measure will be:
  1. **appearance**
  2. **taste**
  3. **texture** (soft & oozy **versus** hard & chewy)
  4. **cost**
- In this situation the components of the cheese blend **cannot** be set independently of one another. For example, if we put 2 ounces of mozzarella cheese into the blend, we must put a total of 4 ounces of the other two cheeses into the blend.
- This is a typical **mixture experiment**.

CRITICAL!

mozzarella + provolone + white cheddar = 6 ounces

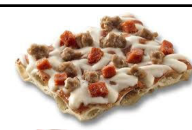
What is a Mixture Experiment?

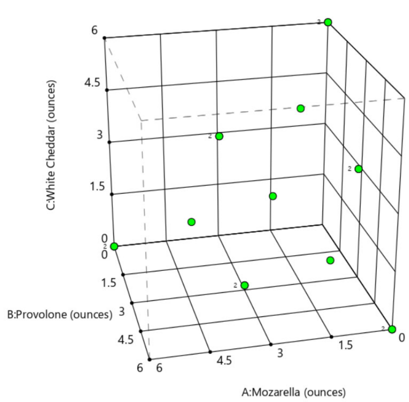
- A typical mixture DOE would look something like this:

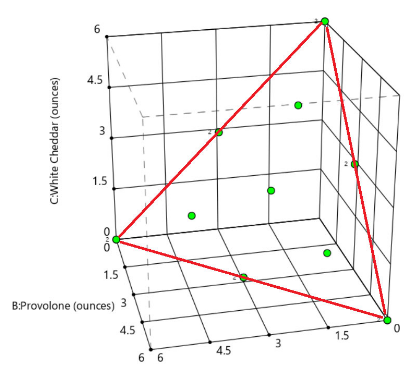
Run	Component 1 A:Mozarella ounces	Component 2 B:Provolone ounces	Component 3 C:White Cheddar ounces	Response 1 appearance	Response 2 taste	Response 3 texture	Response 4 cost
1	0	3	3				
2	4	1	1				
3	3	0	3				
4	0	6	0				
5	2	2	2				
6	1	1	4				
7	6	0	0				
8	1	4	1				
9	0	0	6				
10	3	0	3				
11	3	3	0				
12	0	6	0				
13	3	3	0				
14	0	3	3				
15	6	0	0				
16	0	0	6				

- Note that the **sum of the three cheeses = 6** in each run!

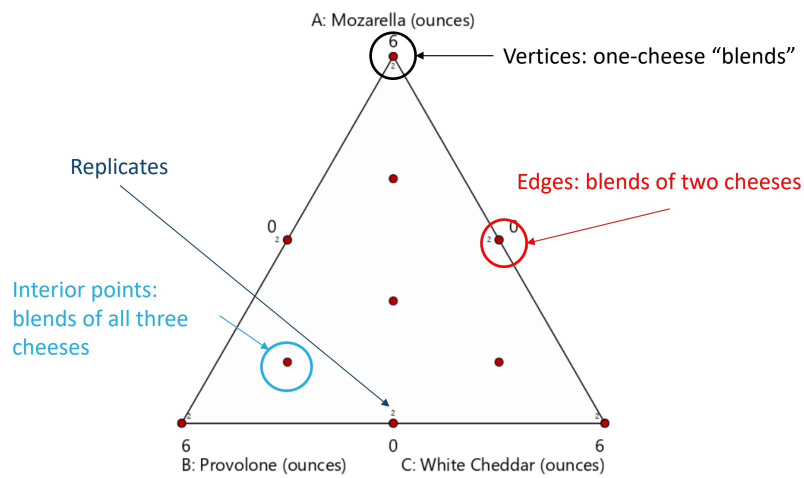
What is a Mixture Experiment?







What is a Mixture Experiment?



Identifying a Mixture Experiment

- Blending experiments should usually be set up as a mixture DOE, but not always.
  - If you are varying concentration or amounts of the components, rather than varying the weight %, volume %, or proportion of total, you may have a response surface experiment.
- The key to verifying whether you need a mixture design is to determine if any of the columns in the design plan **add up to a fixed total** in each run of the experiment.
- Part of an experiment may be a mixture (e.g. a cake formulation) and you may have non-mixture factors as well (e.g. temperature of the oven). This is called a **mixture-process combined design**.

Agenda

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- **Types of Mixture Designs**
- Tips and Tricks
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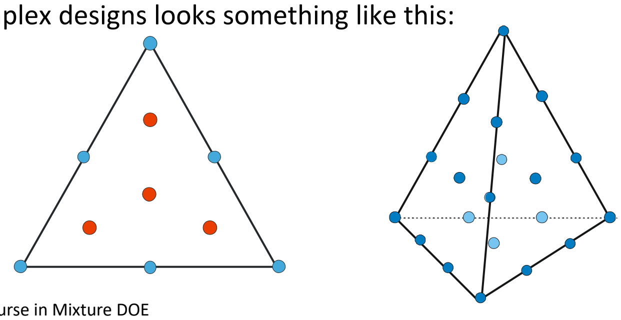
Types of Mixture Designs

- There are two basic categories of mixture DOEs:
  - **Simplex**-based designs (canned)
  - **Optimal** computer-generated designs
- In practice, most of the designs I use are optimal designs due to their flexibility.

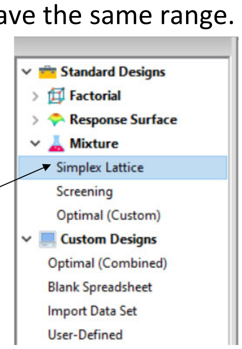
Simplex-Based Designs

- Simplex designs are **canned** and straightforward.
- In order to use a simplex design, one of the following conditions must hold true:
  - All the components have ranges 0 to 100%.
  - All the components must have the same range.
- Simplex designs looks something like this:



Simplex-Based Designs

- Simplex designs are incredibly restrictive and limited purpose.
- It **rarely** makes sense for all components to go from 0% to 100% of the mixture (100% yeast in a bread dough formulation?)
- It's also somewhat rare that all the components have the same range.
- **Do not** force all your components to have the same range so you can use a simplex design!!
- A better option is an **optimal computer-generated** design.



Simplex designs in our software.

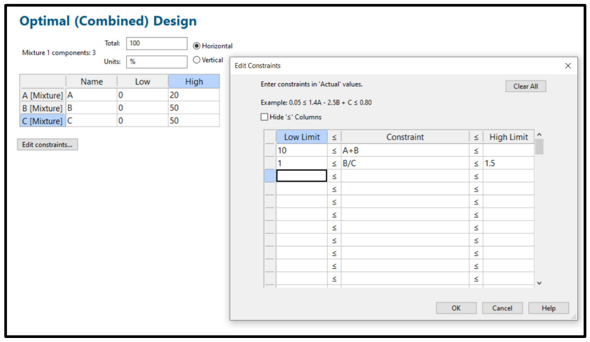
Optimal Design

- Suppose you have the following set of constraints:

  Single component
  - 0% ≤ **A** ≤ 20%
  - 0% ≤ **B** ≤ 50%
  - 0% ≤ **C** ≤ 50%

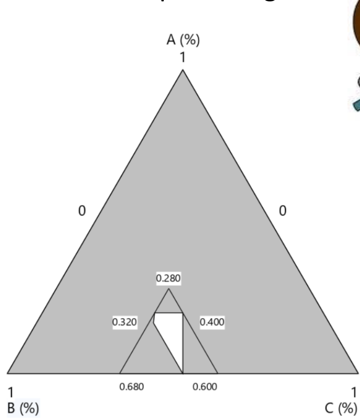
  Multicomponent
  - **A** + **B** ≥ 10%
  - 1 < **B**/**C** < 1.5

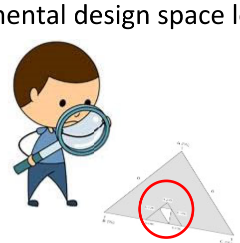
  Equality constraint
  - **A** + **B** + **C** = 100%

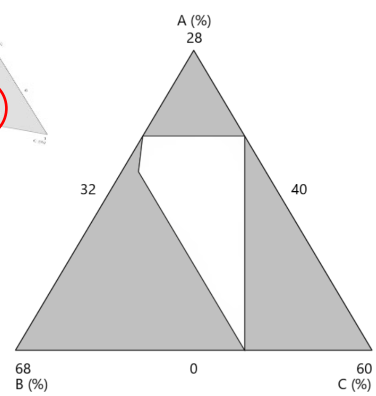


Optimal Design

- This is what the experimental design space looks like. Not a great fit for a simplex design.

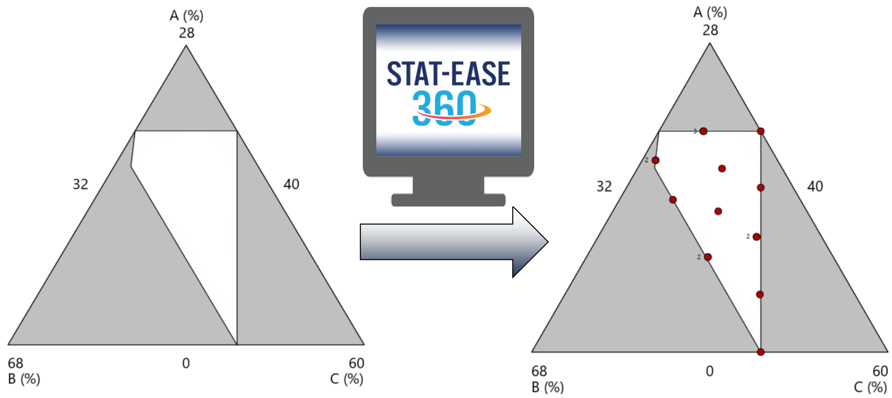






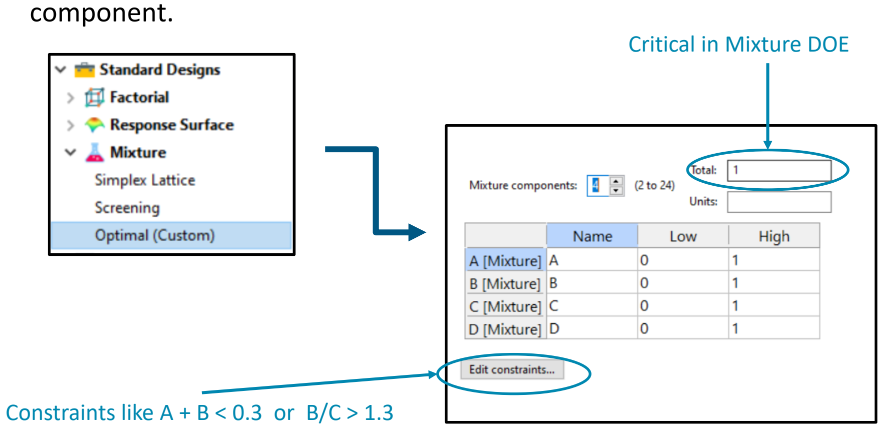
Optimal Design

- Here's what an **optimal computer-generated** design looks like for this complicated design space.



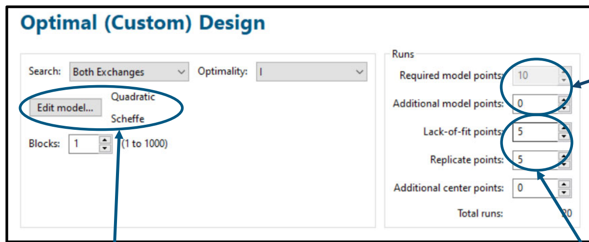
Optimal Design

Optimal designs are straightforward to build. First choose components, set their bounds, and add any constraints involving more than 1 component.



Optimal Design

Next, choose the design size, what types of runs will go into the design, how many blocks you need, what model order you are interested in fitting, and so on…



Runs added to design to estimate the model.

The model you need to be able to fit

Runs to improve properties of the design.

Software Demo

- We'll now work through
  - ✓**Building** a design
  - ✓**Analyzing** the data and building a model
  - ✓**Optimizing** the formulation
- We'll go back to the pizza cheese blend example and use the following components and bounds:

Mozzarella: 2 to 6 ounces

Provolone: 1 to 4 ounces

White Cheddar: 0 to 2 ounces

Total Cheese = 6 ounces

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Tips and Tricks

Here are a few **tips and tricks** to help you get started with mixture experiments.

1. Don't use factorial designs.
2. Don't convert to ratios so that you can use factorial or response surface designs.
3. Spend a lot of time choosing the components and the ranges.
4. Experiment iteratively, especially in new problems.
5. Master building optimal designs.

Tips and Tricks

Tip 1: Don't use factorial designs

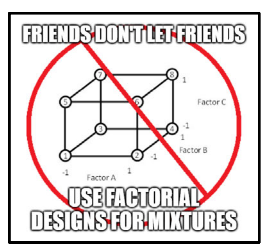
- We often have a situation like this one:
  - Components **A**, **B**, **C** go from 0 to 10%
  - Component **D** is a "filler" to bring the total up to 100%
- Textbooks will often suggest ignoring **D** and performing a 2^3 factorial design on components **A**, **B**, and **C**.
- This approach has two major issues:
  - The design is poor (only looks at extremes of factor ranges).
  - The resulting factorial model is misleading if component **D** actually has an active effect.

Tips and Tricks

Tip 1: Don't use factorial designs

4-component I-optimal design

Run	Component 1 A:A	Component 2 B:B	Component 3 C:C	Component 4 D:D
1	3.6	10	10	76.4
2	0	10	0	90
3	5.6	0.2	5.6	88.6
4	10	3.8	10	76.2
5	0.3	5.5	5.5	88.7
6	5.5	5.3	0	89.2
7	10	10	3.8	76.2
8	10	0	0	90
9	0	0	0	100
10	0	0	10	90



Factorial design ignoring **D**

Factor 1 A:A	Factor 2 B:B	Factor 3 C:C	Response 1 R1
10	10	10	
0	10	10	
10	10	0	
0	10	0	
10	0	10	
0	0	10	
10	0	0	
0	0	0	

Tips and Tricks

Tip 2: Don't use ratios so that you can use factorial or response surface designs.

- To avoid using Mixture DOE, and to overcome the limitations of factorial designs in the previous tip, experimenters will often convert their mixture to problem to a ratio problem.
- Suppose you have three components **A**, **B**, and **C**. A two-factor response surface design can be created, taking the two factors to be **A**/**C** and **B**/**C**.
- In my experience, this is usually a **bad** idea. This approach produces poor designs in the original mixture space, is tedious (requires lots of converting between % and ratios), and once again produces models that may be misleading.

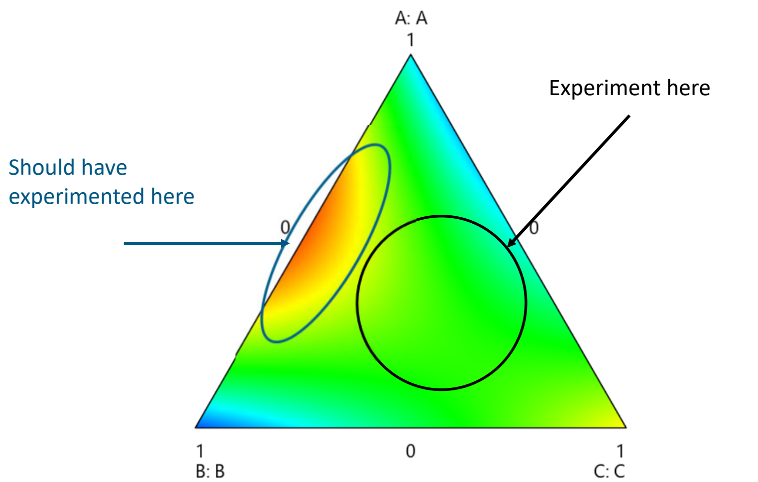
Tips and Tricks

Tip 3: Spend a lot of time choosing the components and the ranges

- The first step in any mixture experiment is choosing what components to blend, and what the upper/lower bounds of each component will be.
- In experience this step is **critical**. Most "failures" (of an experiment to produce results) are due to choosing the wrong mixture components and/or the wrong bounds.
- Components and their bounds are usually chosen using subject-matter knowledge, historical data, and guessing.
- Choosing bounds is tricky with mixtures because of the equality constraint.

Tips and Tricks

Tip 3: Spend a lot of time choosing the components and the ranges



Tips and Tricks

Tip 4: Consider an **iterative** approach

- Design of experiments is often presented as a **one-shot** approach
  - ✓ Build the experiment according to your run budget
  - ✓ Perform the experiment
  - ✓ Analyze data, optimize, and go home
- This is often wasteful in my experience.

Tips and Tricks

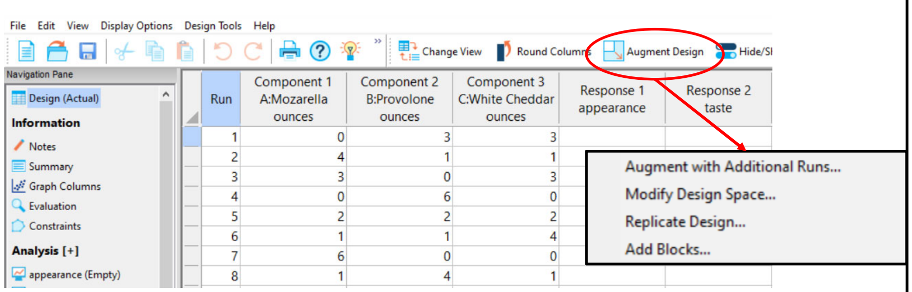
Tip 4: Consider an **iterative** approach

- Instead of depleting your entire run budget on the first pass of the experiment, use a **fraction** of the runs and leave some behind.
- After analyzing the data, you can choose what to do with the remaining runs:
    - **Expand** the mixture space and put the remaining runs in the new area to better optimize the process.
    - **Shrink** the mixture space and put the remaining runs in a smaller area where greater precision is desired.
    - Use the runs to estimate **higher-order models**.
    - Maintain the original design space and use the remaining runs to fill large gaps.

Tips and Tricks

Tip 4: Consider an **iterative** approach

- This is very easy to do in Design-Expert and Stat-Ease® 360:



- Webinar on sequential experimentation: www.youtube.com/watch?v=xiX1VxRPU5k

Tips and Tricks

Tip 5: Master building optimal computer-generated designs.

- Most of the designs you'll build will be optimal computer-generated designs. Even in situations where a canned simplex design can be used, an optimal design may have better properties.
- Learning the ins and outs of these designs will pay huge dividends going forward.
- Building and analyzing and optimal mixture design: www.youtube.com/watch?v=FTKMUNalToU
- Using optimal designs (advanced): www.youtube.com/watch?v=ZPgzc9bH5NA
- Attend a Stat-Ease Mixture DOE workshop: www.statease.com/training/live/mixdl/

Agenda

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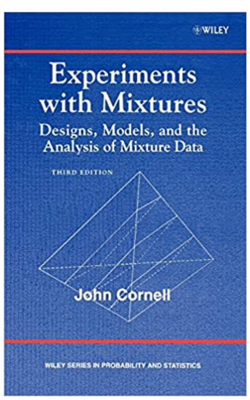
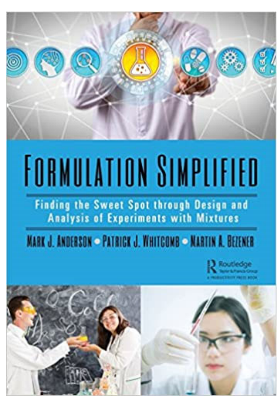
Conclusion

- Mixture DOE is a **very powerful** tool that unfortunately does not receive much attention.
- Design-Expert and Stat-Ease® 360 software contains all the **latest and greatest** tools for building and analyzing mixture experiments.
- The key to recognizing a mixture experiment is determining if there is an **equality constraint**.
- If you enjoyed this presentation and found it useful, consider taking our 4-day distance-learning workshop that dives into more detail on all the topics I discussed, including software use.

Resources





Mixture Design for Optimal Formulations (DL)

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Regular price $1095.

Online
March 20 - 23

REGISTER LEARN MORE

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- Types of Mixture Designs
- Tips and Tricks
- Conclusion
- **Preview of Stat-Ease® 360**

Stat-Ease® 360 Exclusive Preview

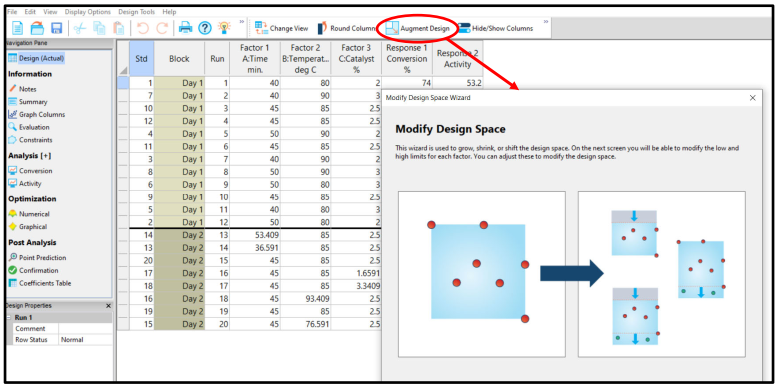
Just Released **Dec 2022!**

Many new, user-requested features!

- **Modify Design Space Wizard**
- **Round Columns**
- **Python Scripting (SE360)**
- Space-Filling Designs & Gaussian Process Models (SE360)

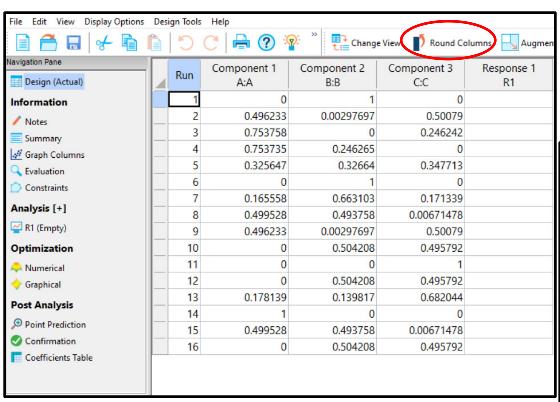
Stat-Ease® 360 Preview

Modify Design-Space Augment Wizard



Stat-Ease® 360 Preview

Round Columns



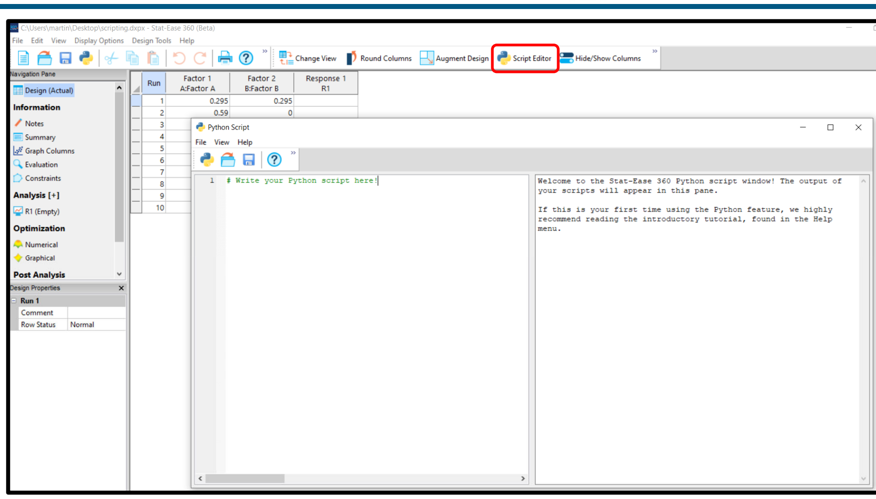
Run	Component 1 A:A	Component 2 B:B	Component 3 C:C	Response 1 R1
1	0	1	0	
2	0.496233	0.00297697	0.50079	
3	0.753758	0	0.246242	
4	0.753735	0.246265	0	
5	0.325647	0.32664	0.347713	
6	0	1	0	
7	0.165558	0.663103	0.171339	
8	0.499528	0.493758	0.00671478	
9	0.496233	0.00297697	0.50079	
10	0	0.504208	0.495792	
11	0	0	1	
12	0	0.504208	0.495792	
13	0.178139	0.139817	0.682044	
14	1	0	0	
15	0.499528	0.493758	0.00671478	
16	0	0.504208	0.495792	

Run	Component 1 A:A	Component 2 B:B	Component 3 C:C
1	0	1	0
2	0.5	0	0.5
3	0.75	0	0.25
4	0.75	0.25	0
5	0.32	0.33	0.35
6	0	1	0
7	0.17	0.66	0.17
8	0.5	0.49	0.01
9	0.5	0	0.5
10	0	0.5	0.5
11	0	0	1
12	0	0.5	0.5
13	0.18	0.14	0.68
14	1	0	0
15	0.5	0.49	0.01
16	0	0.5	0.5

Python Scripting Capabilities

- Here is just a small sampling of what you will be able to do:
  - Write scripts to automate routine processes
  - Create simulations
  - Combine features of Stat-Ease 360 with features from relevant Python packages
  - Create infinitely customizable plots and graphs
  - Facilitate import/export of data between Stat-Ease 360 and other software

Python Scripting Capabilities



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Make the most from every experiment!℠

Thanks for listening!

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