

Multifactor RSM Tutorial

(Optimal design)

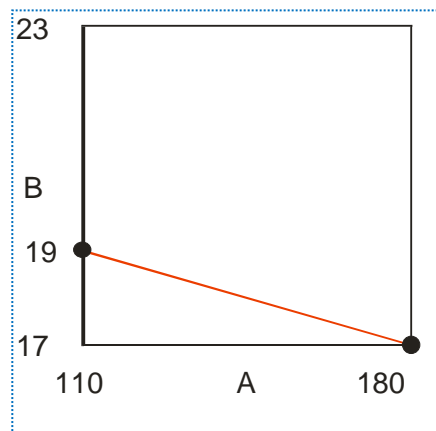
This tutorial details how Design-Expert® software crafts a response surface method (RSM) experiment within an irregular process space.

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® software 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, or select **File, New Design**, or simply click **New Design** on our opening page.

Welcome to Design-Expert® Software from Stat-Ease, Inc.

To get started, click on the File menu and select either

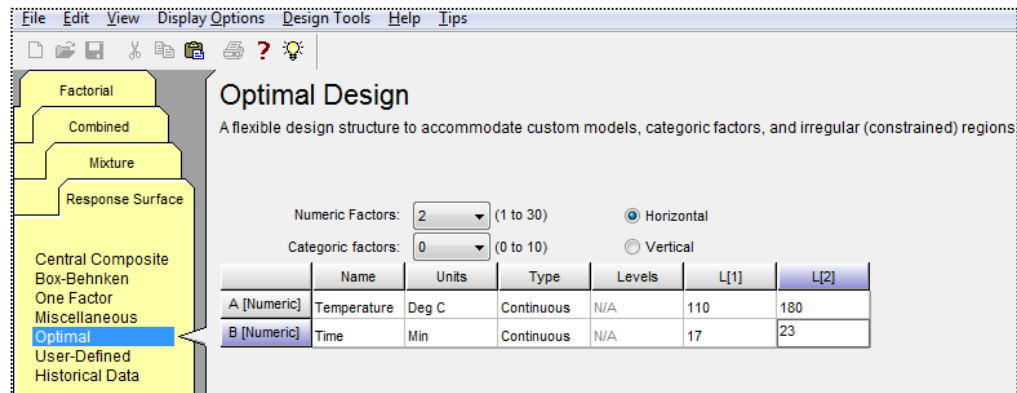
1. [New Design](#)

or

2. [Open Design](#)

Handy New Design or Open Design options

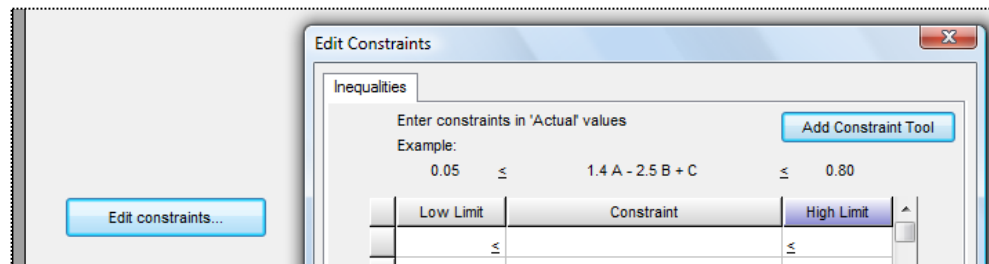
Click the yellow **Response Surface** folder tab, select **Optimal** as the design, and enter the **L[1]** (lower) and **L[2]** (upper) limits as shown below.



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.

The Mathematics

Multifactor constraints like that pictured above must be entered as an equation taking the form of:

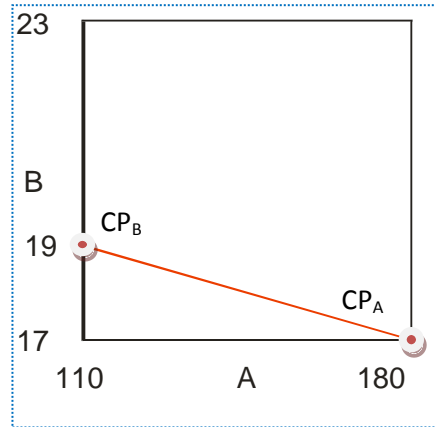
$$\beta_L \leq \beta_1 A + \beta_1 B \dots \leq \beta_U$$

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:

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

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

$$\begin{aligned} 1 &\leq \frac{A - 110}{70} + \frac{B - 17}{2} \\ (70)(2)(1) &\leq 2(A - 110) + 70(B - 17) \\ 140 &\leq 2A - 220 + 70B - 1190 \\ 1550 &\leq 2A + 70B \end{aligned}$$

Dividing both sides by 2 simplifies the equation to $775 \leq A + 35B$

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

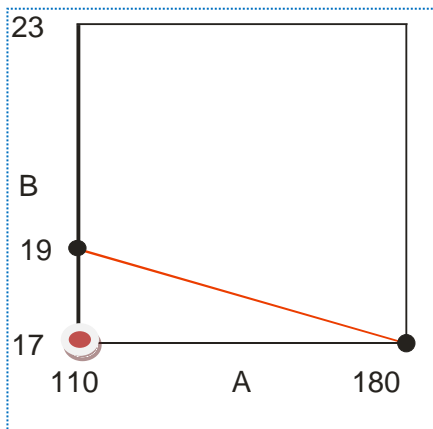
Constraint Tool

In the Vertex field enter the coordinates in actual values for the combination you want to exclude. Then enter in the Constraint Point field the level for each factor where it becomes feasible to run. Finally, click the '<> skip' field to designate for each factor whether it must exceed (>) the Constraint Point or fall below it (<). If a factor is not involved, leave it as is or set it to 'skip'. When done, click the OK button. Press Help for further guidance and examples.

	Name	Low Actual	High Actual	Vertex	< > skip	Constraint Point
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 **A** and change it to **110**.

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

Specifying the vertex coordinate for factor A

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

Constraint Tool

In the Vertex field enter the coordinates in actual values for the combination you want to exclude.
Then enter in the Constraint Point field the level for each factor where it becomes feasible to run.
Finally, click the '<> skip' field to designate for each factor whether it must exceed (>) the Constraint Point or fall below it (<). If a factor is not involved, leave it as is or set it to 'skip'.
When done, click the OK button. Press Help for further guidance and examples.

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

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.

B:	Time	17	23	17	B >	19
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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.

Edit Constraints

Inequalities

Enter constraints in 'Actual' values

Example:
 $0.05 \leq 1.4 A - 2.5 B + C \leq 0.80$

Add Constraint Tool

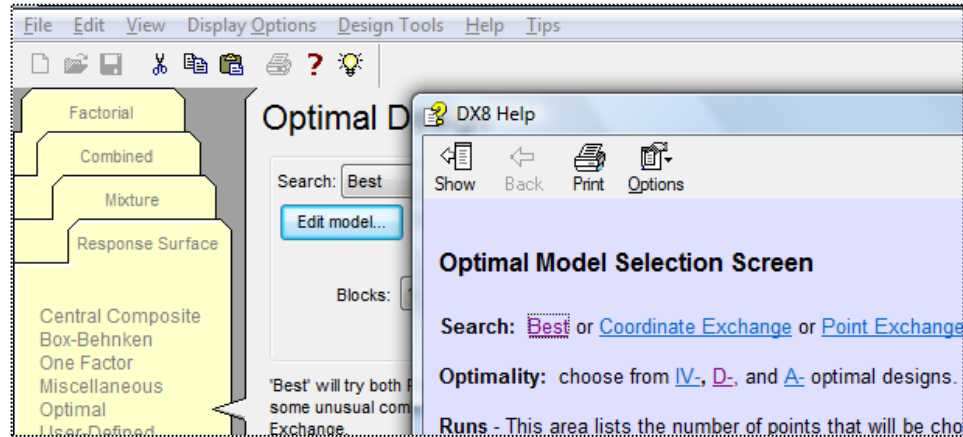
Low Limit	Constraint	High Limit
775	$\leq + A + 35 B$	\leq

Resulting multilinear constraint equation

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

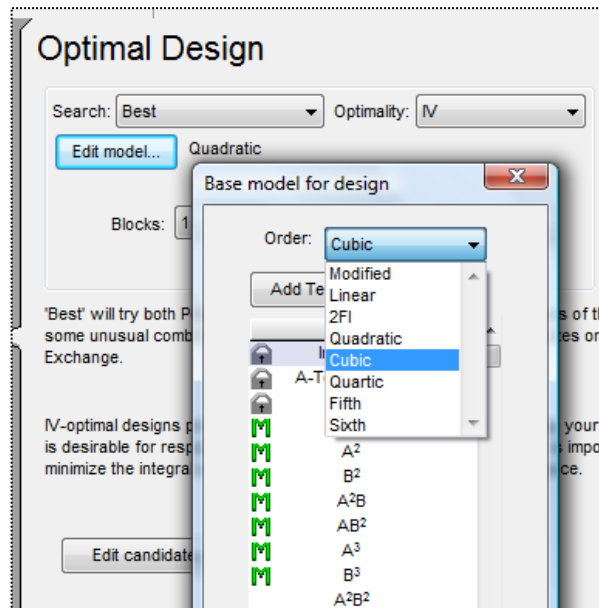
Building an optimal design

Leave the Search option default of “Best” and Optimality on the “IV” criterion. 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 IV optimal for response surface designs like this. In the next tutorial, which shows how to handle a categorical factor for RSM, you will use an alternative criterion called “D-optimal.” Press screen tips (light-bulb icon) for more details about the “Optimal Model Selection Screen.”



Screen tips provide detail on all the choices for optimal design specifications

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 “Optimal Model 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 meager for lack of fit and replicates. The experimenter would like to bolster the design a bit with one more run **To estimate lack of fit** – change this from 3 (by default) to **4**. Also increase the **Replicates** to **4**.

Optimal Design

Search: Best Optimality: IV

Edit model... Cubic

Blocks: 1 Options...

Runs

Model points: 10

To estimate lack of fit: 4

Replicates: 4

Additional center points: 0

Total runs: 18

'Best' will try both Point Exchange and Coordinate Exchange searches of the design space. This could result in some unusual combinations of factors. If you require certain candidates or combinations of factors, switch to Point Exchange.

IV-optimal designs provide lower average prediction variance across your region of experimentation. IV-optimality is desirable for response surface methods (RSM) where prediction is important. The algorithm picks points that minimize the integral of the prediction variance across the design space.

Edit candidate points...

Lack of fit and replicates increased

Press **Continue** to the response entry – leave this at the generic default of “R1” (we will not look at the experimental results). Then **Continue** on to build the optimal design for the constrained process space. 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.

Select	Std	Run	Factor 1 A:Temperature Deg C	Factor 2 B:Time Min	Response 1 R1
<input checked="" type="checkbox"/>	2	1	180.00	17.00	
<input type="checkbox"/>	18	2	180.00	23.00	
<input type="checkbox"/>	14	3	110.00	23.00	
<input type="checkbox"/>	3	4	147.90	17.92	
<input type="checkbox"/>	8	5	127.50	20.00	
<input type="checkbox"/>	6	6	110.00	19.00	
<input type="checkbox"/>	13	7	110.00	23.00	
<input type="checkbox"/>	11	8	180.00	21.38	
<input type="checkbox"/>	4	9	180.00	18.65	

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 click off the **Std** column,
- repeat the **Select** operation to pick **Design ID**,
- right-click the header for the **Id** column and **Sort by Design ID**,
- right-click the **Select** button and click on the **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	Type	Factor 1 A:Temperature Deg C	Factor 2 B:Time Min	Response 1 R1
1	1	Vertex	180.00	17.00	
1	18	Vertex	180.00	17.00	
2	4	Vertex	147.90	17.92	
3	9	Edge	180.00	18.65	
4	6	Vertex	110.00	19.00	
4	14	Vertex	110.00	19.00	
5	12	Interior	147.80	19.67	
6	5	Interior	127.50	20.00	
7	10	Interior	167.75	20.00	
8	11	Edge	110.00	20.99	
9	8	Edge	180.00	21.38	
10	15	Interior	145.00	21.59	
11	3	Vertex	110.00	23.00	
11	7	Vertex	110.00	23.00	
12	13	Edge	129.60	23.00	
13	17	Edge	161.10	23.00	
14	2	Vertex	180.00	23.00	
14	16	Vertex	180.00	23.00	

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

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.

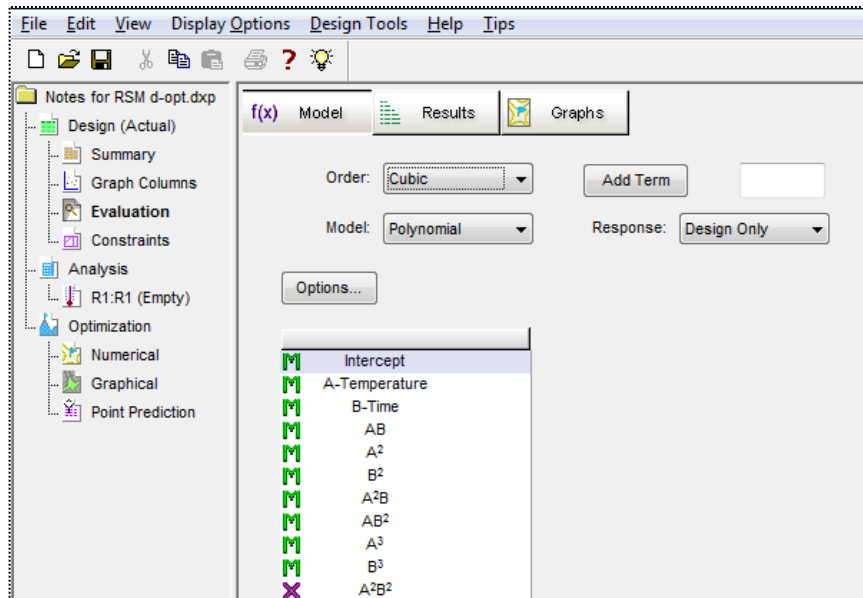
To see how Design-Expert built your design, click the **Summary** node under the Design branch.

Design Summary			
Study Type	Response Surface	Runs	18
Design Type	IV-optimal	Coordinate Exchange Blocks	No Blocks
Design Mode	Cubic	Build Time (ms)	862.28

Summary of design

This IV optimal design was produced via coordinate exchange, which took 862.28 milliseconds to create. Your build may go faster or slower depending on your processor.

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.)

2 Factors: A, B

Design Matrix Evaluation for Response Surface Cubic Model

No aliases found for Cubic Model

Degrees of Freedom for Evaluation

Model	9
Residuals	8
Lack Of Fit	4
Pure Error	4
Corr Total	17

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 ² B	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 %

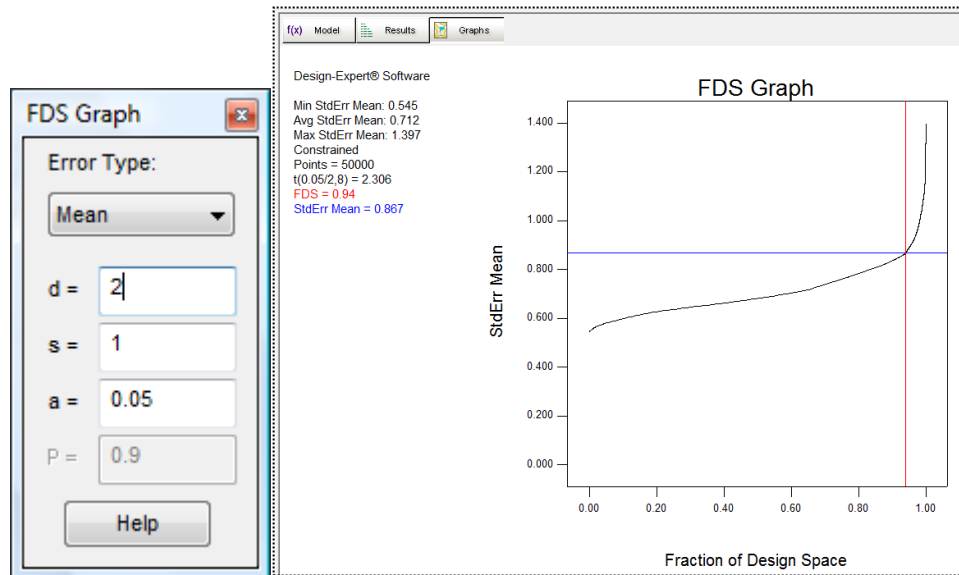
**Basis Std. Dev. = 1.0

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.

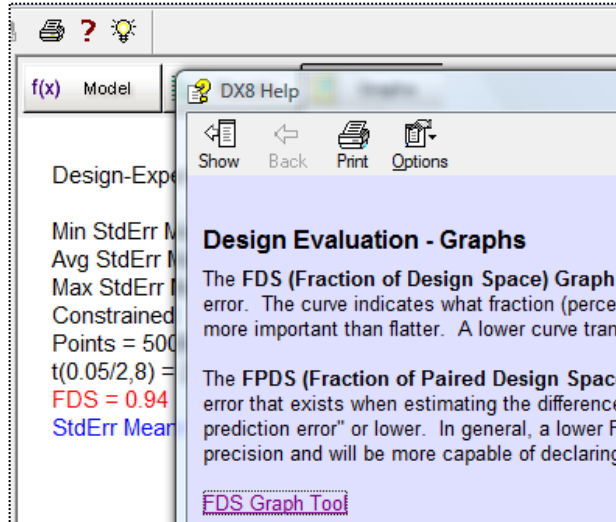
Feel free to press forward to the leverage results by pressing for this on the floating Bookmarks. If you would also like to see matrix measures, go back to the Model screen and change the Options.

Press the **Graphs** button. 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 ration 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.



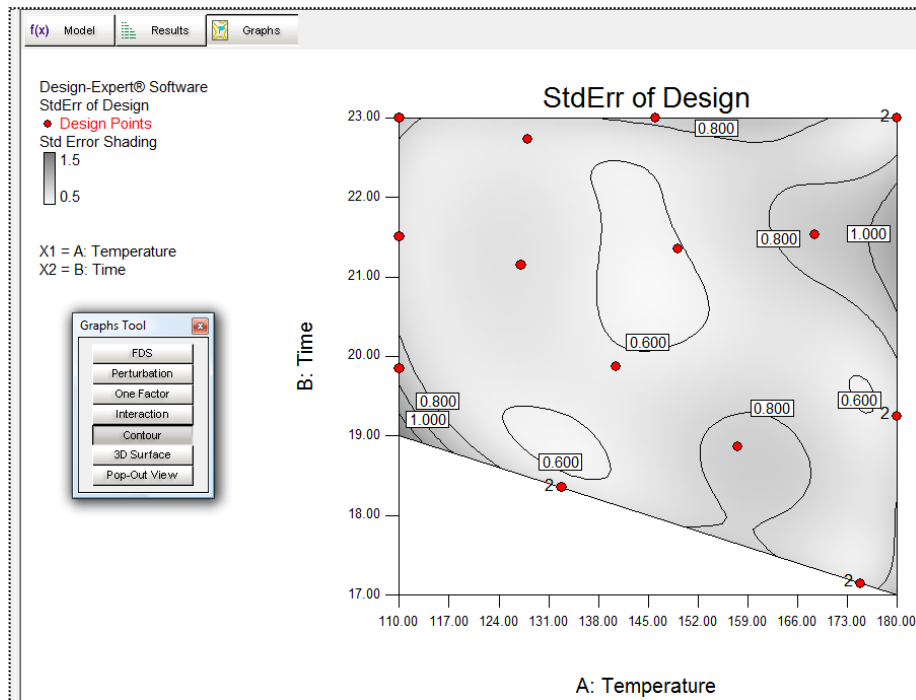
FDS graph

Ideally the FDS, reported in the legend at the left of the graph, will be 0.8 or more. A great deal of information on FDS is available at your fingertips via the screen tips. Take a look at this and click the link to the "FDS Graph Tool."



Screen tips on design evaluation graphs

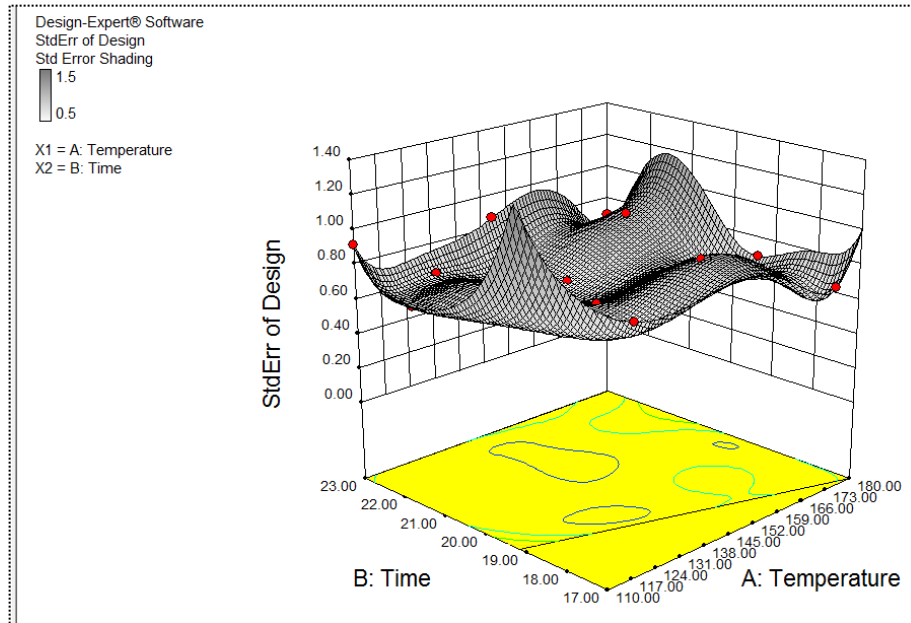
Exit out of the screen-tips help screen. On the floating **Graphs Tool** press **Contour** to see where your points are located (expect these to differ somewhat from those shown below).



Standard error plot

Our points appear to be well-spaced and the choices for replication (points labeled "2") seem reasonable. If we wanted to push the limits of temperature and time, the combinations of at either end of the constraint line could be added to the design layout.

Select **View, 3D Surface** (or choose this off the Graphs Tool) to see the surface for standard error.



Response surface for standard error

Notice that our design exhibits a peak in standard error at the constraint point (110, 19) for (A,B). It would be beneficial to add a run at these conditions of temperature and time.

Where to go from here

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. 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).