Multifactor RSM Tutorial

Optimal Design

Introduction

This tutorial details how Design-Expert® software crafts a response surface method (RSM) experiment within an irregular process space. If you are in a hurry to learn only the bare essentials of computer-based optimal design, then bypass the sidebars. However, they are well worth the time spent to explore things.

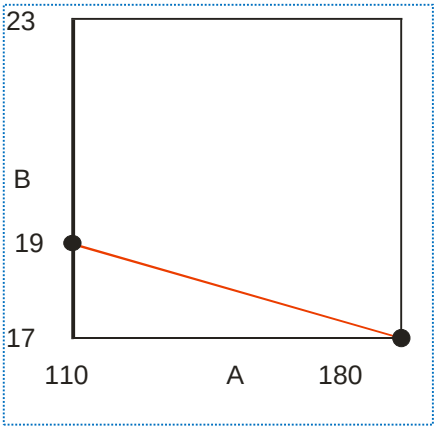
A food scientist wants to optimize a wheat product cooked at varying times versus temperatures. After a series of screening and in-depth factorial designs, the search for a process optimum has been narrowed to two factors, ranging as follows:



A. Temperature, 110 to 180 degrees C.

B. Time, 17 to 23 minutes.

However, it's been discovered that to initiate desirable starch gelatinization, time must be at least 19 minutes when temperature is at 110 degrees C—the low end of its experimental range. On the other hand, when the temperature is increased to 180 degrees, the starch will gel in only 17 minutes.



Constraint at lower levels of factors

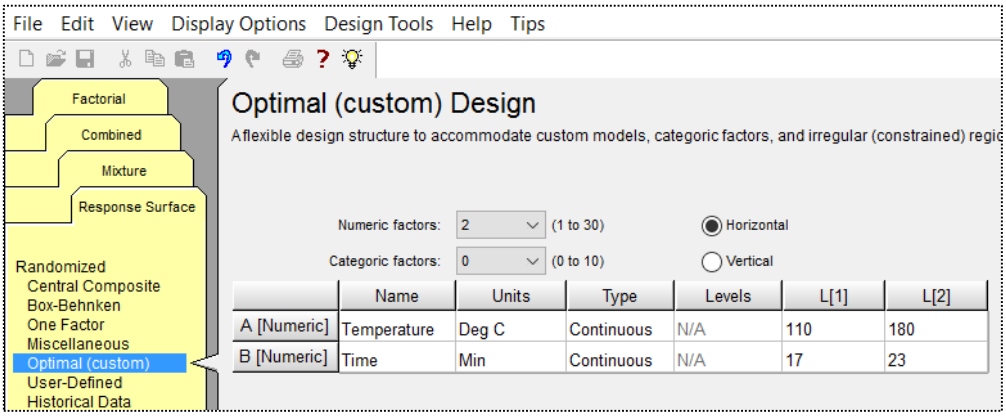
To recap: At the lowest level of A, factor B must be at least 19, while at the lowest level of B, factor A must be at least 180. To complicate matters further, the experimenter suspects that the response surface may be wavy. That is, the standard quadratic model used for response surface methods (RSM) may fall short for providing accurate predictions. Therefore, a cubic model is recommended for the design.

A problem like this can be handled by Design-Expert via its constraint tools and optimal design capability.

Design the Experiment

Start Design-Expert and initiate the design process by clicking the blank-sheet icon 🗋 on the left of the toolbar.

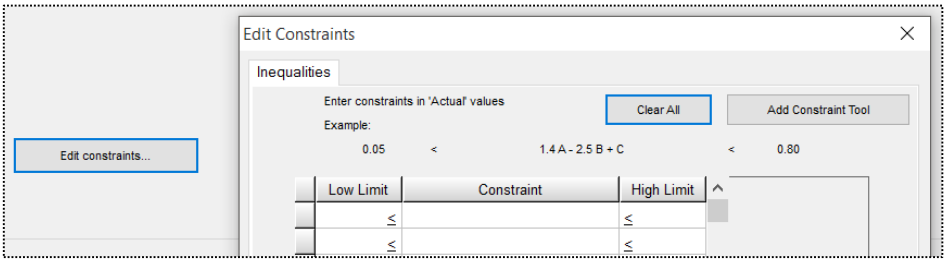
Click the **Response Surface** tab, select **Optimal (custom)** as the design, and enter the **L[1]** (lower) and **L[2]** (upper) limits as shown below.



Entering factor levels for optimal design

Create the multilinear constraint

Press the **Edit Constraints** button at the bottom of the screen.



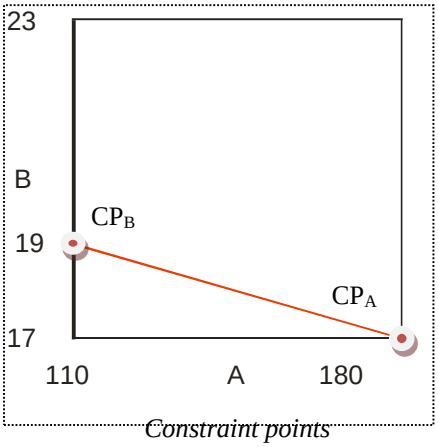
Edit constraints fields for entering equations

At this stage, if you know the multilinear constraint(s), you can enter them directly by doing some math.

☒ ***Explore the mathematics for multifactor constraints:*** Multifactor constraints must be entered as an equation taking the form of: $\beta_L \leq \beta_1 A + \beta_1 B \ldots \leq \beta_U$, where β_L and β_U are lower and upper limits, respectively. Anderson and Whitcomb provide guidelines for developing constraint equations in Appendix 7A of their book *RSM Simplified*. If, as in this case for both A and B, you want factors to exceed their constraint points (CP), this equation describes the boundary for the experimental region:

$$1 \leq \frac{A - LL_A}{CP_A - LL_A} + \frac{B - LL_B}{CP_B - LL_B}$$

where LL is the lower level. In this case, lower levels are 110 for factor A and 17 for factor B. These factors' CPs are 180 for factor A and 19 for factor B (the endpoints on the diagonal constraint line shown in the figure below).



Constraint points

Plugging in these values produces this equation:

$$1 \le \frac{A-110}{180-110} + \frac{B-17}{19-17}$$

However, the software requires formatting as a linear equation. This is accomplished using simple arithmetic as shown below.

$$1 \le \frac{A-110}{70} + \frac{B-17}{2}$$

$$(70)(2)(1) \le 2(A-110) + 70(B-17)$$

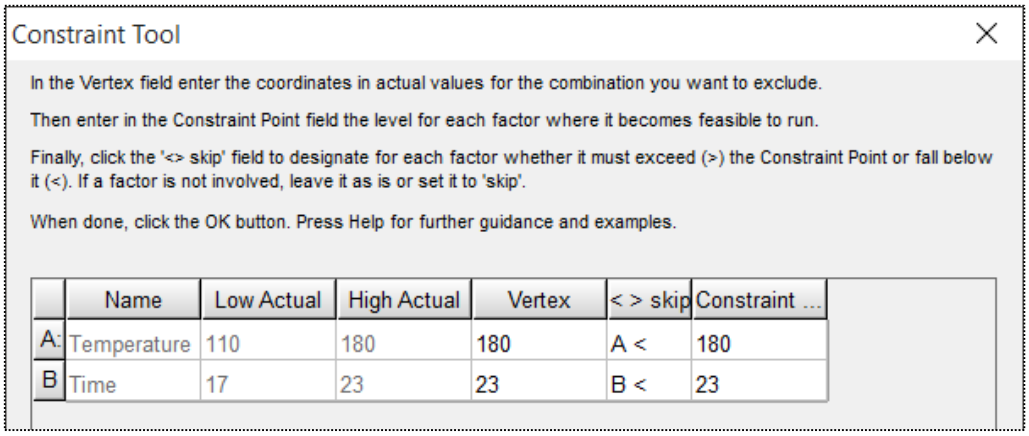
$$140 \le 2A - 220 + 70B - 1190$$

$$1550 \le 2A + 70B$$

Dividing both sides by 2 simplifies the equation to $775 \le A + 35B$. This last equation can be entered directly, or it can be derived by Design-Expert from the constraint points while setting up a RSM design.

Using the Constraint Tool

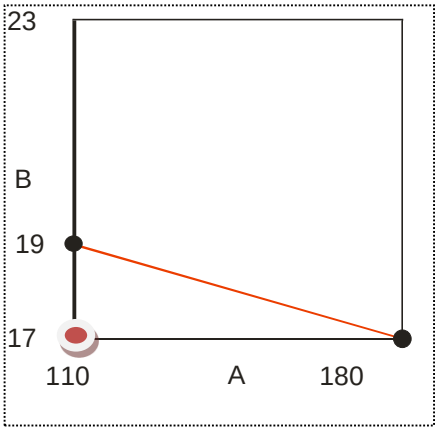
Rather than entering this in directly, let's make Design-Expert do the math. Click the **Add Constraint Tool** button. It's already set up with the appropriate defaults based on what you've entered so far for the design constraints.



	Name	Low Actual	High Actual	Vertex	< > skip	Constraint ...
A:	Temperature	110	180	180	A <	180
B	Time	17	23	23	B <	23

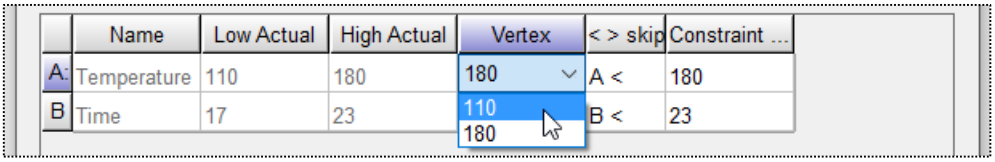
Constraints tool

As directed by the on-screen instructions, start by specifying the combination, or **Vertex** in geometric terminology, that must be excluded – shown in red below.



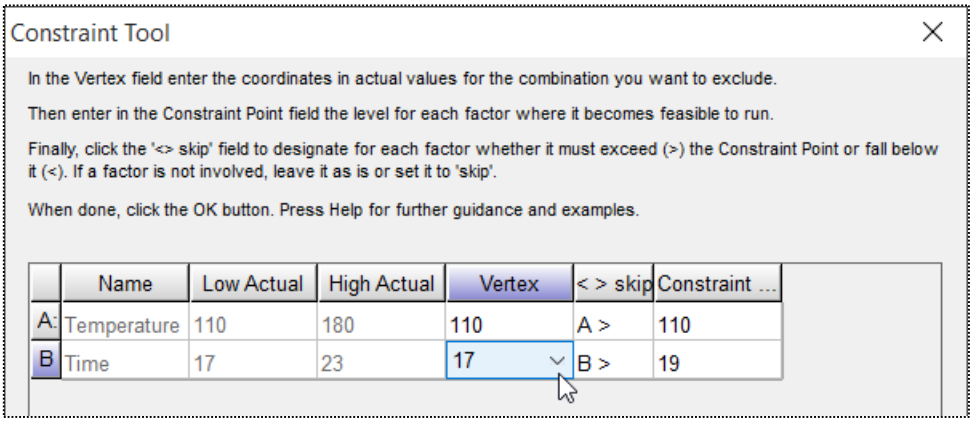
Vertex to be excluded

Click the downlist for vertex **A** and change it to **110**.



Specifying the vertex coordinate for factor A

Then change the **Vertex** coordinate for **B** to **17**.



Vertex coordinate B specified

The next step indicated by the instructions is to enter in the **Constraint Point** field the level for **B** (time) which becomes feasible when the temperature is at its low level of 110. Enter **19** – the time need at a minimum to initiate gelatinization of the starch.



Constraint point entered for factor B

Notice that Design-Expert correctly changed the inequality to greater than (>).

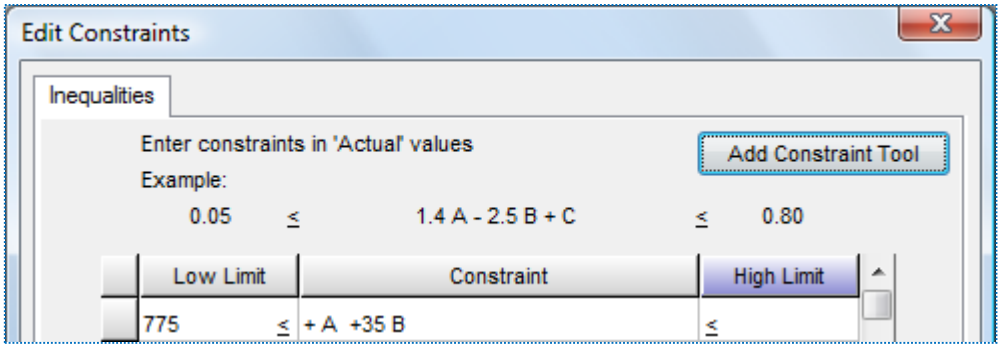
Now we turn our attention back to factor **A** (temperature) and its **Constraint Point**. It must be at least **180** when B (time) is at its vertex (low) level.

	Name	Low Actual	High Actual	Vertex	< > skip	Constraint Point
A:	Temperature	110	180	110	A >	180
B:	Time	17	23	17	B >	19

Constraint point set for A

Notice that Design-Expert previously changed the inequality to greater than (>), which is correct.

Press **OK** to see that Design-Expert calculated the same multilinear constraint equation that we derived mathematically.



Resulting multilinear constraint equation

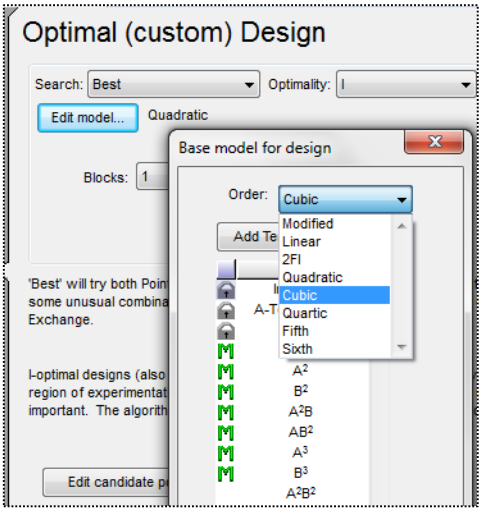
Press **OK** to accept this inequality constraint. Then press **Continue.**

Building an optimal design

Leave the Search option default of "Best" and Optimality on the "I" criterion.

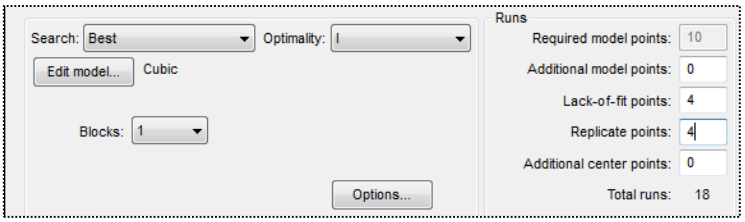
☒ ***Explore details on optimal design options:*** Take a moment now to read the helpful information provided on screen, which provide some pros and cons to these defaults. Note that we recommend the I optimal for response surface designs like this. Press screen tips (light bulb icon) for more details about the "Optimal Model Selection Screen." Feel free to click the link that explains how Design-Expert uses the "Best" search from coordinate and point exchange. Exit out (**X**) of the tips for the "Optimal (custom) Design Selection Screen."

Press the **Edit Model** button to upgrade the default model of quadratic to **Cubic**. (Recall that the experimenter suspects the response might be 'wavy' — a surface that may not get fit adequately with only the default quadratic model.)



Cubic model specified

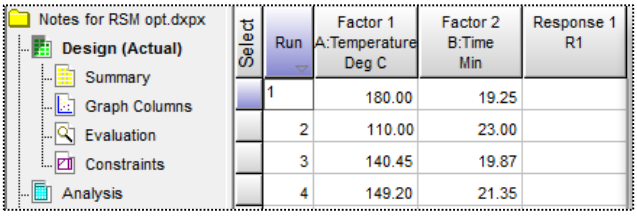
The defaults for the runs are a bit more than the experimenter would like to run for lack of fit and replicates. To limit the number of runs, change the **Lack-of-fit points** — from 5 (by default) to **4**. Also decrease the **Replicate points** to **4**. The experimenter realizes this will decrease the robustness of the design, but decides that runs are too costly, so they need to be limited.



Lack of fit and replicates decreased

Press **Continue** to the response entry — leave this at the generic default of "R1" (we will not look at the experimental results). Then press **Finish** to build the optimal design for the constrained process space.

☒ ***Explore how the program arrives at an optimal design:*** At this stage, Design-Expert randomly chooses a set of design points called the "bootstrap." It then repeatedly exchanges alternative points until achieving a set that meets the specifications established in the model selection screen.



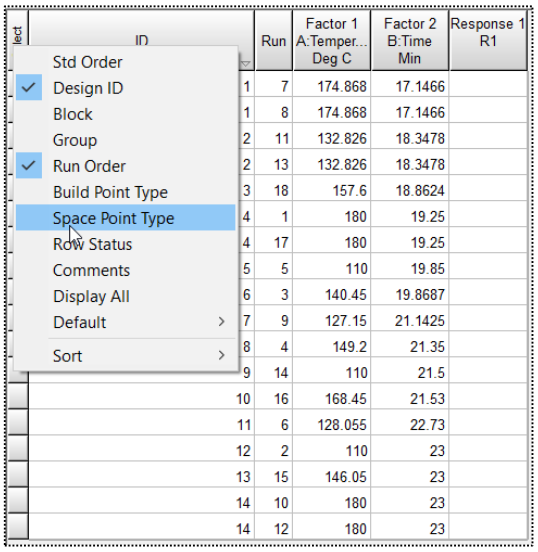
The optimal design (builds may vary due to random bootstraps)

Because of the random bootstraps, design builds vary, but all will be essentially (for all practical purposes) as optimal. Then to see the selection of points:

- right-click the **Select** button and pick **Design ID**,

- right-click the header for the **Id** column and **Sort Ascending** (or double-click the column header),
- right-click the **Select** button and click on the **Space Point Type**.

You should now see a list of design points that are identified and sorted by their geometry. Due to the random bootstraps, your points may vary from those shown below.



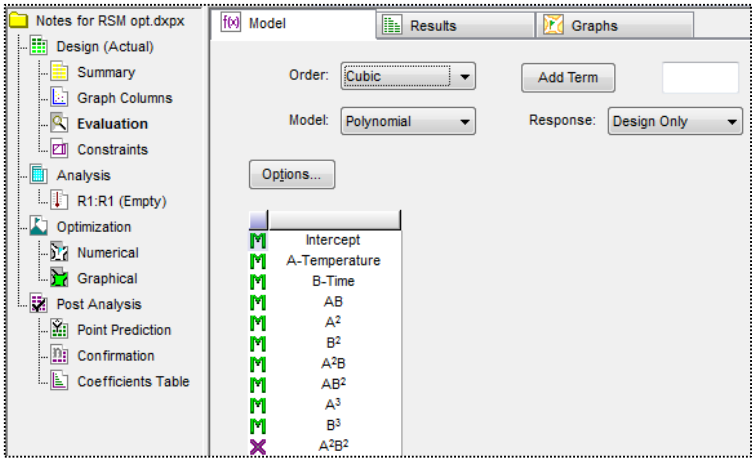
ID	Run	Factor 1 A:Temper... Deg C	Factor 2 B:Time Min	Response 1 R1
1	7	174.868	17.1466	
1	8	174.868	17.1466	
2	11	132.826	18.3478	
2	13	132.826	18.3478	
3	18	157.6	18.8624	
4	1	180	19.25	
4	17	180	19.25	
5	5	110	19.85	
6	3	140.45	19.8687	
7	9	127.15	21.1425	
8	4	149.2	21.35	
9	14	110	21.5	
10	16	168.45	21.53	
11	6	128.055	22.73	
12	2	110	23	
13	15	146.05	23	
14	10	180	23	
14	12	180	23	

Design layout sorted by ID with point type shown (your design may vary)

☒ ***Explore the factor combinations selected by the program:*** Look over the design and, in particular, the point types labeled as "vertex": Is the combination of (110, 17) for (A,B) excluded? It should be – this is too low a temperature and too short a time for the starch to gel.

P.S. To see how Design-Expert built your design, click the **Summary** node under the Design branch.

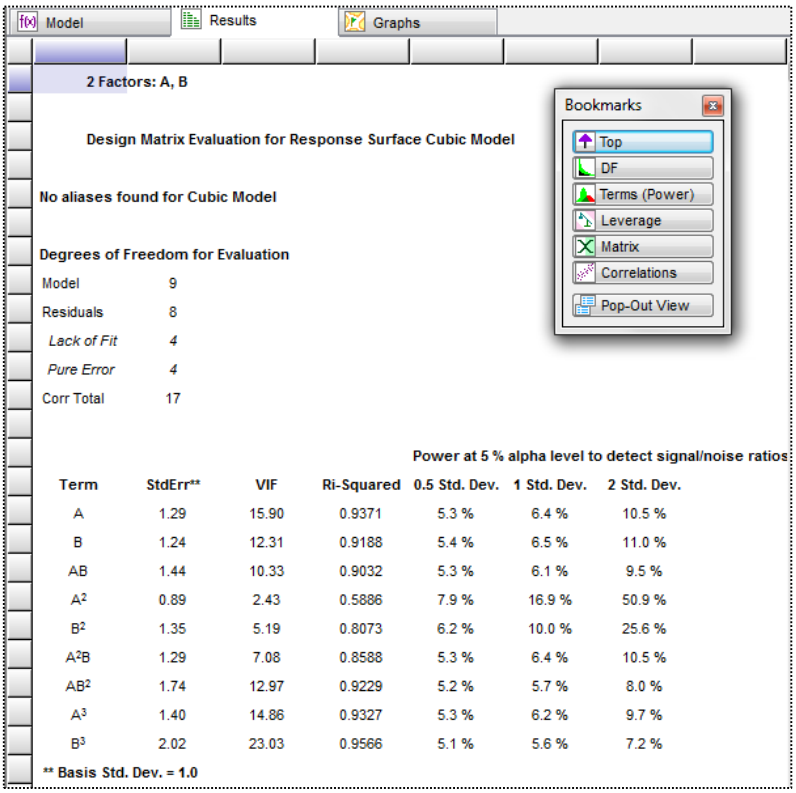
To accurately assess whether these combinations of factors provide sufficient information to fit a cubic model, click the design **Evaluation** node.



Design evaluation for cubic model

Based on the design specification, the program automatically chooses the cubic order for evaluation. Press **Results** to see how well it designed the experiment.

(We went to View and turned off the Annotated Evaluation option before making the screen shot below, but you may want to keep this informative feature enabled.)



Power at 5 % alpha level to detect signal/noise ratios

Term	StdErr**	VIF	Ri-Squared	0.5 Std. Dev.	1 Std. Dev.	2 Std. Dev.
A	1.29	15.90	0.9371	5.3 %	6.4 %	10.5 %
B	1.24	12.31	0.9188	5.4 %	6.5 %	11.0 %
AB	1.44	10.33	0.9032	5.3 %	6.1 %	9.5 %
A^2	0.89	2.43	0.5886	7.9 %	16.9 %	50.9 %
B^2	1.35	5.19	0.8073	6.2 %	10.0 %	25.6 %
A^2B	1.29	7.08	0.8588	5.3 %	6.4 %	10.5 %
AB^2	1.74	12.97	0.9229	5.2 %	5.7 %	8.0 %
A^3	1.40	14.86	0.9327	5.3 %	6.2 %	9.7 %
B^3	2.02	23.03	0.9566	5.1 %	5.6 %	7.2 %

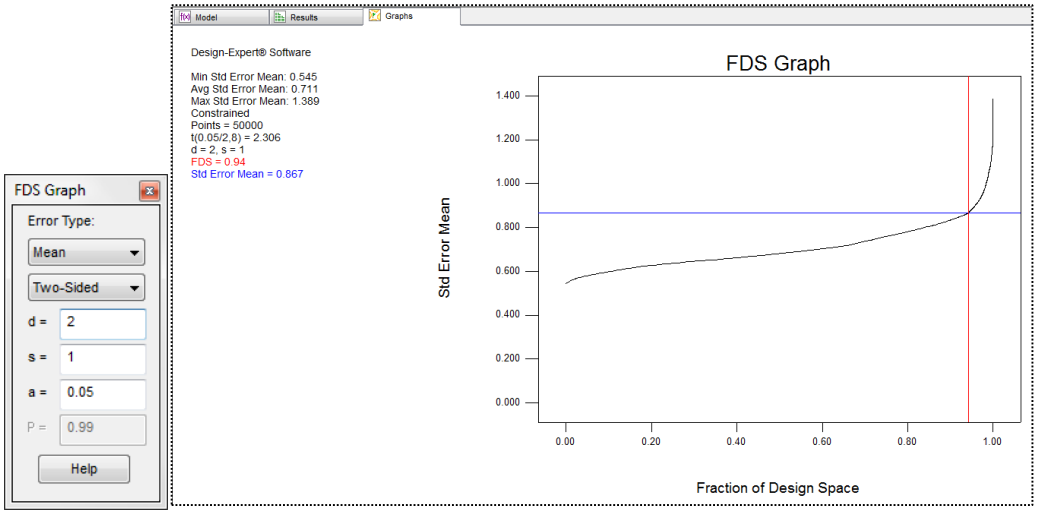
** Basis Std. Dev. = 1.0

Results of design evaluation (yours may vary)

No aliases are found: That's a good start! However, you may be surprised at the low power statistics and how they vary by term. This is fairly typical for designs with multilinear constraints. Therefore, we recommend you use the fraction of design space (FDS) graph as an alternative for assessing the sizing of such experiments. This will come up in just a moment.

☒ ***Explore other aspects of design evaluation:*** Feel free to press forward to the leverage results and beyond by pressing for this on the floating Bookmarks. Look over the annotations. Also press for Tips and look in Help for statistical details.

Press the **Graphs** tab. Let's assume that the experimenter hopes to see differences as small as two standard deviations in the response, in other words a signal-to-noise ratio of 2. In the floating tool for **FDS Graph** enter a **d** of **2**. Press the Tab key to see the fraction of design space that achieves this level of precision for prediction ("d" signifying the response difference) given the standard deviation ("s") of 1.

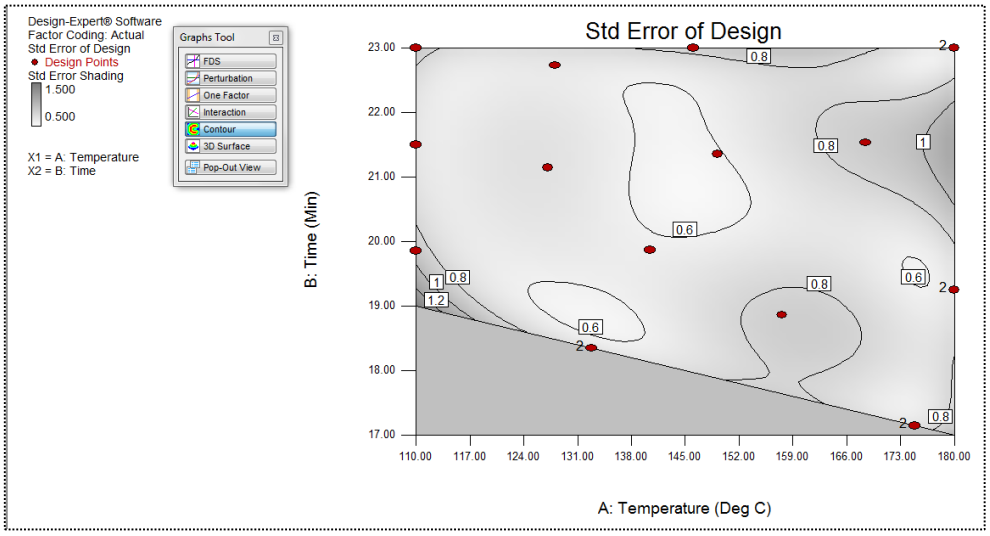


FDS graph

Ideally the FDS, reported in the legend at the left of the graph, will be 0.8 or more as it is in this case. This design is good to go!

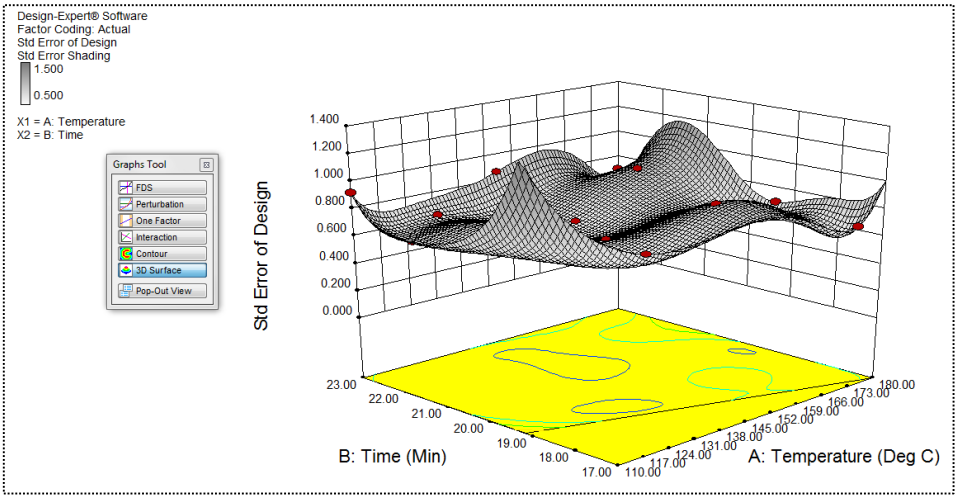
☒ ***Explore details on fraction of design space (FDS):*** A great deal of information on FDS is available at your fingertips via the screen tips. Take a look at this and you will see more on the link to the "FDS Graph Tool." Exit out of the screen-tips help screen.

On the floating **Graphs Tool** press **Contour** to see where your points are located (expect these to differ somewhat from those shown below).



Standard error plot

Our points appear to be well-spaced and the choices for replication (points labeled "2") seem reasonable. Select **View**, **3D Surface** (or choose this off the Graphs Tool) to see the surface for standard error.



Response surface for standard error

This design produces a relatively flat surface on the standard error plot, that is, it provides very similar precision for predictions throughout the experimental region.

This concludes the tutorial on optimal design for response surface methods.

☒ ***Explore what happens if you modify the design:*** You are now on your own. Depending on which points Design-Expert picked for your design, you may want to add a few more runs* at the extreme vertices, along an edge, or in other locations to decrease relatively high prediction variances. If you modify the design, go back and evaluate it. Check the 3D view of standard error and see how much lower it becomes at the point(s) you add. In any case, you can rest assured that, via its optimal design capability, Design-Expert will provide a good spread of processing conditions to fit the model that you specify, and do it within the feasible region dictated by you.

*We detailed how to modify the design layout in Part 2 of General One-Factor Tutorial (Advanced Features).