Multifactor RSM Tutorial

(Part 1/3 – The Basics)

Response Surface Design and Analysis

This tutorial, the first of three in this series, shows how to use Design-Expert® software for response surface methodology (RSM). This class of designs is aimed at process optimization. A case study provides a real-life feel to the exercise.

If you are in a rush to get the gist on design and analysis of RSM, hop past all the sidebars. However, if/when you find the time, it will be well worth the effort to explore these "by-the-ways."

☒ ***Explore more fundamental features of the software***: Due to the specific nature of this case study, a number of features that could be helpful to you for RSM will not be implemented in this tutorial. Many of these features are used in the General One Factor, RSM One Factor, or Two-Level Factorial tutorials. If you have not completed all these tutorials, consider doing so before starting this one.

We will presume that you are knowledgeable of the statistical aspects of RSM. For a good primer on the subject, see *RSM Simplified* (Anderson and Whitcomb, Productivity, Inc., New York, 2005). You will find overviews on RSM and how it's done via Design-Expert in the on-line Help system. To gain a working knowledge of RSM, we recommend you attend our Response Surface Methods for Process Optimization workshop. Call Stat-Ease or visit our website for a schedule at www.statease.com.

The case study in this tutorial involves production of a chemical. The two most important responses, designated by the letter "y", are:

- y_1 - Conversion (% of reactants converted to product)
- y_2 - Activity.

The experimenter chose three process factors to study. Their names and levels are shown in the following table.

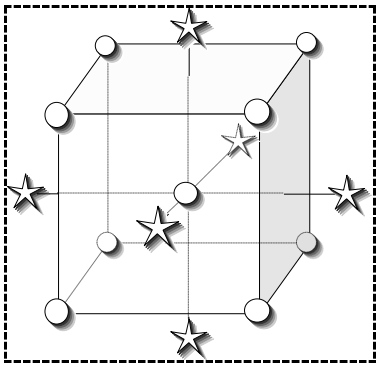
Factor	Units	Low Level (-1)	High Level (+1)
A – Time	minutes	40	50
B – Temperature	degrees C	80	90
C – Catalyst	percent	2	3

Factors for response surface study

You will study the chemical process using a standard RSM design called a central composite design (CCD). It's well suited for fitting a quadratic surface, which usually works well for process optimization.

☒ ***Explore the makeup of a CCD***: The three-factor layout for this CCD is pictured below. It is composed of a core factorial that forms a cube with sides that are two coded units in length (from -1 to +1 as noted in the table above). The stars represent axial points. How far out from the cube these should go is a matter for much discussion between

statisticians. They designate this distance "alpha" – measured in terms of coded factor levels. As you will see, Design-Expert offers a variety of options for alpha.



Central Composite Design for three factors

Assume that the experiments will be conducted over a two-day period, in two blocks:

1. Twelve runs: composed of eight factorial points, plus four center points.
2. Eight runs: composed of six axial (star) points, plus two more center points.

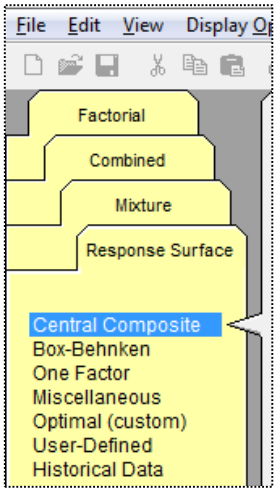
Design the Experiment

Start the program by finding and double clicking the Design-Expert software icon.



Welcome screen

Click the blank-sheet icon 🗋 on the left of the toolbar and then pick the **Response Surface** folder tab to show the designs available for RSM.

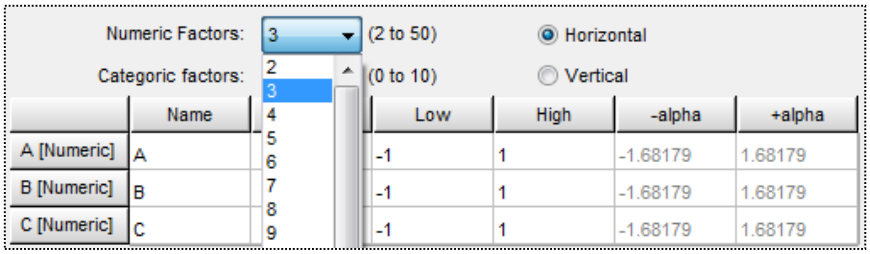


Response surface design tab

The default selection is the Central Composite design, which is used in this case study.

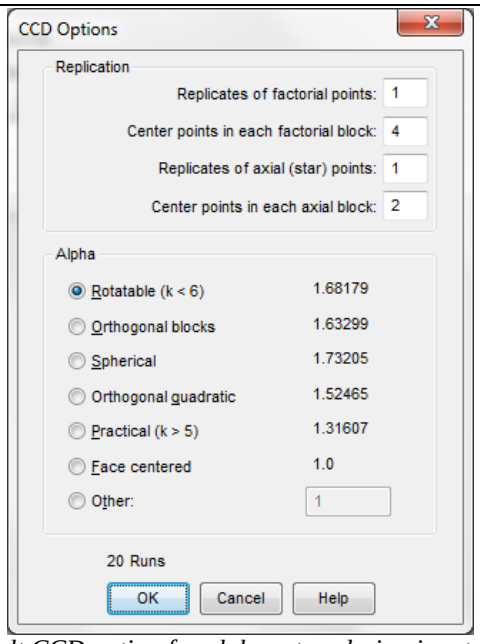
☒ ***Explore some other RSM design choices***: To see alternative RSM designs for three factors, click at far left on **Box-Behnken** (notice 17 runs near the screen bottom) and **Miscellaneous** designs, where you find the 3-Level Factorial option (32 runs, including 5 center points). Now go back and re-select **Central Composite** design.

Click the down arrow in the **Numeric Factors** entry box and Select **3** as shown below.



Selecting three numeric factors

☒ ***Explore options for CCD construction***: Before entering factors and ranges, click **Options** near the bottom of the CCD screen. Notice that it defaults to a **Rotatable** design with the axial (star) points set at 1.68179 coded units from the center – a conventional choice for the CCD.



Default CCD option for alpha set so design is rotatable

Many options are statistical in nature, but one that produces less extreme factor ranges is the "Practical" value for alpha. This is computed by taking the fourth root of the number of factors (in this case $3^{1/4}$ or 1.31607). See *RSM Simplified* Chapter 8 "Everything You Should Know About CCDs (but dare not ask!)" for details on this practical versus other levels suggested for alpha in CCDs – the most popular of which may be the "Face Centered" (alpha equals one). Press **OK** to accept the rotatable value. (Note: you won't get the "center points in each axial block" option until you change to 2 blocks in this design, as below).

Using the information provided in the table on page 1 of this tutorial (or on the screen capture below), type in the details for factor **Name** (A, B, C), **Units,** and **Low** and **High** levels.

Numeric Factors: 3 (2 to 50) Horizontal
Categoric factors: 0 (0 to 10) Vertical

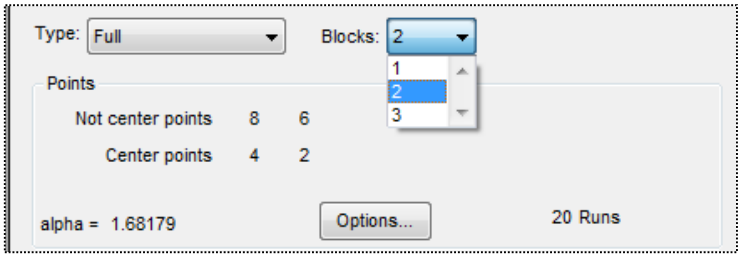
	Name	Units	Low	High	-alpha	+alpha
A [Numeric]	Time	min.	40	50	36.591	53.409
B [Numeric]	Temperature	deg C	80	90	76.591	93.409
C [Numeric]	Catalyst	%	2	3	2.3409	0.659104

Completed factor form

You've now specified the cubical portion of the CCD. As you did this, Design-Expert calculated the coded distance "alpha" for placement on the star points in the central composite design.

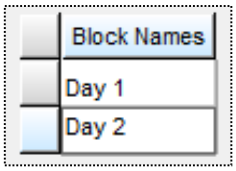
☒ ***Explore an alternative way to lay out a CCD***: Alternatively, by clicking the "entered factor ranges in terms of alphas" option you can control how far out the runs will go for each of your factors.

Now return to the bottom of the central composite design form. Leave **Type** at its default value of **Full** (the other option is a "small" CCD, which we do not recommend unless you must reduce the number of runs to the bare minimum). You will need two blocks for this design, one for each day, so click the **Blocks** field and select **2**.



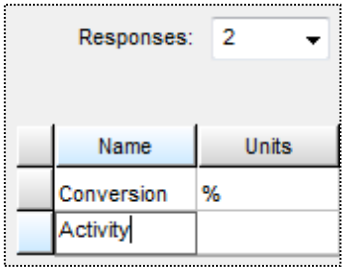
Selecting the number of blocks

Notice the software displays how this CCD will be laid out in the two blocks – for example, 4 center points will go in one and 2 in the other. Click **Continue** to reach the second page of the "wizard" for building a response surface design. You now have the option of identifying **Block Names**. Enter **Day 1** and **Day 2** as shown below.



Block names

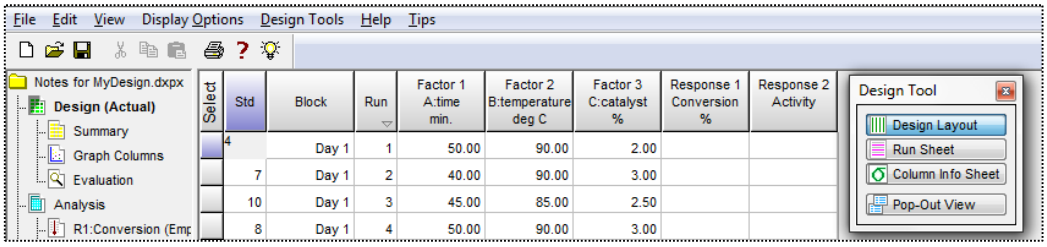
Press **Continue** to enter **Responses**. Select **2** from the pull down list. Now enter the response **Name** and **Units** for each response as shown below.



Completed response form

At any time in the design-building phase, you can return to the previous page by pressing the Back button. Then you can revise your selections. Press **Finish** to view the design layout (*your run order may differ due to randomization*).

☒ ***Explore options for modifying the design***: Design-Expert offers many ways to modify the design and how it's laid out on-screen. Preceding tutorials, especially Part 2 for General One Factor, delved into this in detail, so go back and look this over if you haven't already. Click the Tips (light bulb icon) button for a refresher.



Design layout (only partially shown, your run order may differ due to randomization)

Save the Data to a File

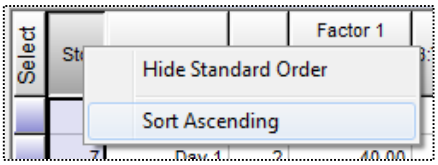
Now that you've invested some time into your design, it would be prudent to save your work. Click the **File** menu item and select **Save As**.

You can now specify your **File name** (we suggest **tut-RSM**) to Save as type "*.dxpx" in the Data folder for Design-Expert (or wherever you want to Save in).

Enter the Response Data – Create Simple Scatter Plots

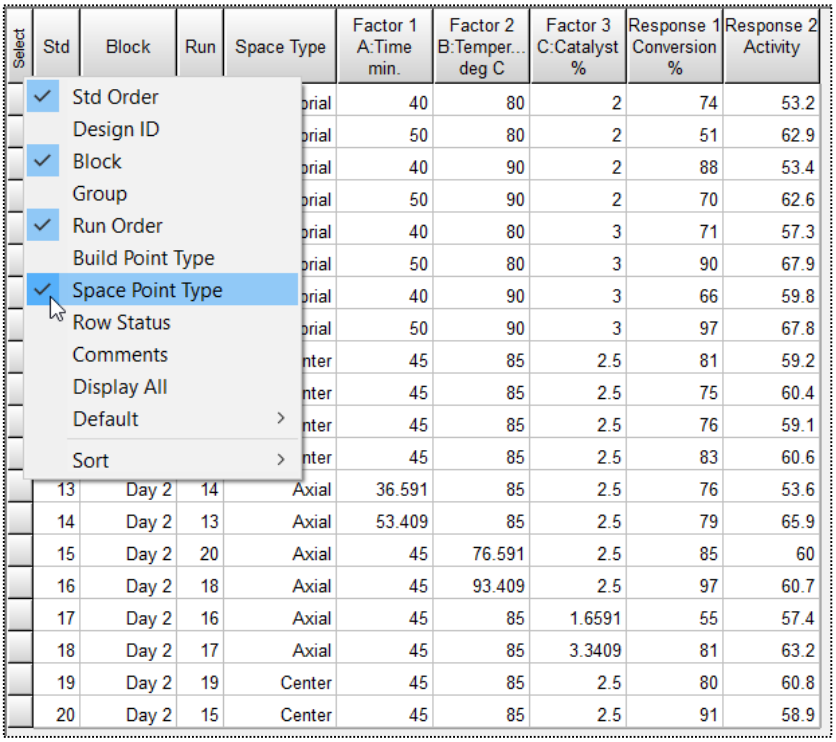
Assume that the experiment is now completed. At this stage, the responses must be entered into Design-Expert. We see no benefit to making you type all the numbers, particularly with the potential confusion due to differences in randomized run orders. Therefore, use the **File**, **Open Design** menu and select **RSM.dxpx** from the Design-Expert program **Data** directory. Click **Open** to load the data.

Let's examine the data, which came in with the file you opened (no need to type it in!). Move your cursor to **Std** column header and right-click to bring up a menu from which to select **Sort Ascending** (this can also be done via a double-click on the header).



Sorting by Standard (Std) Order

Now right-mouse click the **Select** column header and choose **Space Point Type**.



Std	Block	Run	Space Type	Factor 1 A:Time min.	Factor 2 B:Temper... deg C	Factor 3 C:Catalyst %	Response 1 Conversion %	Response 2 Activity
			brial	40	80	2	74	53.2
			brial	50	80	2	51	62.9
			brial	40	90	2	88	53.4
			brial	50	90	2	70	62.6
			brial	40	80	3	71	57.3
			brial	50	80	3	90	67.9
			brial	40	90	3	66	59.8
			brial	50	90	3	97	67.8
			nter	45	85	2.5	81	59.2
			nter	45	85	2.5	75	60.4
			nter	45	85	2.5	76	59.1
			nter	45	85	2.5	83	60.6
13	Day 2	14	Axial	36.591	85	2.5	76	53.6
14	Day 2	13	Axial	53.409	85	2.5	79	65.9
15	Day 2	20	Axial	45	76.591	2.5	85	60
16	Day 2	18	Axial	45	93.409	2.5	97	60.7
17	Day 2	16	Axial	45	85	1.6591	55	57.4
18	Day 2	17	Axial	45	85	3.3409	81	63.2
19	Day 2	19	Center	45	85	2.5	80	60.8
20	Day 2	15	Center	45	85	2.5	91	58.9

Displaying the Point Type

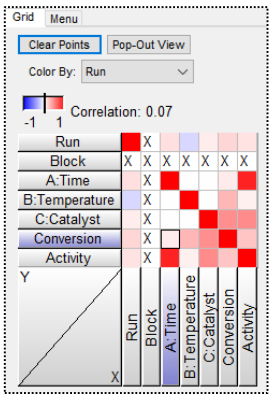
Notice the new column identifying points as "Factorial," "Center" (for center point), and so on. Notice how the factorial points align only to the Day 1 block. Then in Day 2 the axial points are run. Center points are divided between the two blocks.

Unless you change the default setting for the Select option, do not expect the Type column to appear the next time you run Design-Expert. It is only on temporarily at this stage for your information.

Before focusing on modeling the response as a function of the factors varied in this RSM experiment, it will be good to assess the impact of the blocking via a simple scatter plot. Click the **Graph Columns** node branching from the design 'root' at the upper left of your screen. You should see a scatter plot with factor A:Time on the X-axis and the Conversion response on the Y-axis.

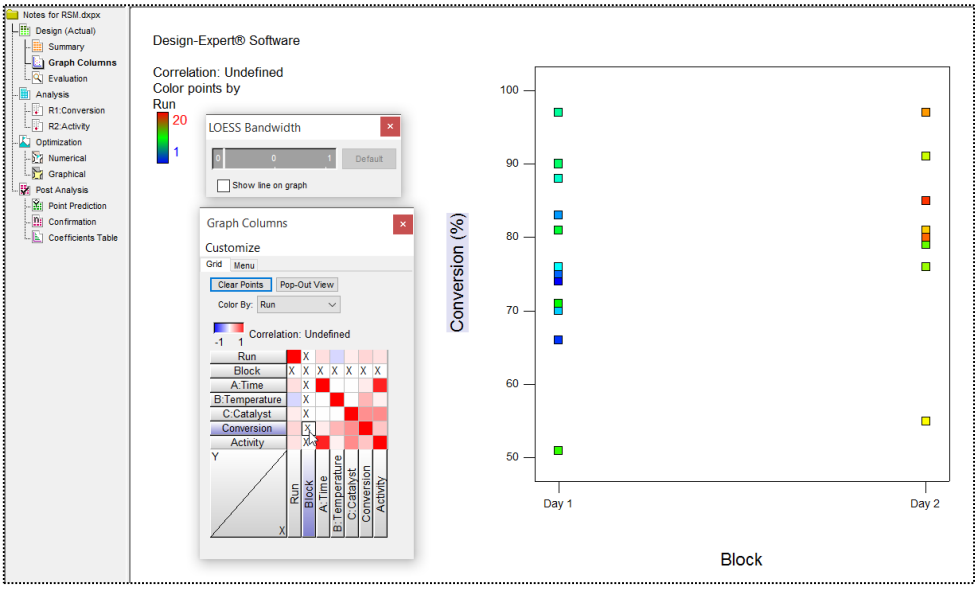
☒ ***Explore the color-coded correlation grid***: The correlation grid that pops up with the Graph Columns can be very interesting. First off, observe that it exhibits red along the diagonal—indicating the complete (r=1) correlation of any variable with itself (Run vs Run, etc). Block versus run (or, conversely, run vs block) is also highly correlated due to this restriction in randomization (runs having to be done for day 1 before day 2). It is good to see so many white squares because these indicate little or no correlation between factors, thus they can be estimated independently.

For now, it is most useful to produce a plot showing the impact of blocks because this will be literally blocked out in the analysis. Therefore, on the floating **Graph Columns** tool click the button where **Conversion** intersects with **Block** as shown below.



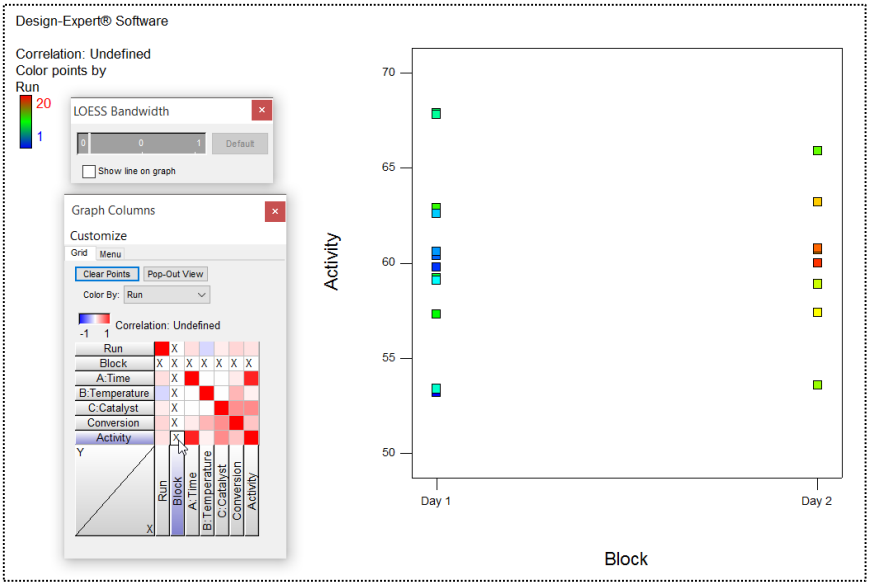
Plotting the effect of Block on Conversion

The graph visually shows there is not much of a difference between block 1 and 2. The points on Day 1 and Day 2 are both spread around about the same average value. Bear in mind that whatever the difference may be between blocks, it will be filtered out mathematically so as not to bias the estimation of factor effects.



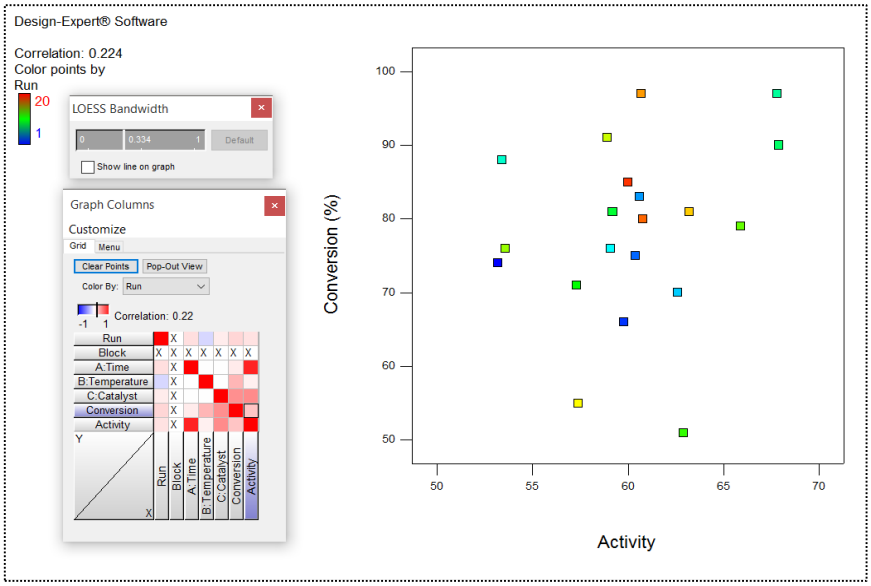
Graph Columns feature for design layout

Change the Y Axis to **Activity** (by clicking down the column one box) to see how it's affected by the day-to-day blocking (not much, either!).



Changing response (resulting graph not shown)

Finally, to see how the responses correlate, change the X Axis to **Conversion**. Now that we have 2 numeric factors along the axes, we can see the correlation between them. In the upper left of the legend you will see the correlation number is 0.224, showing slight correlation.

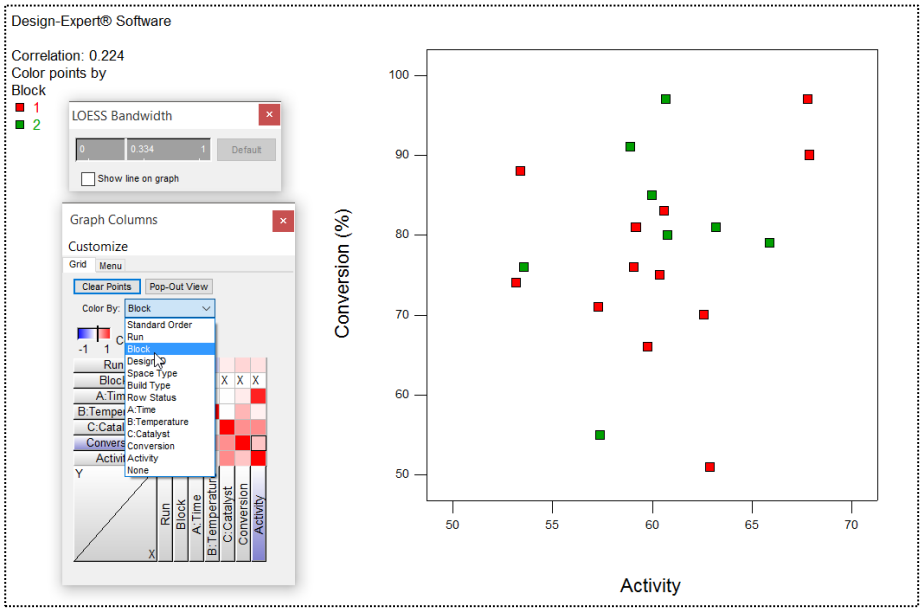


Plotting one response versus the other (resulting graph not shown)

You may also note there is a faded pink color in the box you clicked in the grid to get this graph, denoting a slight upward correlation as you go from left to right on the graph.

Feel free to make other scatter plots, but the ones done thus far will be most valuable so it will be best to move on from here.

☒ ***Explore the color-by tool***: Notice you can also color selected factors, including run (default). For example, choose **Color by Block** to see which points were run in block 1 (black) and block 2 (red).

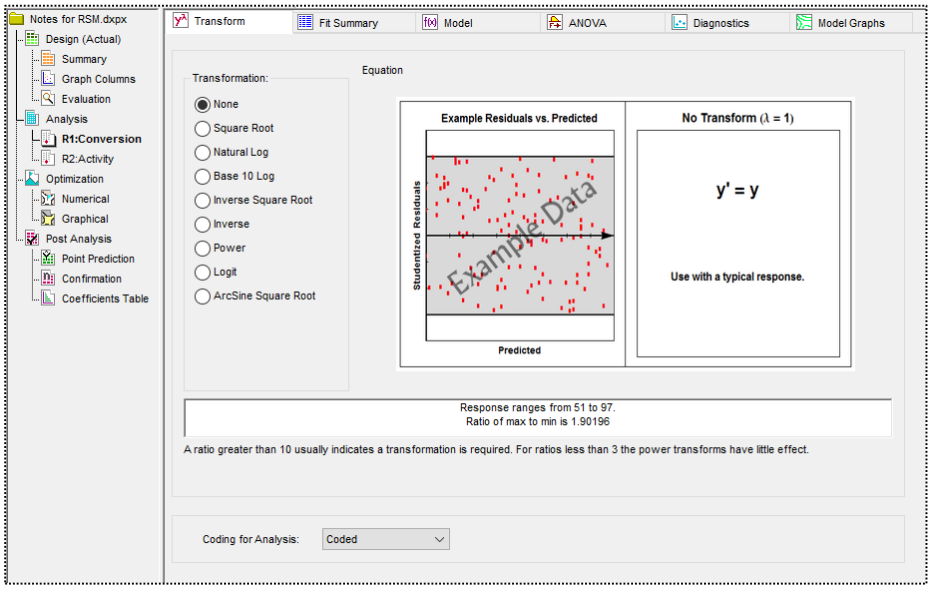


Graph columns with points colored by Block

However, do not get carried away with this, because it will be much more productive to do statistical analysis first – before drawing any conclusions.

Analyze the Results

Now let's start analyzing the responses numerically. Under the **Analysis** branch click the node labeled **Conversion**. A new set of tabs appears at the top of your screen. They are arranged from left to right in the order needed to complete the analysis. What could be simpler?



Begin analysis of Conversion

Design-Expert provides a full array of response transformations via the **Transform** option. Click Tips for details. For now, accept the default transformation selection of **None**.

Now click the ***Fit Summary*** tab. At this point Design-Expert fits linear, two-factor interaction (2FI), quadratic, and cubic polynomials to the response. At the top is the response identification, immediately followed below, in this case, by a warning: "The Cubic Model and higher are Aliased." Do not be alarmed. By design, the central composite matrix provides too few unique design points to determine all the terms in the cubic model. It's set up only for the quadratic model (or some subset).

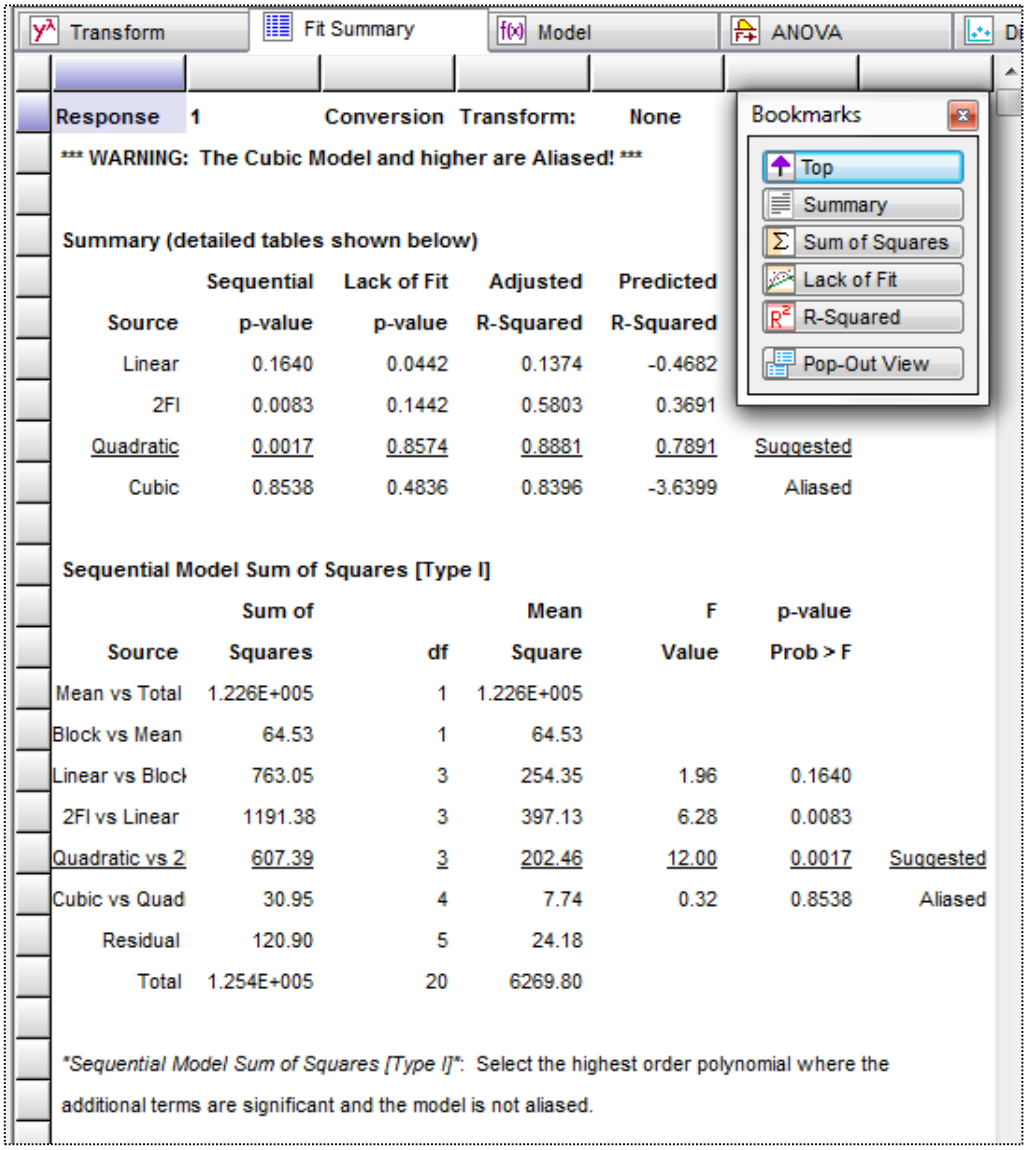
Next you will see several extremely useful tables for model selection. (To move through the display, use the floating Bookmarks palette or the side/bottom scroll bars). Each table is discussed briefly via sidebars in this tutorial on RSM.

The table of "Sequential Model Sum of Squares" (technically "Type I") shows how terms of increasing complexity contribute to the total model.

☒ ***Explore the Sequential Model Sum of Squares table***: The model hierarchy is described below:

- "Linear vs Block": the significance of adding the linear terms to the mean and blocks,
- "2FI vs Linear": the significance of adding the two factor interaction terms to the mean, block, and linear terms already in the model,
- "Quadratic vs 2FI": the significance of adding the quadratic (squared) terms to the mean, block, linear, and two-factor interaction terms already in the model,

- "Cubic vs Quadratic": the significance of the cubic terms beyond all other terms.



Transform | Fit Summary | Model | ANOVA | D

Response 1 Conversion Transform: None

*** WARNING: The Cubic Model and higher are Aliased! ***

Bookmarks: Top | Summary | Sum of Squares | Lack of Fit | R-Squared | Pop-Out View

Summary (detailed tables shown below)

Source	Sequential p-value	Lack of Fit p-value	Adjusted R-Squared	Predicted R-Squared	
Linear	0.1640	0.0442	0.1374	-0.4682	
2FI	0.0083	0.1442	0.5803	0.3691	
Quadratic	0.0017	0.8574	0.8881	0.7891	Suggested
Cubic	0.8538	0.4836	0.8396	-3.6399	Aliased

Sequential Model Sum of Squares [Type I]

Source	Sum of Squares	df	Mean Square	F Value	p-value Prob > F	
Mean vs Total	1.226E+005	1	1.226E+005			
Block vs Mean	64.53	1	64.53			
Linear vs Block	763.05	3	254.35	1.96	0.1640	
2FI vs Linear	1191.38	3	397.13	6.28	0.0083	
Quadratic vs 2	607.39	3	202.46	12.00	0.0017	Suggested
Cubic vs Quad	30.95	4	7.74	0.32	0.8538	Aliased
Residual	120.90	5	24.18			
Total	1.254E+005	20	6269.80			

*"Sequential Model Sum of Squares [Type I]": Select the highest order polynomial where the additional terms are significant and the model is not aliased.

Sequential Model Sum of Squares

For each source of terms (linear, etc.), examine the probability ("Prob > F") to see if it falls below 0.05 (or whatever statistical significance level you choose). So far, Design-Expert is indicating (via underline) the quadratic model looks best – these terms are significant, but adding the cubic order terms will not significantly improve the fit. (Even if they were significant, the cubic terms would be aliased, so they wouldn't be useful for modeling purposes.) Use the handy **Bookmarks** tool to advance to the next table for **Lack of Fit** tests on the various model orders.

Lack of Fit Tests

Source	Sum of Squares	df	Mean Square	F Value	p-value Prob > F	
Linear	1845.37	11	167.76	6.38	0.0442	
2FI	653.99	8	81.75	3.11	0.1442	
Quadratic	46.60	5	9.32	0.35	0.8574	Suggested
Cubic	15.65	1	15.65	0.59	0.4836	Aliased
Pure Error	105.25	4	26.31			

*"Lack of Fit Tests": Want the selected model to have insignificant lack-of-fit.

Summary Table: Lack of Fit Tests

The "Lack of Fit Tests" table compares residual error with "Pure Error" from replicated design points. If there is significant lack of fit, as shown by a low probability value ("Prob>F"), then be careful about using the model as a response predictor. In this case, the linear model definitely can be ruled out, because its Prob > F falls below 0.05. The quadratic model, identified earlier as the likely model, does not show significant lack of fit. Remember that the cubic model is aliased, so it should not be chosen.

Look over the last table in the Fit Summary report, which provides "Model Summary Statistics" for the 'bottom line' on comparing the options.

Model Summary Statistics

Source	Std. Dev.	R-Squared	Adjusted R-Squared	Predicted R-Squared	PRESS	
Linear	11.40	0.2812	0.1374	-0.4682	3984.14	
2FI	7.95	0.7202	0.5803	0.3691	1711.98	
Quadratic	4.11	0.9440	0.8881	0.7891	572.20	Suggested
Cubic	4.92	0.9554	0.8396	-3.6399	12591.11	Aliased

*"Model Summary Statistics": Focus on the model maximizing the "Adjusted R-Squared" and the "Predicted R-Squared".

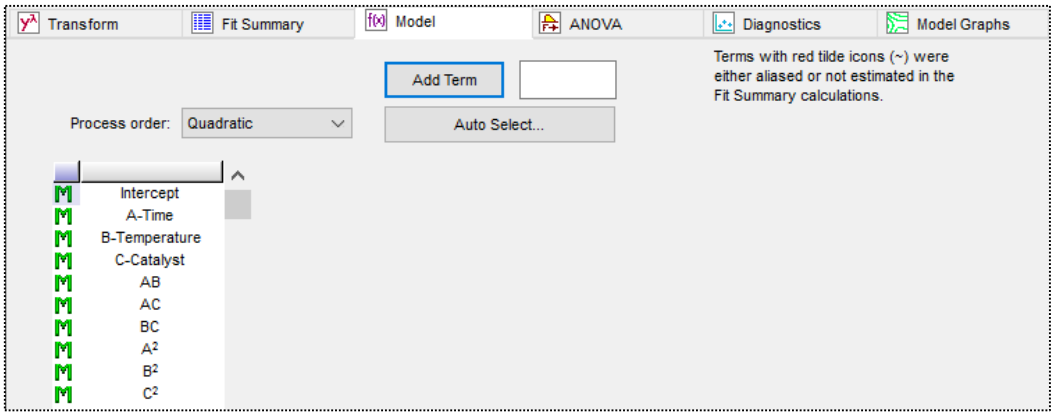
Summary Table: Model Summary Statistics

The quadratic model comes out best: It exhibits low standard deviation ("Std. Dev."), high "R-Squared" values, and a low "PRESS."

The program automatically underlines at least one "Suggested" model. Always confirm this suggestion by viewing these tables.

☒ ***Explore more details on model selection***: From the main menu select **Tips**, **Screen Tips** or simply press the light-bulb icon (💡) for more information about the procedure for choosing model(s).

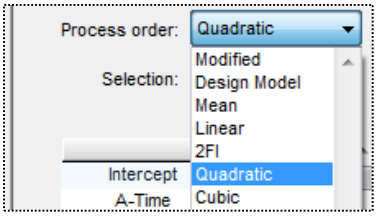
Design-Expert allows you to select a model for in-depth statistical study. Click the **Model** tab at the top of the screen to see the terms in the model.



Model results

The program defaults to the "Suggested" model shown in the earlier Fit Summary table.

☒ ***Explore more details on model selection***: If you want, you can choose an alternative model from the Process Order pull-down list. (Be sure to try this in the rare cases when Design-Expert suggests more than one model.)

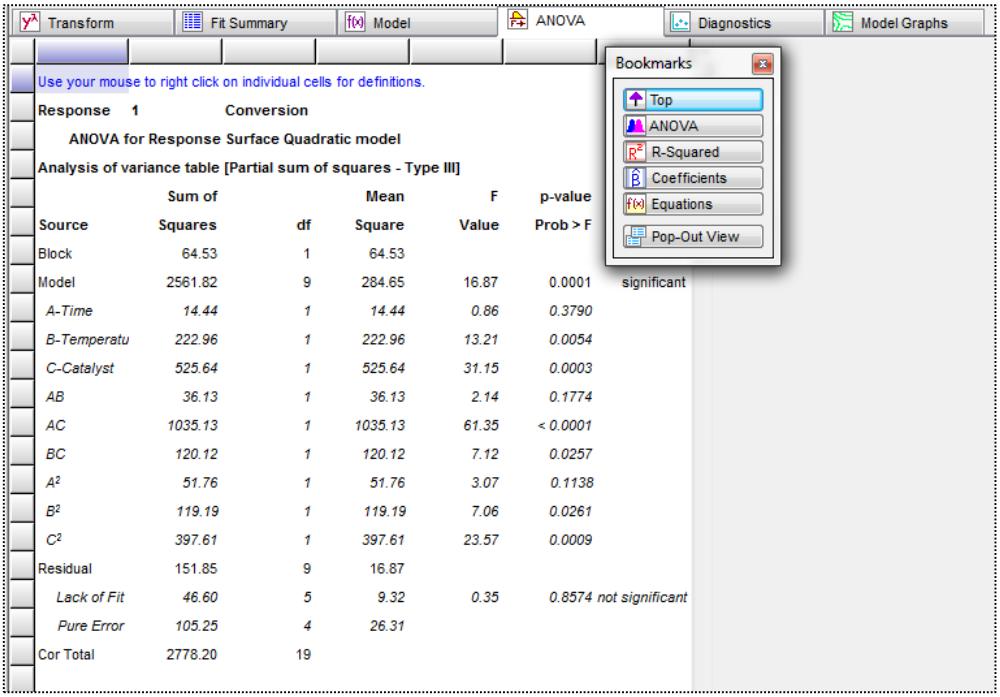


The options for process order

At this stage you could make use of the Add Term feature. This is subject to limitations that you'd best ask about via statehelp@statease.com.

Also, you could now manually reduce the model by clicking off insignificant effects. For example, you will see in a moment that several terms in this case are marginally significant at best. Design-Expert provides several automatic reduction algorithms as alternatives to the "Manual" method: "Backward," "Forward," and "Stepwise." Click the "Auto Select…" button to see these. From more details, try Screen Tips and/or search Help.

Click the **ANOVA** tab to produce the analysis of variance for the selected model.



Statistics for selected model: ANOVA table

The ANOVA in this case confirms the adequacy of the quadratic model (the Model Prob>F is less than 0.05.) You can also see probability values for each individual term in the model. You may want to consider removing terms with probability values greater than 0.10. Use process knowledge to guide your decisions.

Next, press the **Bookmarks** button for **R-Squared** to see that Design-Expert presents various statistics to augment the ANOVA. The R-Squared statistics are very good — near to 1.

Std. Dev.	4.11	R-Squared	0.9440
Mean	78.30	Adj R-Squared	0.8881
C.V. %	5.25	Pred R-Squared	0.7891
PRESS	572.20	Adeq Precision	16.294

Post-ANOVA statistics

Press forward to **Coefficients** to bring the following details to your screen, including the mean effect-shift for each block, that is, the difference from Day 1 to Day 2 in the response.

Factor	Coefficient Estimate	df	Standard Error	95% CI Low	95% CI High	VIF
Intercept	81.60	1	1.69	77.77	85.43	
Day 1	-1.92	1				
Day 2	1.92					
A-Time	1.03	1	1.11	-1.49	3.54	1.00
B-Temperature	4.04	1	1.11	1.53	6.55	1.00
C-Catalyst	6.20	1	1.11	3.69	8.72	1.00
AB	2.13	1	1.45	-1.16	5.41	1.00
AC	11.38	1	1.45	8.09	14.66	1.00
BC	-3.87	1	1.45	-7.16	-0.59	1.00
A^2	-1.90	1	1.08	-4.34	0.55	1.02
B^2	2.88	1	1.08	0.43	5.33	1.02
C^2	-5.25	1	1.08	-7.70	-2.81	1.02

Coefficients for the quadratic model

Press **Equations** to bring the next section to your screen — the predictive models in terms of coded versus actual factors (shown side-by-side below). Block terms are left out. These terms can be used to re-create the results of this experiment, but they cannot be used for modeling future responses.

Final Equation in Terms of Coded Factors:

Conversion =
+81.60
+1.03 * A
+4.04 * B
+6.20 * C
+2.13 * A * B
+11.38 * A * C
-3.87 * B * C
-1.90 * A^2
+2.88 * B^2
-5.25 * C^2

Final Equation in Terms of Actual Factors:

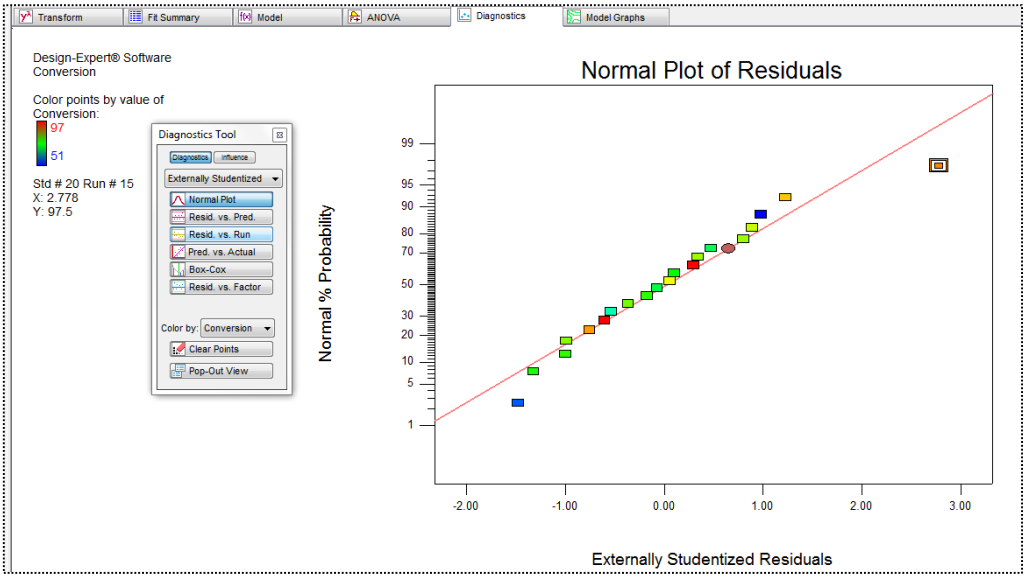
Conversion =
+1026.77403
-11.56883 * Time
-18.70551 * Temperature
+44.50242 * Catalyst
+0.085000 * Time * Temperature
+4.55000 * Time * Catalyst
-1.55000 * Temperature * Catalyst
-0.075839 * $Time^2$
+0.11508 * $Temperature^2$
-21.01890 * $Catalyst^2$

Final equation: coded versus actual

You cannot edit any ANOVA outputs. However, you can copy and paste the data to your favorite word processor or spreadsheet. Also, as detailed in the One-Factor RSM tutorial, Design-Expert provides a tool to export equations directly to Excel in a handy format that allows you to 'plug and chug', that is, enter whatever inputs you like to generate predicted response. This might be handy for clients who are phobic about statistics. ;)

Diagnose the Statistical Properties of the Model

The diagnostic details provided by Design-Expert can best be grasped by viewing plots available via the **Diagnostics** tab. The most important diagnostic — normal probability plot of the residuals — appears by default.



Normal probability plot of the residuals

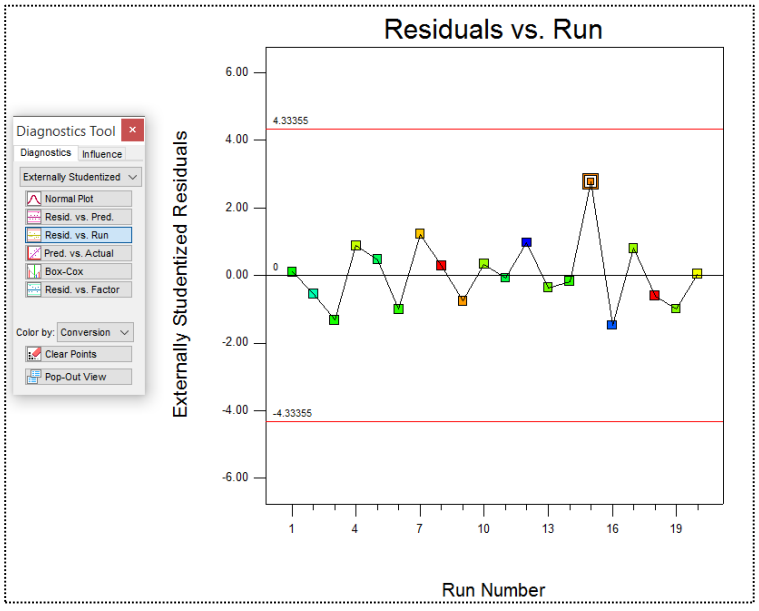
Data points should be approximately linear. A non-linear pattern (such as an S-shaped curve) indicates non-normality in the error term, which may be corrected by a transformation. The only sign of any problems in this data may be the point at the far right. Click this on your screen to highlight it as shown above.

Find the floating **Diagnostics Tool** palette on your screen.

☒ ***Explore details on how Design-Expert displays residuals***: Notice that residuals are "externally studentized" unless you change their form on the floating tool palette (not advised). This has been discussed in prior tutorials. To recap:

- Externally calculating residuals increases the sensitivity for detecting outliers.
- Studentized residuals counteract varying leverages due to design point locations. For example, center points carry little weight in the fit and thus exhibit low leverage.

Now go to the Diagnostics Tool and click **Resid. vs Run**.

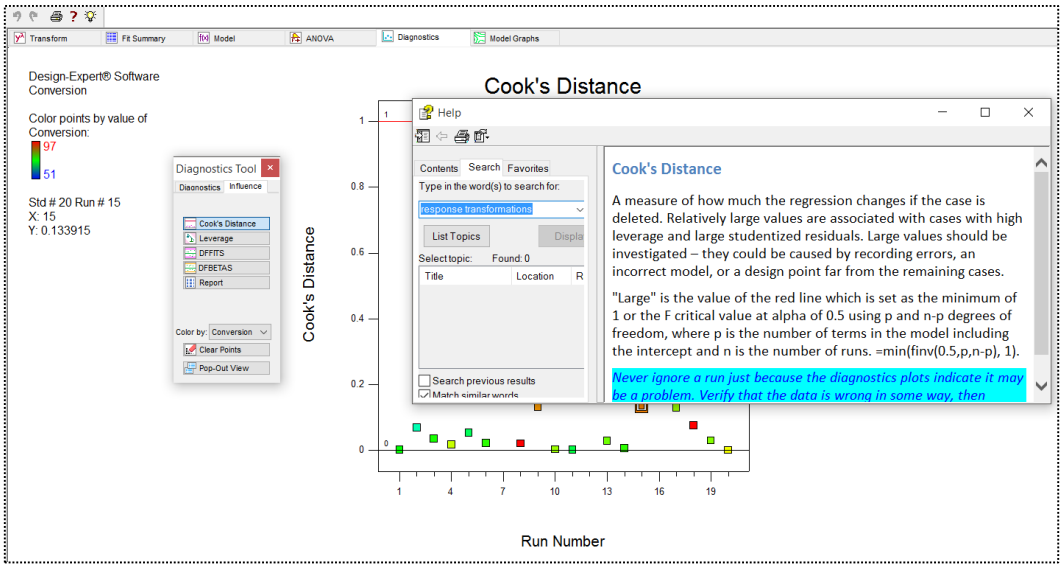


Residuals versus run

Now you can see that, although the highlighted run does differ more from its predicted value than any other, there is really no cause for alarm.

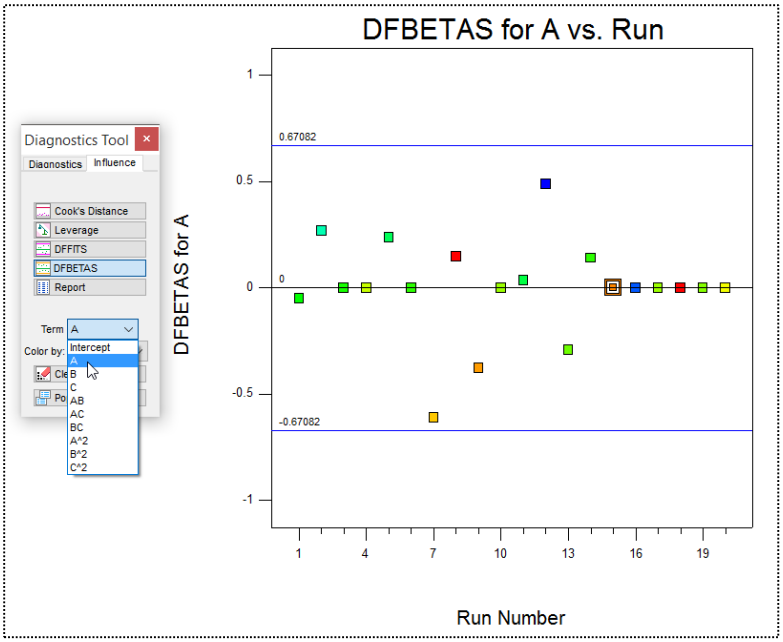
☒ ***Explore details on how Design-Expert displays residuals***: Each button on the palette represents a different diagnostics graph. Check out the other graphs if you like. Press Screen Tips along the way to get helpful details and suggestions on interpretation. In this case, none of the graphs really indicates anything that invalidates the model, so press ahead.

Next press the **Influence** side for another set of diagnostics, including a report detailed case-by-case residual statistics. Press the Screen Tips light-bulb icon for details on the Cook's Distance that now displays.



Cook's Distance — the first of the Influence diagnostics

Exit (X) out of the Screen Tips and move on to **Leverage**. This is best explained by the previous tutorial on One-Factor RSM so go back to that if you did not already go through it. Then skip ahead to **DFBETAS**, which breaks down the changes in the model to each coefficient, which statisticians symbolize with the Greek letter β, hence the acronym DFBETAS — the difference in betas. For the **Term** click the down-list arrow (▼) and select **A** as shown in the following screen shot.



DFBETAS for term A

You can evaluate ten model terms (including the intercept) for this quadratic predictive model (see sidebar below for help).

☒ ***Explore DFBETAS***: Click outside the Term field, reposition your mouse over the **Term** field and simply scroll your mouse wheel to quickly move up and down the list. In a similar experiment to this one, where the chemist changed catalyst, the DFBETAS plot for that factor exhibited an outlier for the one run where its level went below a minimal level needed to initiate the reaction. Thus, this diagnostic proved to be very helpful in seeing where things went wrong in the experiment.

Now move on to the **Report** to bring up detailed case-by-case diagnostic statistics, many which have already been shown graphically.

Diagnostics Case Statistics

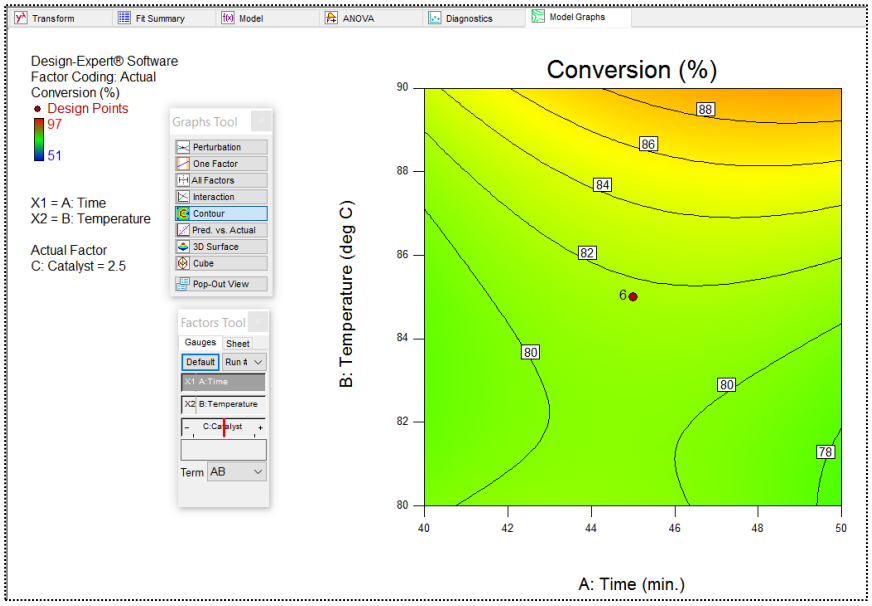
Run Order	Actual Value	Predicted Value[1]	Residual	Leverage	Internally Studentized Residual	Externally Studentized Residual	Cook's Distance	Influence on Fitted Value DFFITS	Standard Order
1	74.00	73.76	0.24	0.706	0.107	0.101	0.003	0.157	1
2	66.00	67.25	-1.25	0.706	-0.561	-0.538	0.069	-0.834	7
3	75.00	79.68	-4.68	0.194	-1.270	-1.322	0.035	-0.649	10
4	83.00	79.68	3.32	0.194	0.900	0.889	0.018	0.437	12
5	70.00	68.90	1.10	0.706	0.494	0.472	0.053	0.732	4
6	76.00	79.68	-3.68	0.194	-0.999	-0.999	0.022	-0.491	11
7	88.00	85.34	2.66	0.706	1.193	1.226	0.310	1.899	3
8	97.00	96.31	0.69	0.706	0.311	0.295	0.021	0.457	8
9	90.00	91.73	-1.73	0.706	-0.774	-0.756	0.131	-1.171	6
10	81.00	79.68	1.32	0.194	0.357	0.339	0.003	0.167	9
11	71.00	71.17	-0.17	0.706	-0.076	-0.071	0.001	-0.111	5
12	51.00	48.82	2.18	0.706	0.979	0.977	0.209	1.513	2
13	79.00	79.89	-0.89	0.679	-0.382	-0.363	0.028	-0.529	14
14	76.00	76.43	-0.43	0.679	-0.185	-0.175	0.007	-0.254	13
15	91.00	83.52	7.48	0.250	2.102	2.778	0.134	1.604	20
16	55.00	58.23	-3.23	0.679	-1.387	-1.474	0.370	-2.146	17
17	81.00	79.09	1.91	0.679	0.820	0.803	0.129	1.169	18
18	97.00	98.45	-1.45	0.679	-0.625	-0.603	0.075	-0.878	16
19	80.00	83.52	-3.52	0.250	-0.990	-0.989	0.030	-0.571	19
20	85.00	84.86	0.14	0.679	0.058	0.055	0.001	0.080	15

Diagnostics report

☒ ***Explore a footnote on the diagnostics report***: The note below the table ("Predicted values include block corrections.") alerts you that any shift from block 1 to block 2 will be included for purposes of residual diagnostics. (Recall that block corrections did not appear in the predictive equations shown in the ANOVA report.)

Examine Model Graphs

The residuals diagnosis reveals no statistical problems, so now let's generate response surface plots. Click the **Model Graphs** tab. The 2D contour plot of factors A versus B comes up by default in graduated color shading.



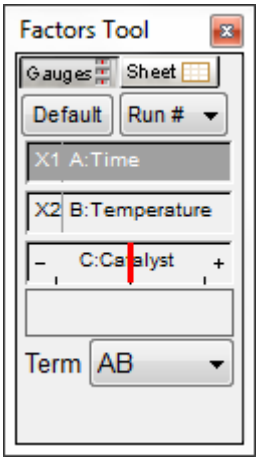
Response surface contour plot

☒ ***Explore how to visualize design point in multifactor space***: Note that Design-Expert displays any actual point included in the design space shown. In this case you see a plot of conversion as a function of time and temperature at a mid-level slice of catalyst. This slice includes six center points as indicated by the dot at the middle of the contour plot. By replicating center points, you get a very good power of prediction at the middle of your experimental region.

The floating **Factors Tool** palette appears with the default plot. Move this floating tool as needed by clicking and dragging the top blue border. The tool controls which factor(s) are plotted on the graph.

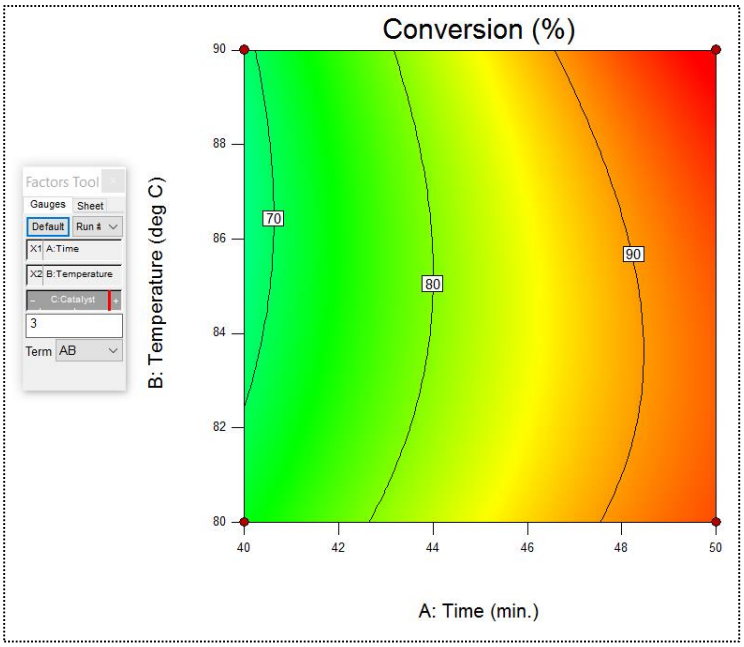
☒ ***Explore the Factors Tool features***: The Gauges option near the top of the tool is the default. Each factor listed has either an axis label, indicating that it is currently shown on the graph, or a red slider bar, which allows you to choose specific settings for the factors that are not currently plotted. All red slider bars default to midpoint levels of those factors not currently assigned to axes. You can change factor levels by dragging their red slider bars or by right-clicking factor names to make them active (they become highlighted) and then typing desired levels into the numeric space near the bottom of the tool palette. Give this a try.

Click the **C:Catalyst** toolbar to see its value. Don't worry if the red slider bar shifts a bit — we will instruct you how to re-set it in a moment.



Factors tool showing factor C highlighted and value displayed

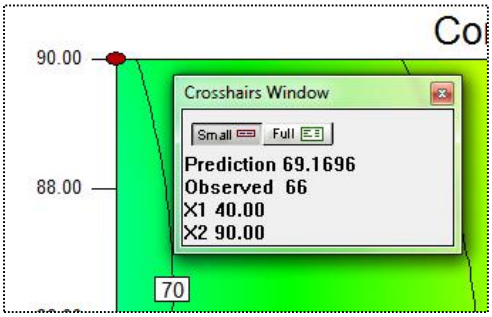
Left-Click the red bar with your mouse and drag it to the right.



Slide bar for C pushed right to higher value

As indicated by the color key on the left, the surface becomes 'hot' at higher response levels, yellow in the '80's, and red above 90 for conversion.

☒ ***Explore coordinates on the graph using a crosshairs tool***: To enable a handy tool for reading coordinates off contour plots, go to **View**, **Show Crosshairs Window**. Now move your mouse over the contour plot and notice that Design-Expert generates the predicted response for specific factor values corresponding to that point. If you place the crosshair over an actual point, for example – the one at the far upper left corner of the graph now on screen, you also see that observed value (in this case: 66).

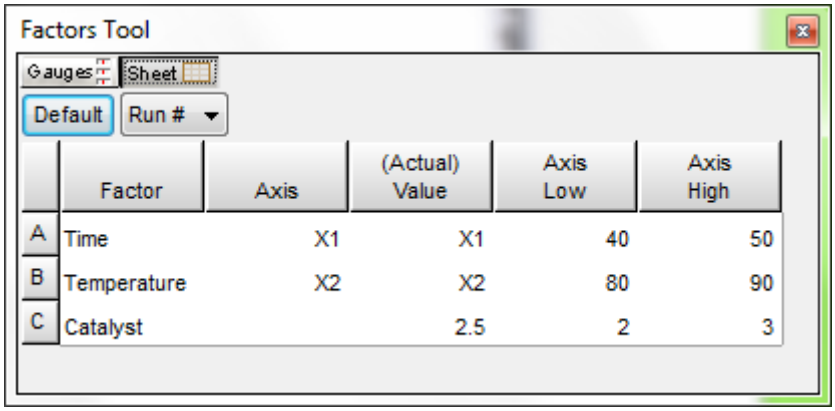


Prediction at coordinates of 40 and 90 where an actual run was performed

P.S. See what happens when you press the Full option for crosshairs.

Now press the **Default** button on the floating Factors Tool to place factor C back at its midpoint.

☒ ***Explore Sheet View on Factors Tool***: Switch to Sheet View on the **Factors Tool** by clicking the **Sheet** button.



	Factor	Axis	(Actual) Value	Axis Low	Axis High
A	Time	X1	X1	40	50
B	Temperature	X2	X2	80	90
C	Catalyst		2.5	2	3

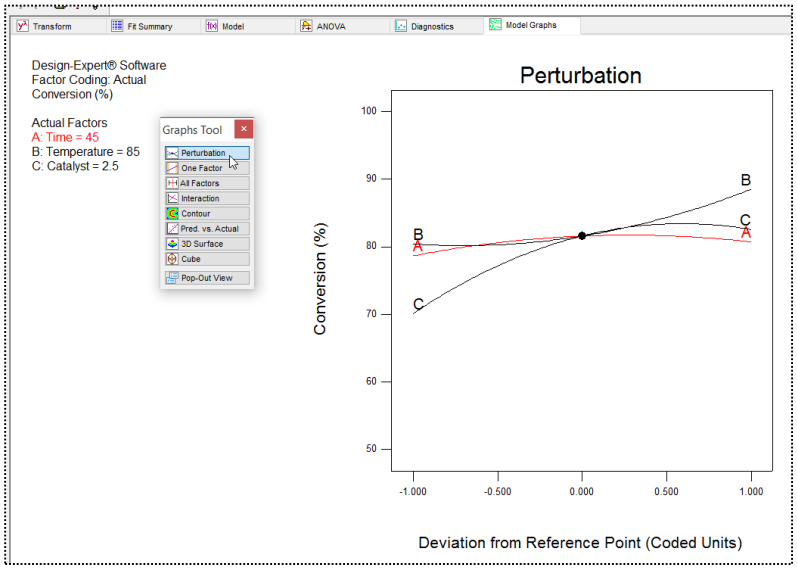
Factors tool – Sheet view

In the columns labeled Axis and Value you can change the axes settings or type in specific values for factors. Give this a try. Then return to the **Gauges** view and press the **Default** button.

P.S. At the bottom of the Factors Tool is a pull-down list from which you can also select the factors to plot. Only the terms that are in the model are included in this list. At this point in the tutorial this should be set at AB. If you select a single factor (such as A) the graph changes to a One-Factor Plot. Try this if you like, but notice how Design-Expert warns if you plot a main effect that's involved in an interaction.

Perturbation Plot

Wouldn't it be handy to see all your factors on one response plot? You can do this with the perturbation plot, which provides silhouette views of the response surface. The real benefit of this plot is when selecting axes and constants in contour and 3D plots. See it by mousing to the **Graphs Tool** and pressing **Perturbation** or pull it up via View from the main menu.



The Perturbation plot with factor A clicked to highlight it

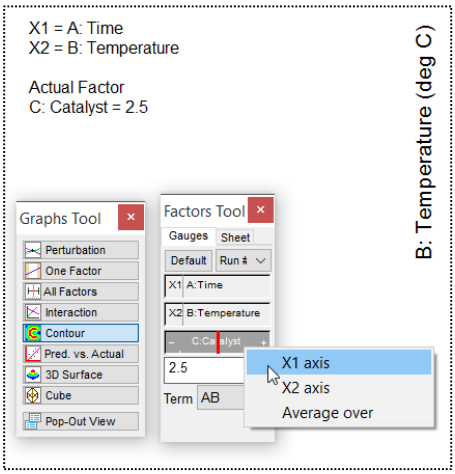
For response surface designs, the perturbation plot shows how the response changes as each factor moves from the chosen reference point, with all other

factors held constant at the reference value. Design-Expert sets the reference point default at the middle of the design space (the coded zero level of each factor).

Click the curve for factor A to see it better. The software highlights it in a different color as shown above. It also highlights the legend. (You can click it also – it is interactive!) In this case, at the center point, you see that factor A (time) produces a relatively small effect as it changes from the reference point. Therefore, because you can only plot contours for two factors at a time, it makes sense to choose B and C – and slice on A.

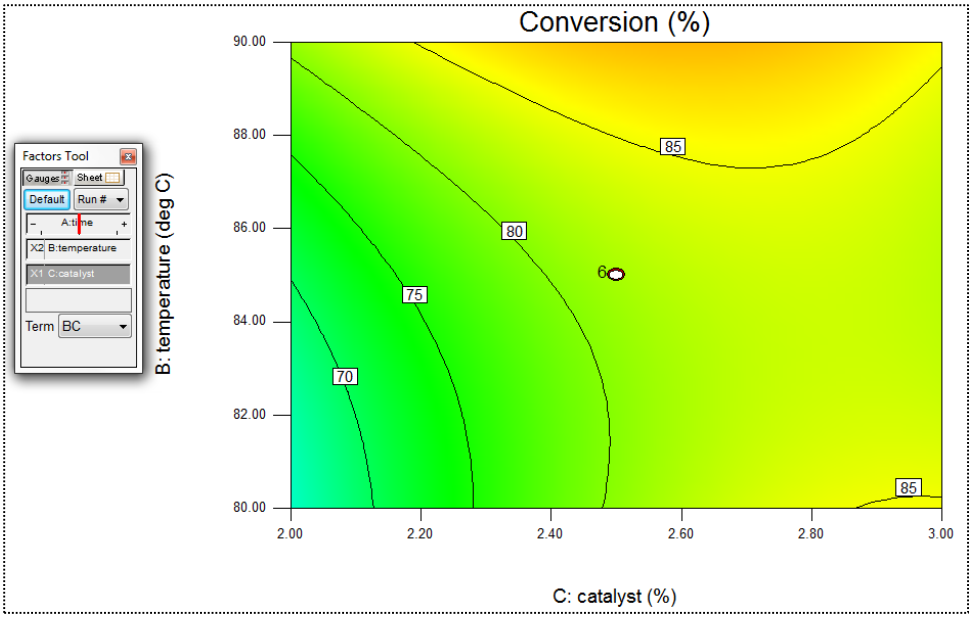
Contour Plot: Revisited

Let's look at the plot of factors B and C. Start by clicking **Contour** on the floating Graphs tool. Then in the **Factors Tool** right-click the **Catalyst** bar and select **X1 axis** by left clicking it.



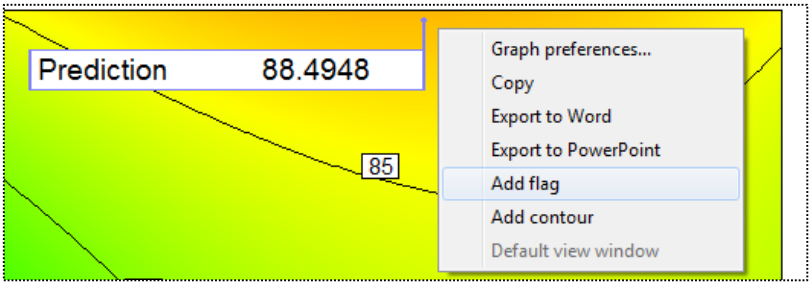
Making factor C the x1-axis

You now see a catalyst versus temperature plot of conversion, with time held as a constant at its midpoint.



Contour plot of B:temperature versus C:catalyst

Design-Expert contour plots are highly interactive. For example, right-click up in the hot spot at the upper middle and select **Add Flag.**

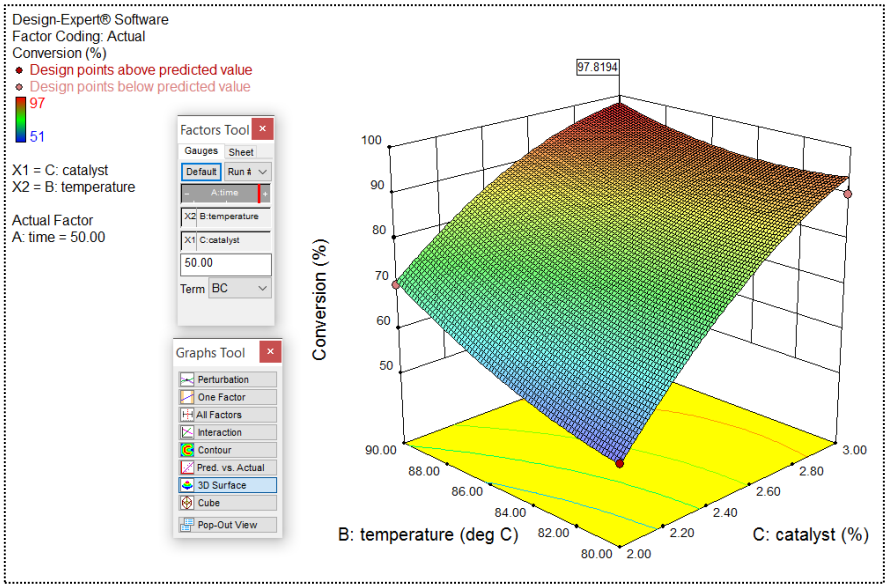


Adding a flag

That's enough on the contour plot for now — hold off until Part 3 of this tutorial to learn other tips and tricks on making this graph and others more presentable. Right-click and **Delete flag** to clean the slate.

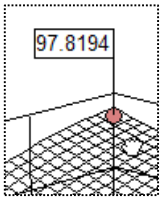
3D surface plot

Now to really get a feel for how the response varies as a function of the two factors chosen for display, select from the floating **Graphs Tool** the **3D Surface**. You then will see three-dimensional display of the response surface. If the coordinates encompass actual design points, these will be displayed. On the **Factors Tool** move the slide bar for **A:time** to the right. This presents a very compelling picture of how the response can be maximized. Right-click at the peak to set a flag.



3D response surface plot with A:time at high level

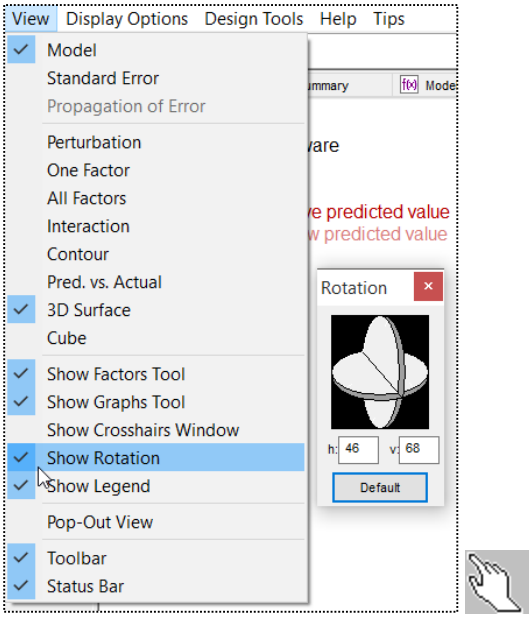
You can see points below the surface by rotating the plot. Move your mouse over the graph. When the cursor turns into a hand click and hold the left mouse-button and then drag.



Seeing a point beneath the surface

Seeing an actual result predicted so closely lends credence to the model. Things are really looking up at this point!

☒ ***Explore another way to rotate the 3D graph***: Another way to do this is to select **View**, **Show Rotation** to bring up a handy tool for this.



Rotation tool

Move your cursor over the tool. The pointer changes to a hand. Now use the hand to rotate the vertical or horizontal wheel. Whether you use the rotation tool or simply grab the plot with your mouse, watch the 3D surface change. It's fun! What's really neat is how it becomes transparent so you can see hidden points falling below the surface. Notice how the points below the surface are shown with a lighter shade. The Stat-Ease program developers thought of everything! Before moving on from here, go back to the **Rotation** tool and press **Default** to put the graph back in its original angle. Notice that you can also specify the horizontal ("h") and vertical ("v") coordinates.

Remember that you're only looking at a 'slice' of factor A (time). Normally, you'd want to make additional plots with slices of A at the minus and plus one levels, but let's keep moving — still lots to be done for making the most of this RSM experiment.

Analyze the Data for the Second Response

This step is a BIG one. Analyze the data for the second response, activity. Be sure you find the appropriate polynomial to fit the data, examine the residuals and plot the response surface. *Hint: The correct model is linear.*

Before you quit, do a **File**, **Save** to preserve your analysis. Design-Expert will save your models. To leave Design-Expert, use the File, Exit menu selection. The program will warn you to save again if you've modified any files.

Multifactor RSM Tutorial
(Part 2/3 – Optimization)

Introduction

This tutorial shows how to use Design-Expert software for optimization experiments. It's based on the data from Multifactor RSM Tutorial Part 1. You should go back to that tutorial if you've not completed it.

For details on optimization, see our on-line program help. Also, Stat-Ease provides in-depth training in our Response Surface Methods for Process Optimization workshop. Call or visit our web site for information on content and schedules.

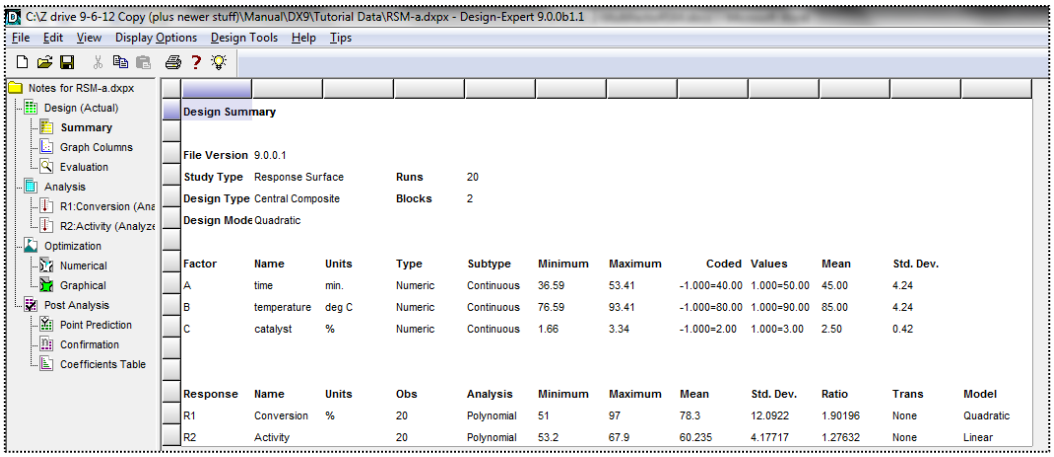
In this section, you will work with predictive models for two responses, yield and activity, as a function of three factors: time, temperature, and catalyst. These models are based on results from a central composite design (CCD) on a chemical reaction.

Click the open design icon (see below) and load the case study data modeled by Stat-Ease and saved to a file named **RSM-a.dxpx**.



Open design icon

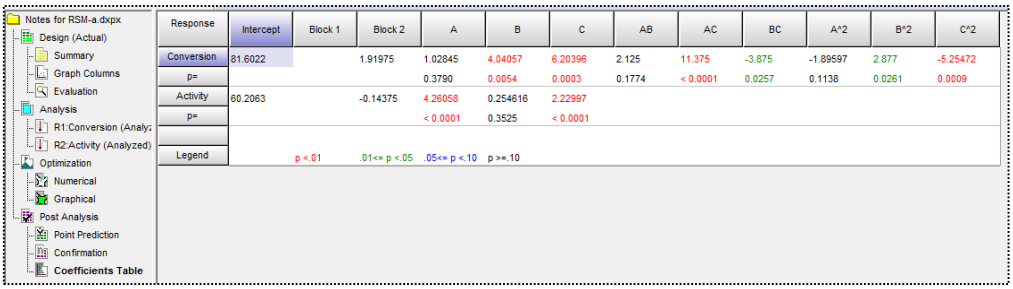
To see a description of the file contents, click the **Summary** node under the Design branch at the left of your screen. Within the design status screen you can see we modeled conversion with a quadratic model and activity with a linear model, as shown below.



Design summary

☒ ***Explore making tables easier to read on screen***: Drag the left border and open the window to better see the branch/node menu. You can also re-size columns with your mouse.

Click on the **Coefficients Table** node at the bottom branch.



Coefficients Table

This table provides a convenient comparison of the coefficients for all of the responses.

☒ ***Explore how to compare models***: Because the Coefficients Table is laid in terms of coded factors you can make inferences about the relative effects. For instance, notice that the coefficient for AC (11.375) in the conversion equation is much higher than the coefficients for Factor B (4.04057). This shows, for the region studied, that the AC interaction influences conversion more than Factor B. The coefficients in the table are color-coded by p-value, making it easy to see each term's significance at a glance. In our example, we chose to use the full quadratic model. Therefore, some less significant terms (shown in black) are retained, even though they are not significant at the 0.10 level.

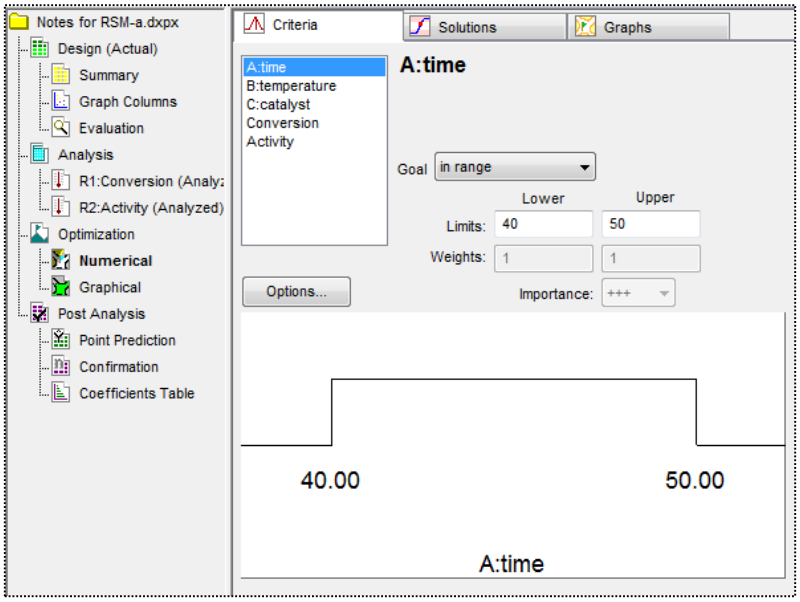
P.S. Right-click any cell to export this report to PowerPoint or Word for your presentation or report. Check it out: This is very handy!

Numerical Optimization

Design-Expert software's numerical optimization will maximize, minimize, or target:

- A single response
- A single response, subject to upper and/or lower boundaries on other responses
- Combinations of two or more responses.

Under the Optimization branch to the left of the screen, click the **Numerical** node to start.



Setting numerical optimization criteria

Setting the Optimization Criteria

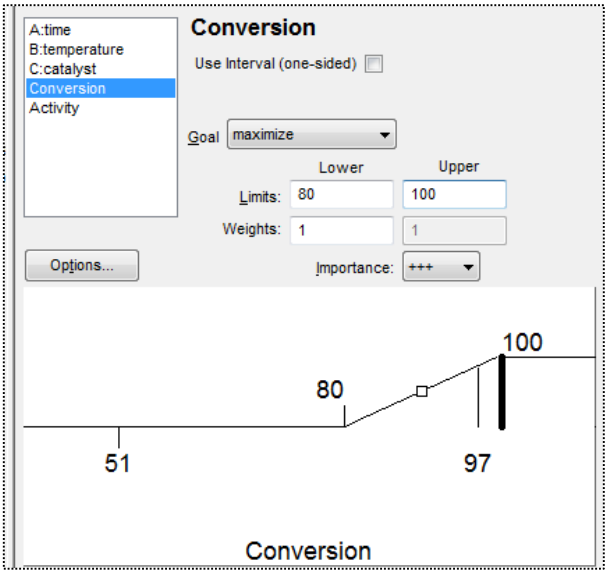
Design-Expert allows you to set criteria for all variables, including factors and propagation of error (POE). (We will detail POE later.) The program restricts factor ranges to factorial levels (plus one to minus one in coded values) — the region for which this experimental design provides the most precise predictions. Response limits default to observed extremes. In this case, you should leave the settings for time, temperature, and catalyst factors alone, but you will need to make some changes to the response criteria.

Now you get to the crucial phase of numerical optimization: assigning "Optimization Parameters." The program uses five possibilities as a "Goal" to construct desirability indices (d_i):

- Maximize,
- Minimize,
- Target->,
- In range,
- Equal to -> *(factors only)*.

Desirabilities range from zero to one for any given response. The program combines individual desirabilities into a single number and then searches for the greatest overall desirability. A value of one represents the ideal case. A zero indicates that one or more responses fall outside desirable limits. Design-Expert uses an optimization method developed by Derringer and Suich, described by Myers, Montgomery and Anderson-Cook in *Response Surface Methodology*, 3rd edition, John Wiley and Sons, New York, 2009.

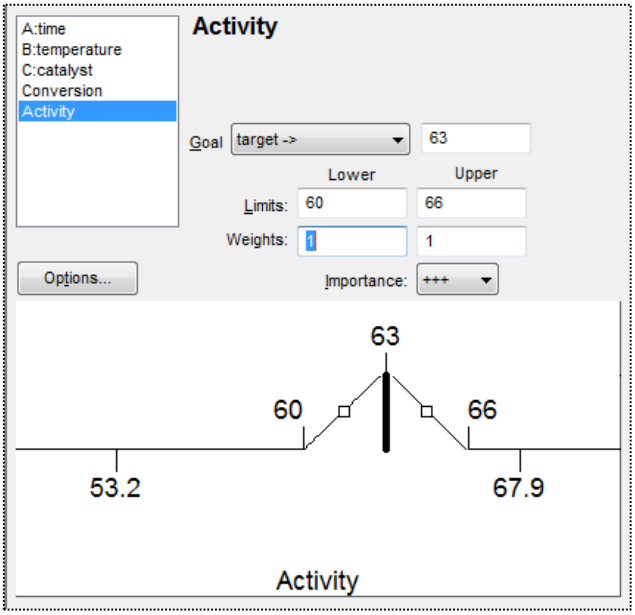
For this tutorial case study, assume you need to increase conversion. Click **Conversion** and set its **Goal** to **maximize**. As shown below, set **Lower Limit** to **80** (the lowest acceptable value, and **Upper Limit** to **100**, the theoretical high.



Conversion criteria settings

You must provide both these thresholds so the desirability equation works properly. By default, thresholds will be set at the observed response range, in this case 51 to 97. By increasing the upper end for desirability to 100, we put in a 'stretch' for the maximization goal. Otherwise we may come up short of the potential optimum.

Now click the second response, **Activity**. Set its **Goal** to **target->** of **63**. Enter **Lower Limits** and **Upper Limits** of **60** and **66**, respectively. These limits indicate that it is most desirable to achieve the targeted value of 63, but values in the range of 60-66 are acceptable. Values outside that range are not acceptable.



Activity criteria settings

The above settings create the following desirability functions:

1. Conversion:

- if less than 80%, desirability (d_i) equals zero
- from 80 to 100%, d_i ramps up from zero to one
- if over 100%, d_i equals one

2. Activity:

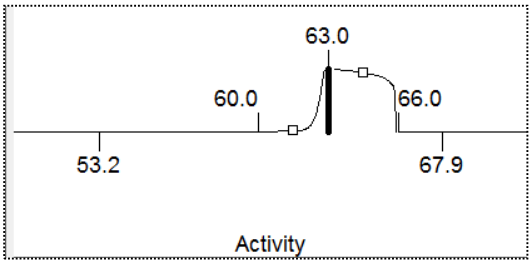
- if less than 60, d_i equals zero
- from 60 to 63, d_i ramps up from zero to one
- from 63 to 66, d_i ramps back down to zero
- if greater than 66, d_i equals zero

☒ ***Explore details on features available for numerical optimization***: Recall that at your fingertips you'll find advice for using sophisticated Design-Expert software features by pressing the 💡 button to see Screen Tips on Numerical Optimization. Close out Screen Tips by pressing **X** at the upper-right corner of its screen.

Changing Desirability Weights and the (Relative) Importance of Variables

You can select additional parameters called "weights" for each response. Weights give added emphasis to upper or lower bounds or emphasize target values. With a weight of 1, d_i varies from 0 to 1 in linear fashion. Weights greater than 1 (maximum weight is 10) give more emphasis to goals. Weights less than 1 (minimum weight is 0.1) give less emphasis to goals.

☒ ***Explore changing weights***: Weights can be quickly changed by 'grabbing' (clicking and dragging) the handles (squares ▫) on desirability ramps. Try pulling the square on the left down and the square on the right up as shown below.



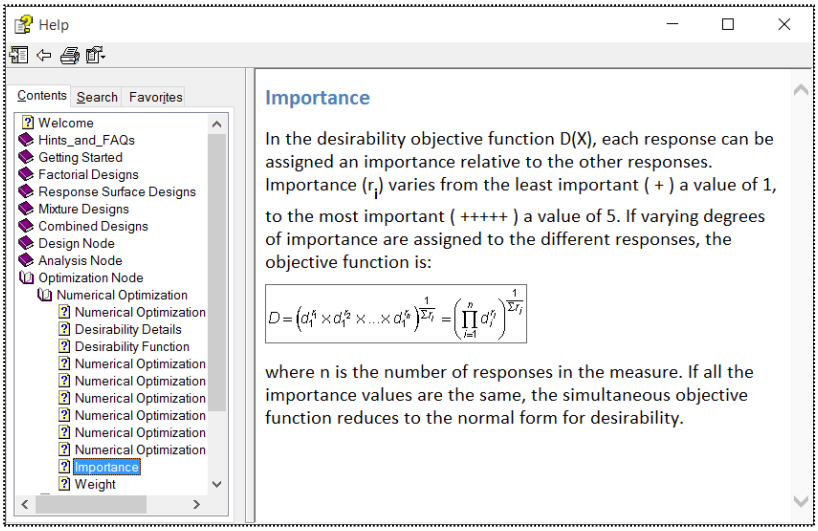
Weights change by grabbing handles with mouse

This might reflect a situation where your customer says they want the targeted value (63), but if it must be missed due to a trade-off necessary for other specifications, it would be better to err to the high side. Before moving on from here, re-enter the **Lower** and **Upper Weights** at their default values of **1** and **1**; respectively. This straightens them to their original 'tent' shape (🗠).

"Importance" is a tool for changing relative priorities to achieve goals you establish for some or all variables. If you want to emphasize one over the rest, set its importance higher. Design-Expert offers five levels of importance ranging from 1 plus (+) to 5 plus (+++++). For this study, leave the **Importance** field at **+++**, a medium setting. By leaving all importance criteria at their defaults, no goals are favored over others.

☒ ***Explore details on desirability functions***: For statistical details about how desirability functions are constructed – and formulas for weights and importance – click on the tips (light bulb icon). Then, click **Contents**. The **Optimization** branch is intuitively already expanded for you, so choose **Numerical Optimization "Statistical Details"** then

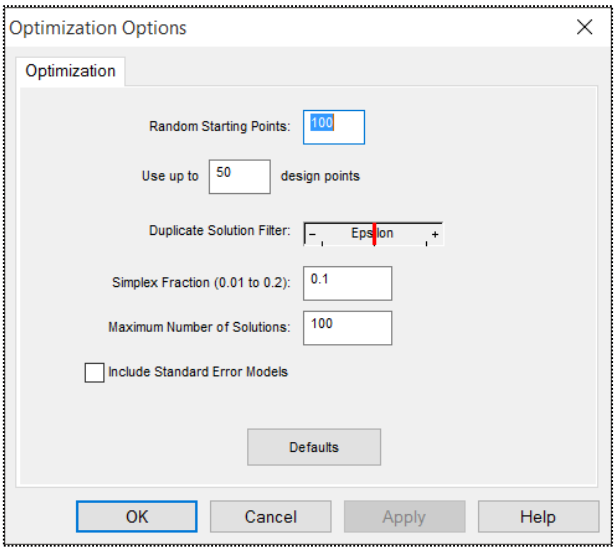
Importance as shown on the screen-shot below. From here you can open various topics and look for any details you need.



Details about optimization criterion "importance" found in program Help

When you are done viewing Help, close it by pressing **X** at the upper-right corner of the screen.

Now click the **Options** button to see what you can control for the numerical optimization.



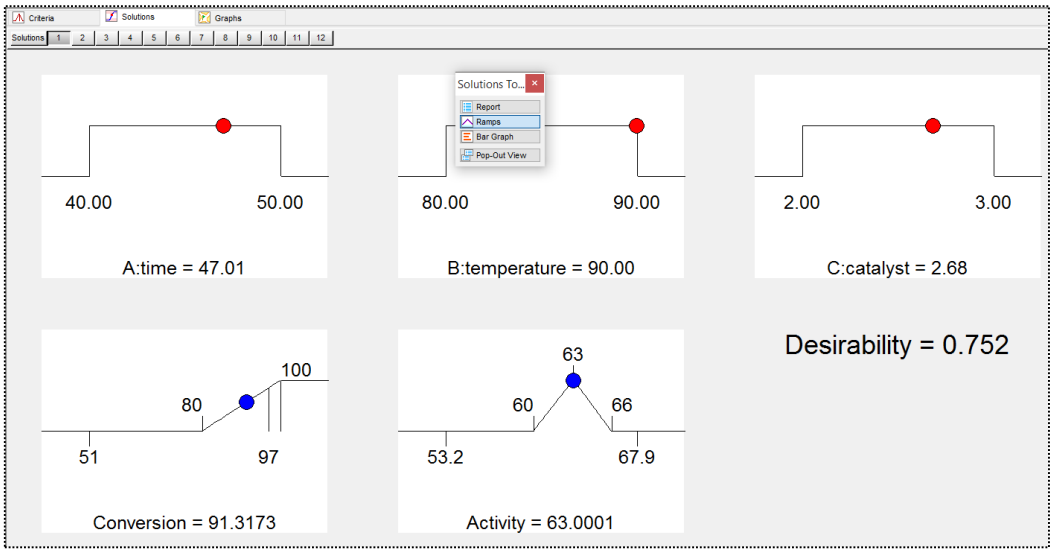
Optimization Options dialog box

☒ ***Explore options for numerical optimization***: Press **Help** to get details on these options. One that you should experiment with is the Duplicate Solution Filter, which establishes the "epsilon" (minimum difference) for eliminating essentially identical solutions. After doing your first search for the optimum, go back to this Option and slide it one way and the other. Observe what happens to the solutions presented by Design-Expert. If you move the Filter bar to the right, you decrease the number. Conversely, moving the bar to the left increases the solutions.

Click **OK** to close Optimization Options.

Running the optimization

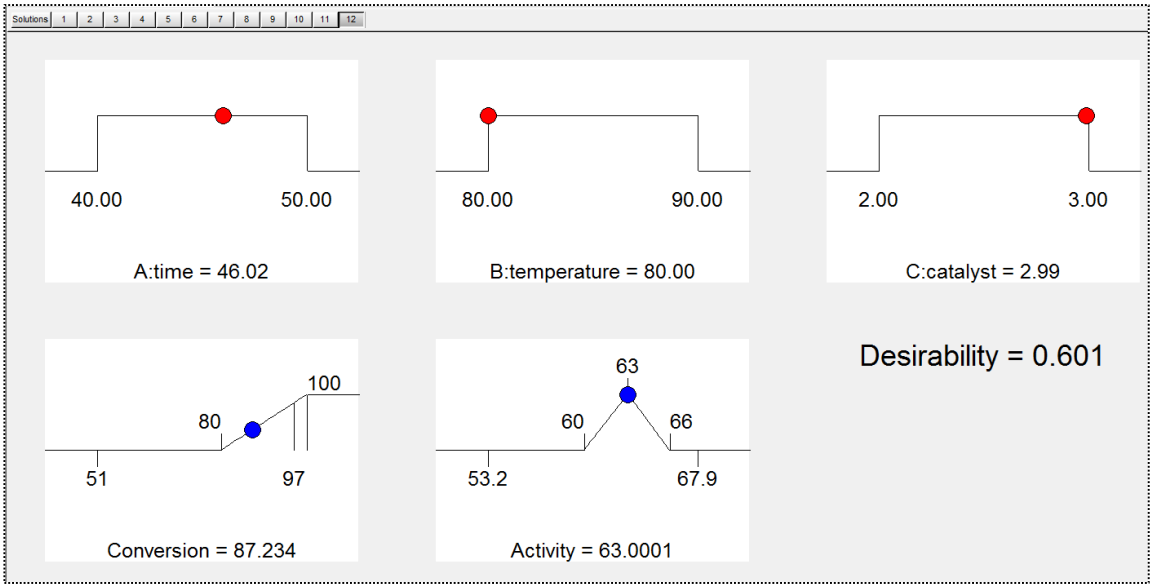
Start the optimization by clicking the **Solutions** tab. It defaults to the Ramps view so you get a good visual on the best factor settings and the desirability of the predicted responses.



Numerical Optimization Ramps view for Solutions (Your results may differ)

The program randomly picks a set of conditions from which to start its search for desirable results – your results may differ. Multiple cycles improve the odds of finding multiple local optimums, some of which are higher in desirability than others. Design-Expert then sorts the results from most desirable to least. Due to random starting conditions, your results are likely to be slightly different from those in the report above.

☒ ***Explore various solutions via Ramps view***: The ramp display combines individual graphs for easier interpretation. The colored dot on each ramp reflects the factor setting or response prediction for that solution. The height of the dot shows how desirable it is. Press the different solution buttons (1, 2, 3,…) or use the arrow keys to cycle through the list and watch the dots. They may move only very slightly from one solution to the next. However, if you look closely at temperature, you should find two distinct optimums, the first few near 90 degrees; further down the solution list, others near 80 degrees. (You may see slight differences in results due to variations in approach from different random starting points.) For example, click the last solution on your screen. Does it look something like the one below?



Second optimum at lower temperature, but conversion drops, so it is inferior

If your search also uncovered this local optimum, note that conversion falls off, thus making it less desirable than the higher-temperature option.

The Solutions Tool provides three views of the same optimization. (Drag the tool to a convenient location on the screen.) Click the **Solutions Tool** view option **Report**.

Constraints

Name	Goal	Lower Limit	Upper Limit	Lower Weight	Upper Weight	Importance
A:time	is in range	40	50	1	1	3
B:temperature	is in range	80	90	1	1	3
C:catalyst	is in range	2	3	1	1	3
Conversion	maximize	80	100	1	1	3
Activity	is target = 63	60	66	1	1	3

Solutions To... × Report Ramps Bar Graph Pop-Out View

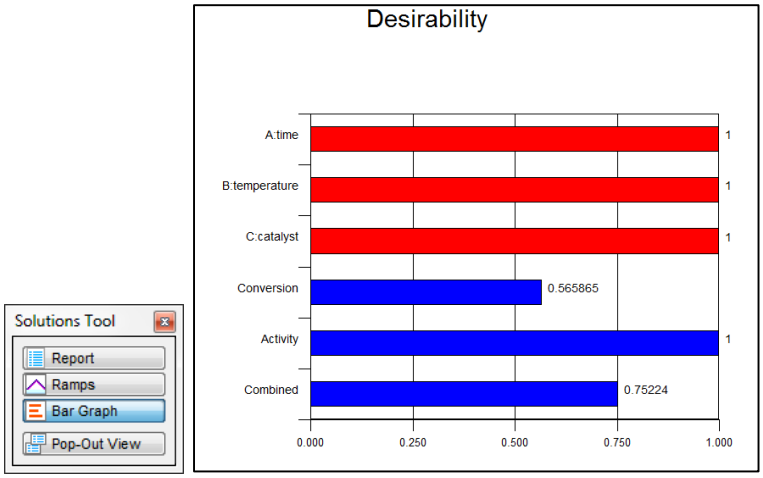
Solutions

Number	time	temperature	catalyst	Conversion	Activity	Desirability	
1	47.014	90.000	2.685	91.317	63.000	0.752	Selected
2	46.944	90.000	2.698	91.308	63.000	0.752	
3	47.096	90.000	2.669	91.306	63.000	0.752	
4	47.444	90.000	2.602	91.003	63.000	0.742	
5	46.995	90.000	2.674	91.229	62.937	0.741	
6	46.323	80.000	2.931	87.392	63.000	0.608	
7	46.343	80.000	2.927	87.391	63.000	0.608	
8	46.300	80.000	2.935	87.391	63.000	0.608	
9	46.252	80.000	2.944	87.383	63.000	0.608	
10	46.159	80.000	2.962	87.346	63.000	0.606	
11	46.109	80.000	2.972	87.313	63.000	0.605	
12	46.019	80.000	2.989	87.234	63.000	0.601	

12 Solutions found

Report on numerical optimization

Now select the **Bar Graph** view from the floating Solutions Tool.

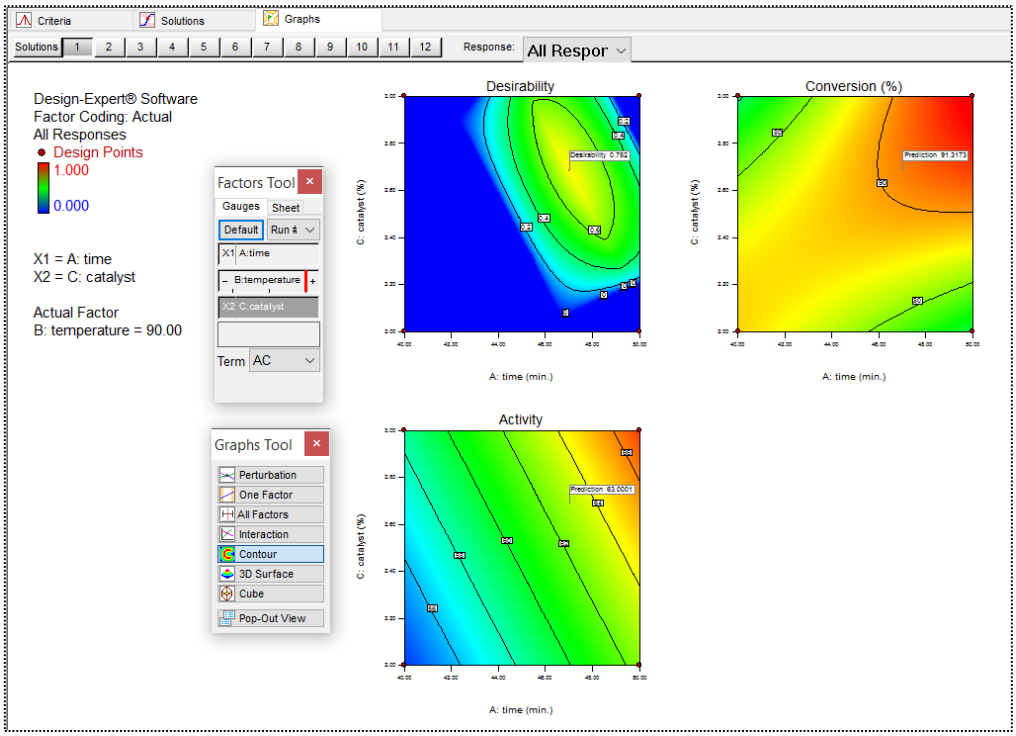


Solution to multiple response optimization — desirability bar graph

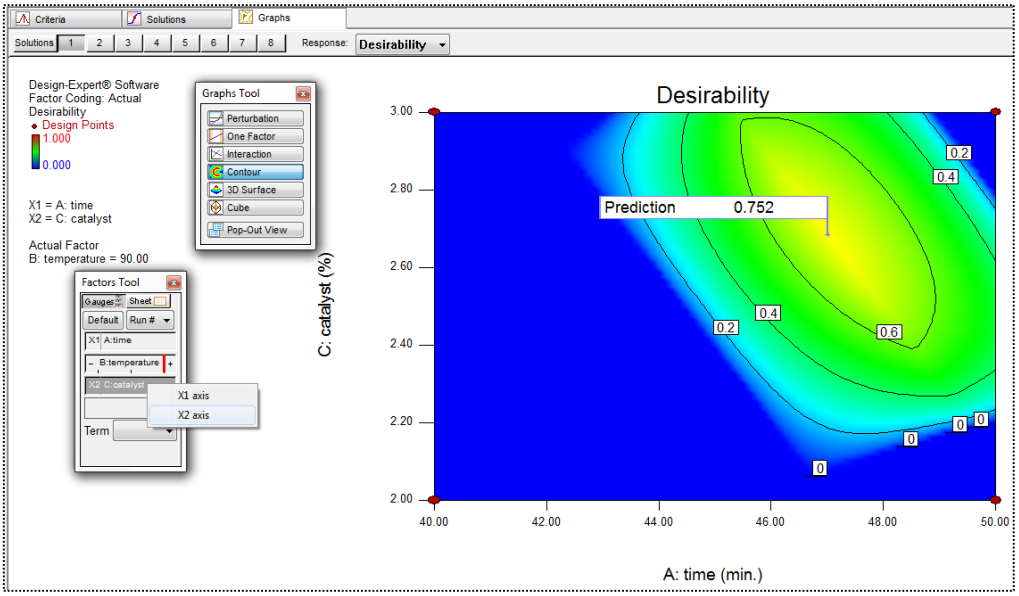
The bar graph shows how well each variable satisfies the criteria: values near one are good.

Optimization Graphs

Press **Graphs** near the top of your screen to view a contour graph of the overall desirability and all of your responses. On the **Factors Tool** palette, right-click **C:Catalyst**. Make it the **X2 axis**. Temperature then becomes a constant factor at 90 degrees (this level is picked automatically by the selected solution #1).



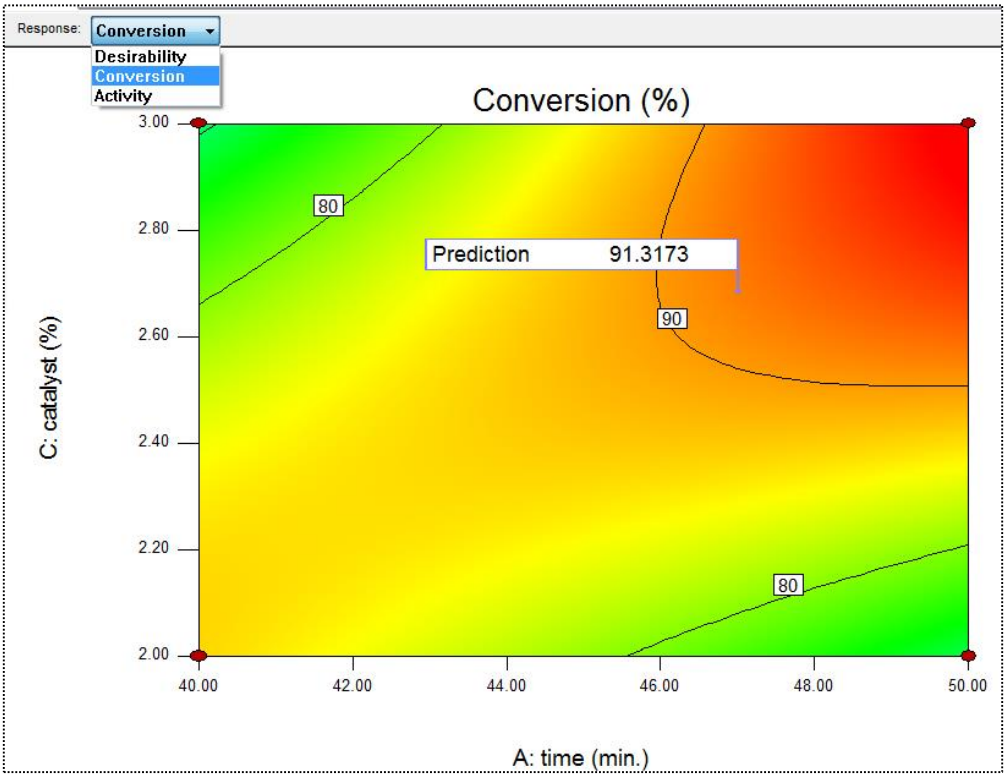
You can also use the droplist to look at bigger versions of each plot, such as the desirability plot below.



Desirability graph (after changing X2 axis to factor C)

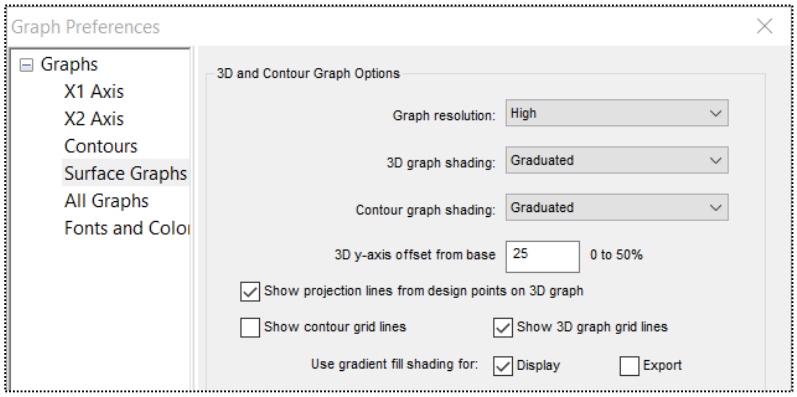
The screen shot above is a graph displaying graduated colors – cool blue for lower desirability and warm yellow for higher.

Design-Expert software sets a flag at the optimal point (as selected by the button bar at the top , number 1 is selected in the screenshot above). To view a response associated with the desirability, select the desired **Response** from its droplist. Take a look at the **Conversion** plot.



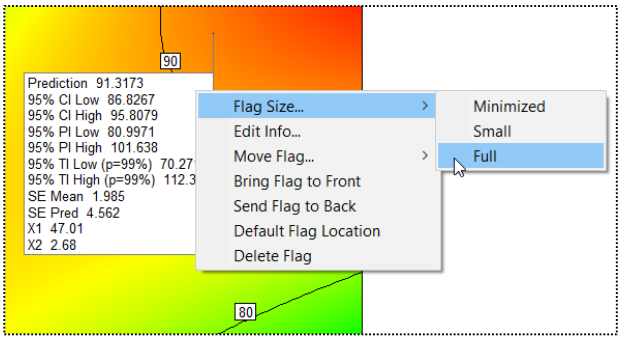
Conversion contour plot (with optimum flagged)

☒ ***Explore Graph Preferences for contour graphs***: Right-click over this graph and choose **Graph Preferences**. Then go to **Surface Graphs** and click **Show contour grid lines**.



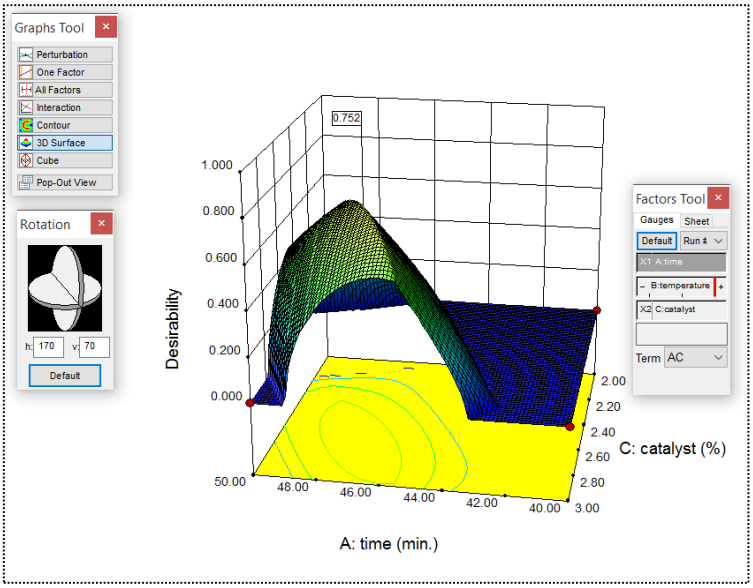
Show contour grid lines option

Grid lines help locate the optimum, but for a more precise locator right-click the flag and **Flag Size->Full** to see the coordinates plus many more predicted outcome details. To get just what you want on the flag, right-click it again and select **Edit Info**.



Flag size toggled to see select detail

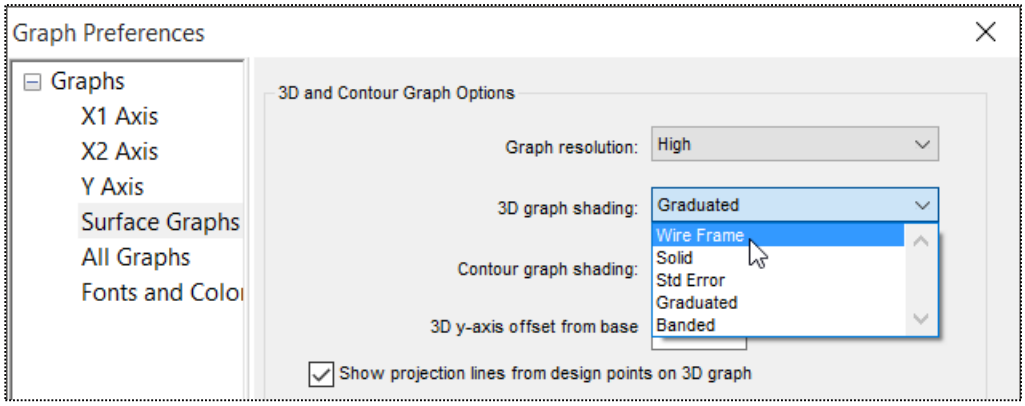
To look at the desirability surface in three dimensions, again click **Response** and choose **Desirability**. Then, on the floating **Graphs Tool,** press **3D Surface**. Next select **View**, **Show Rotation** and change horizontal control **h** to **170.** Press your Tab key or click the graph. What a spectacular view!



3D desirability plot

Now you can see there's a ridge where desirability can be maintained at a high level over a range of catalyst levels. In other words, the solution is relatively robust to factor C.

☒ ***Explore Graph Preferences for 3D graphs***: Right-click over your graph to re-summon **Graph preferences**. Via the **Surface Graphs** tab change the **3D graph shading** option to **Wire Frame**.



3D graph shading changed to wire frame

One way or another, please show your colleagues what Design-Expert software does for pointing out the most desirable process factor combinations. We'd like that! The best way to show what you've accomplished is not on paper, but rather by demonstrating it on your computer screen or by projecting your output to larger audiences. In this case, you'd best shift back to the default colors and other display schemes. Do this by pressing the **Default** button Surface Graphs and any other Graph Preference screens you experimented on.

P.S. Design-Expert offers a very high Graph resolution option. Try this if you like, but you may find that the processing time taken to render this, particularly while rotating the 3D graph, can be a bit bothersome. This, of course, depends on the speed of your computer and the graphics-card capability.

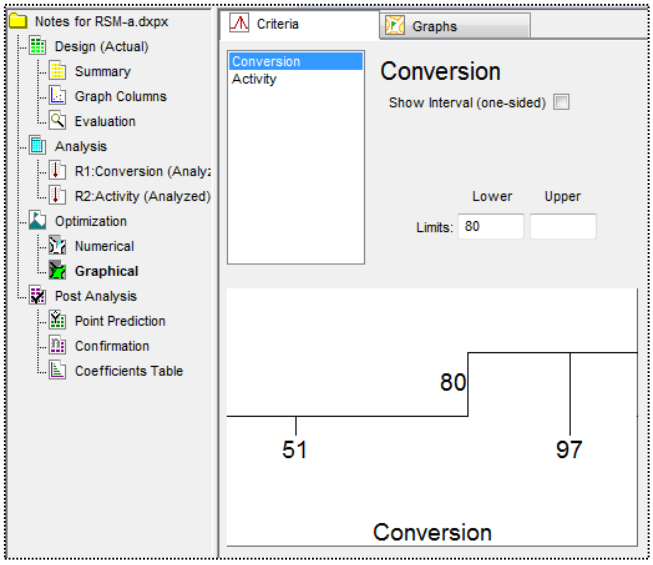
Now move on to graphical optimization—this may the best way to convey the outcome of an RSM experiment by displaying the "sweet spot" for process optimization.

Graphical Optimization

When you generated numerical optimization, you found an area of satisfactory solutions at a temperature of 90 degrees. To see a broader operating window, click the **Graphical** node. The requirements are essentially the same as in numerical optimization:

- 80 < Conversion
- 60 < Activity < 66

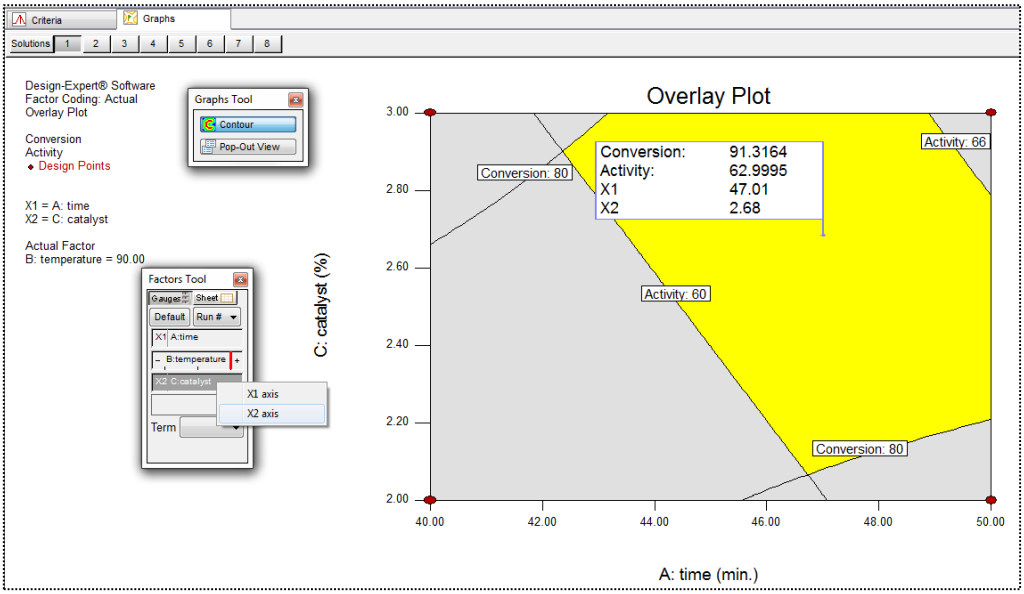
For the first response – **Conversion** (if not already entered), type in **80** for the **Lower Limit**. You need not enter a high limit for graphical optimization to function properly.



Graphical optimization: Conversion criteria

Click **Activity** response. If not already entered, type in **60** for the **Lower Limit** and **66** for the **Upper Limit**.

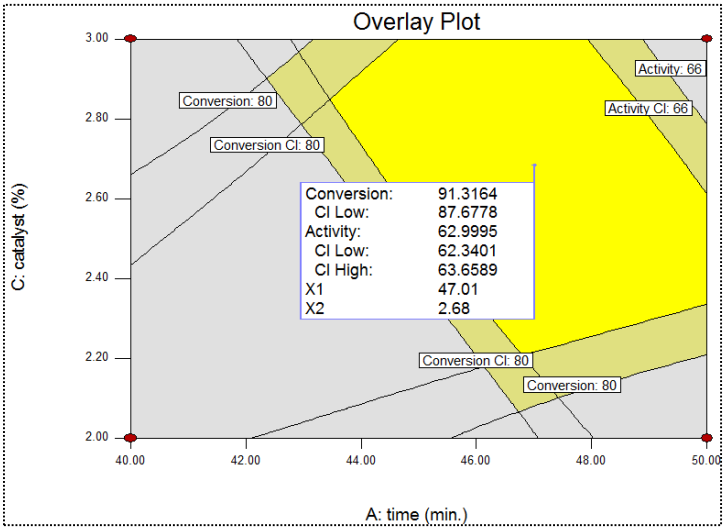
Now click the ***Graphs*** button to produce the "overlay" plot. Notice that regions not meeting your specifications are shaded out, leaving (hopefully!) an operating window or "sweet spot." Now go to the **Factors Tool** palette and right-click **C:Catalyst**. Make it the **X2 axis**. Temperature then becomes a constant factor at 90 degrees as before for Solution 1.



Overlay plot

Notice the flag remains planted at the optimum. That's handy! This Design-Expert display may not look as fancy as 3D desirability but it can be very useful to show windows of operability where requirements simultaneously meet critical properties. Shaded areas on the graphical optimization plot do <u>not</u> meet the selection criteria. The clear "window" shows where you can set factors that satisfy requirements for both responses.

☒ ***Explore adding uncertainty intervals around your window of operability***: Go back to the **Criteria** and click **Show Interval (one-sided)** for both **Conversion** and **Activity**. This provides a measure of uncertainty on the boundaries predicted by the models — a buffer of sorts.



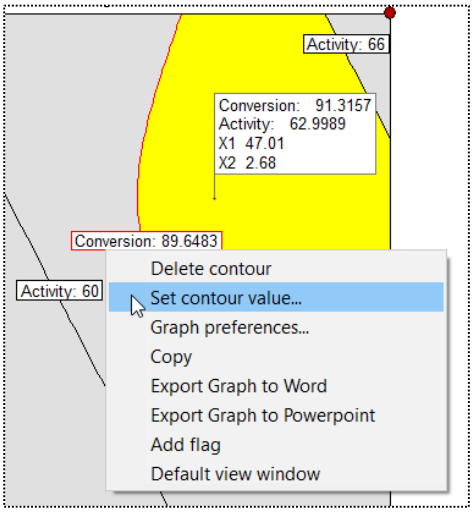
Confidence intervals (CI) superimposed on operating window

After looking at this, go back and turn off the intervals to re-set the graph to the default settings.

P.S. If you are subject to FDA regulation and participate in their quality by design (QBD) initiative, the CI-bounded window can be considered to be a functional design space, that is, a safe operating region for any particular unit operations. However, to establish a manufacturing design space one must impose tolerance intervals. This tutorial

experiment provided too few runs to support imposition of TIs. To size designs properly for manufacturing QBD requires advanced know-how taught by Stat-Ease in its Designed Experiments for Pharma workshop.

Let's say someone wonders whether the 80 minimum for conversion can be increased. What will this do to the operation window? Find out by dragging the 80 conversion contour until it reaches a value near 90. Then right-click it and Set contour value to **90** on the nose.



Changing the conversion specification to 90 minimum

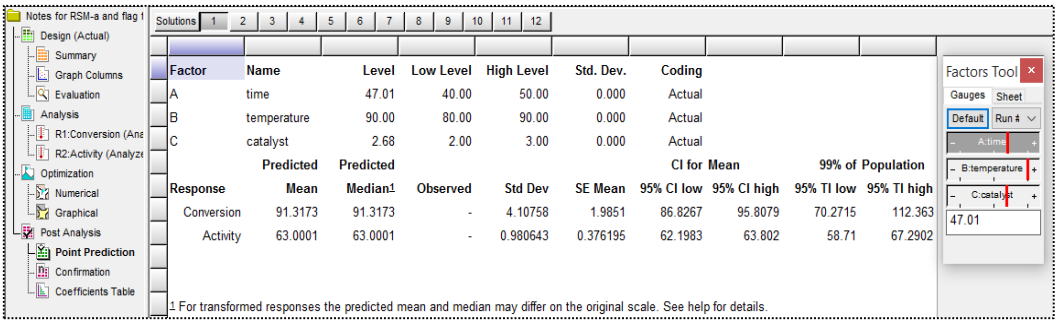
It appears that the more ambitious goal of 90 percent conversion is feasible. This requirement change would make the lower activity specification superfluous as evidenced by it no longer being a limiting level, that is, not a boundary condition on the operating window.

Graphical optimization works great for two factors, but as factors increase, optimization becomes more and more tedious. You will find solutions much more quickly by using the numerical optimization feature. Then return to the graphical optimization and produce outputs at the various optimization solutions for exploration of the processing windows.

Response Prediction and Confirmation

This feature in Design-Expert software allows you to generate predicted response(s) for any set of factors. To see how this works, click on the **Point Prediction** node (lower left on your screen).

Click the **Point Prediction** node (left on your screen). Notice it now defaults to the first solution. (Be thankful Design-Expert programmers thought of this, because it saves you the trouble of dialing it up on the Factors Tool.)



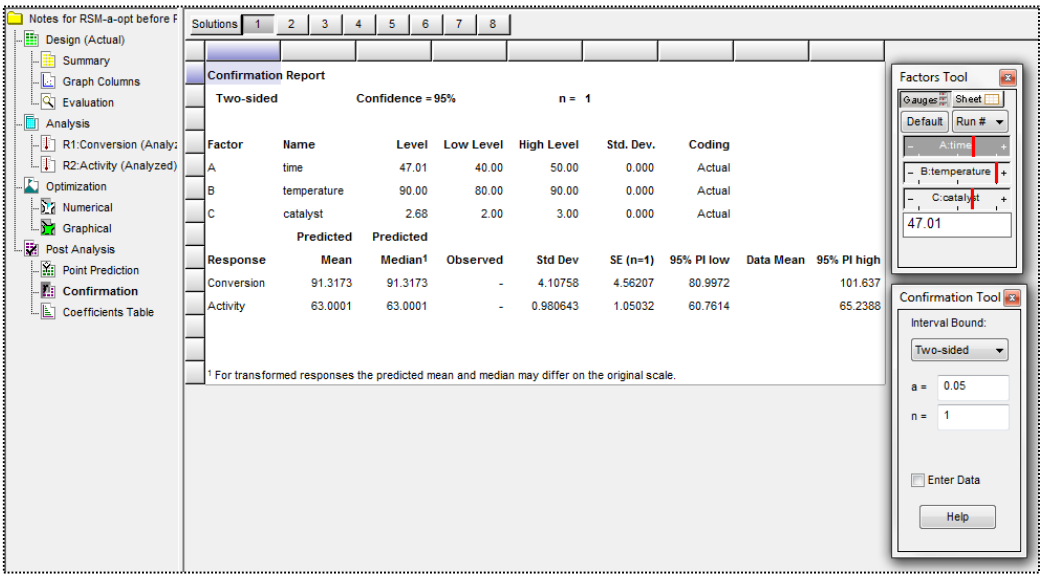
Point prediction set to solution #1

☒ ***Explore other factor settings by moving the slide bar***: The Factors Tool again allows you to adjust the settings to any values you wish. Go ahead and play with them now if you like. You can either move the slider controls, or switch to the Sheet view and enter values.

P.S. Take a moment now to study the screen tips on all the statistical intervals that come up when you press the light-bulb icon (💡).

Confirmation

After finding the optimum settings based on your RSM models, the next step is to confirm that they actually work. To do this, click the **Confirmation** node (left side of your screen).

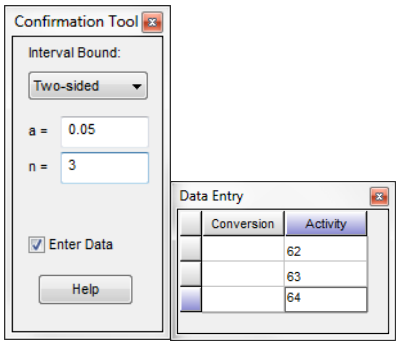


Confirmation predictions set to solution #1

Look at the 95% prediction interval ("PI low" to "PI high") for the Activity response. This tells you what to expect for an individual (n = 1) confirmation test on this product attribute. You might be surprised at the level of variability, but it will help you manage expectations. (Note: block effects, in this case day-by-day, cannot be accounted for in the prediction.)

Of course you would not convince many people by doing only one confirmations run. Doing several would be better. For example, let's say that the experimenters

do three confirmatory tests. Go to the **Confirmation Tool** and enter for **n** the number **3**. Click the **Enter Data** option and type for Activity **62**, **63** and **64**.



Entering confirmation run results

Notice that the prediction interval (PI) narrows as n increases. Does the Data Mean (62.5) fall within this range? If so, the model is confirmed. If not, it will turn red-isn't DX helpful?

Response	Predicted Mean	Predicted Median[1]	Observed	Std Dev	n	SE Pred	95% PI low	Data Mean	95% PI high
Conversion	91.3173	91.3173	-	4.10758	3	3.09	84.32		98.31
Activity	63.0001	63.0001	-	0.980643	2	0.79	61.32	62.50	64.68

Confirmation results are within the interval for activity

☒ ***Explore increasing numbers of confirmation runs***: Keep increasing the value for n. Observe the diminishing returns in terms of the precision, that is, the PI approaches a limit — the confidence interval (CI) that you saw in Point Prediction. The CI is a function of the number of experimental runs from which the model is derived. That is done is this stage, so one can only go so far with the number of confirmation runs. Perhaps half a dozen of these may suffice.

Save the Data to a File

Now that you've invested all this time into setting up the optimization for this design, it would be prudent to save your work. Click the **File** menu item and select **Save As**. You can now specify the **File name** (we suggest **tut-RSM-opt**) for Save as type "*.dxpx" in the Data folder for Design-Expert (or wherever you want to Save in).

If you are not worn out yet, you will need this file in Part 3 of this series of tutorials.

Summary

Numerical optimization becomes essential when you investigate many factors with many responses. It provides powerful insights when combined with graphical analysis. However, subject-matter knowledge is essential to success. For example, a naive user may define impossible optimization criteria that results in zero desirability everywhere! To avoid this, try setting broad acceptable ranges. Narrow them down as you gain knowledge about how changing factor levels affect the responses. Often, you will need to make more than one pass to find the "best" factor levels that satisfy constraints on several responses simultaneously.

This tutorial completes the basic introduction to doing RSM with Design-Expert software. Move on to the next tutorial on advanced topics for more detailing of what the software can do. If you want to learn more about response surface methods (not the software per se), attend our Stat-Ease workshop Response Surface Methods for Process Optimization.

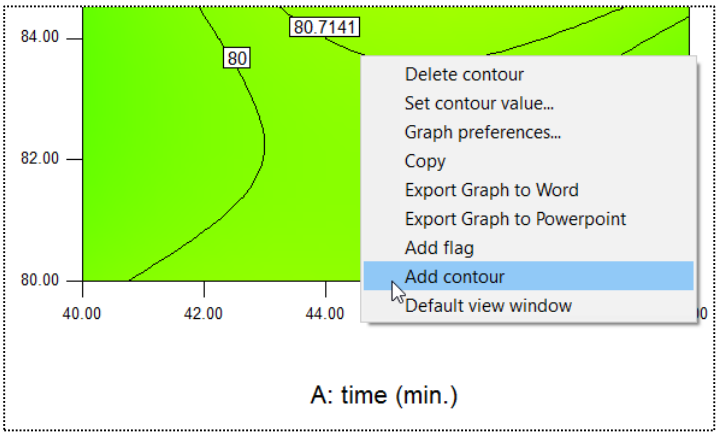
We appreciate your questions and comments on Design-Expert software. E-mail these to stathelp@statease.com along with your dx* file if you've created one. Do so at the design stage to get advice on a planned experiment and/or when you've collected the data and taken a shot at analyzing it. It's always good to get a second opinion from experts in the field. Don't be shy!

Multifactor RSM Tutorial
(Part 3/3 – Advanced Topics)

Tips and Tricks for Making Response Graphs Most Presentable

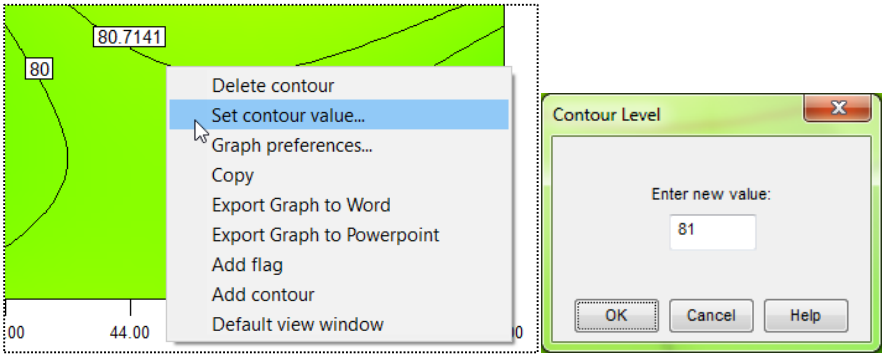
Go back a step and re-open the file named **RSM-a.dxpx**. Then under the Analysis branch click the **R1:Conversion** node and go to **Model Graphs** to bring up the contour plot. Let's quickly try some things here that you may find useful when making a presentation.

In the vacant region of the AB contour plot right-click and select **Add contour**. Then drag the contour around (it will become highlighted). You may get two contours from one click like those with the same response value shown below. (This pattern indicates a shallow valley, which becomes apparent when we get to the 3D view later.)



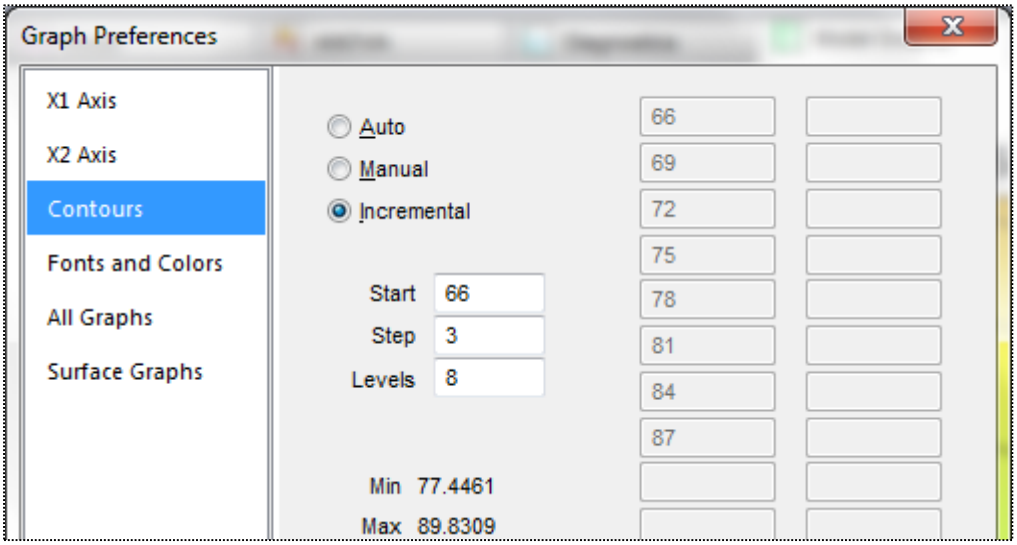
Adding a contour

Click the new contour line to highlight it. Then drag it (place the mouse cursor on the contour and hold down the left button while moving the mouse) to as near to 81 as you can. Now to obtain the precise contour level, right-click the contour you just dragged, choose **Set contour value** and enter **81**.



Setting a contour value

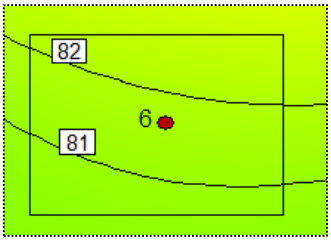
☒ ***Explore another way to set contour values***: Right-click over the plot and choose **Graph Preferences**. Then choose **Contours**. Now select the **Incremental** option and fill in **Start** at **66**, **Step** at **3,** and **Levels** at **8**.



Setting contour values incrementally via Graph Preferences

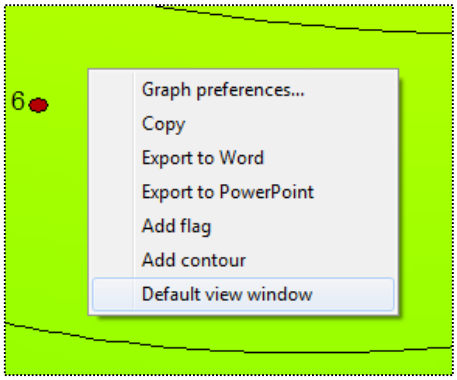
If you go this route, be sure to look over the Min and Max values first. That gives you a clue on where to start and how big to step on the contour values.

To zoom in on the area around the center point (the red dot labeled "6"), position the crosshairs and, while holding down the left mouse button, drag over (rope-off) your desired region of interest.



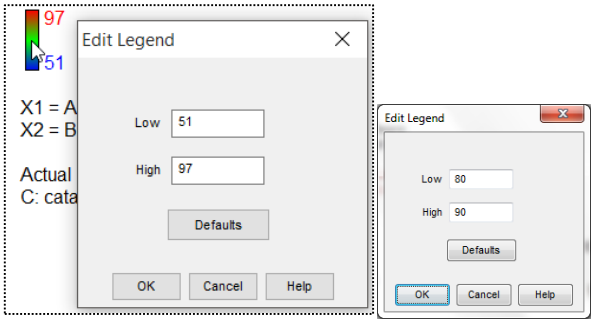
Zooming in on a region of interest by roping off a box

Notice how the graph coordinates change. Obviously you would now want to add more contours using the tools you learned earlier in this tutorial. However, do not spend time on this now: Right-click over the graph and select **Default View Window**.



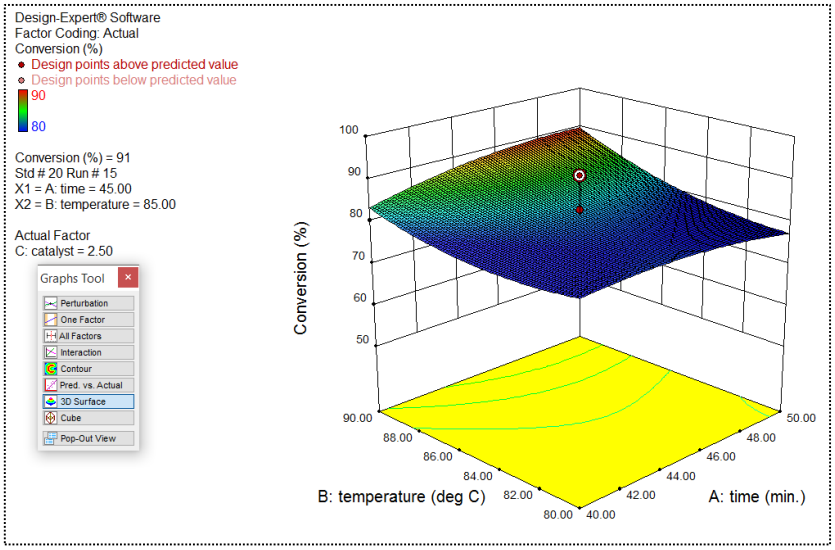
Restoring default region (factorial ranges within CCD)

That's enough for the contours plot for now. On the **Graphs Tool** go to **3D Surface** view. Modify the color range via a click on the color scale gradient, which brings up the **Edit Legend** dialog box. Change the **Low** to **80** and the **High** to **90**. Notice how this makes the graph far more colorful and thus informative on the relative heights.



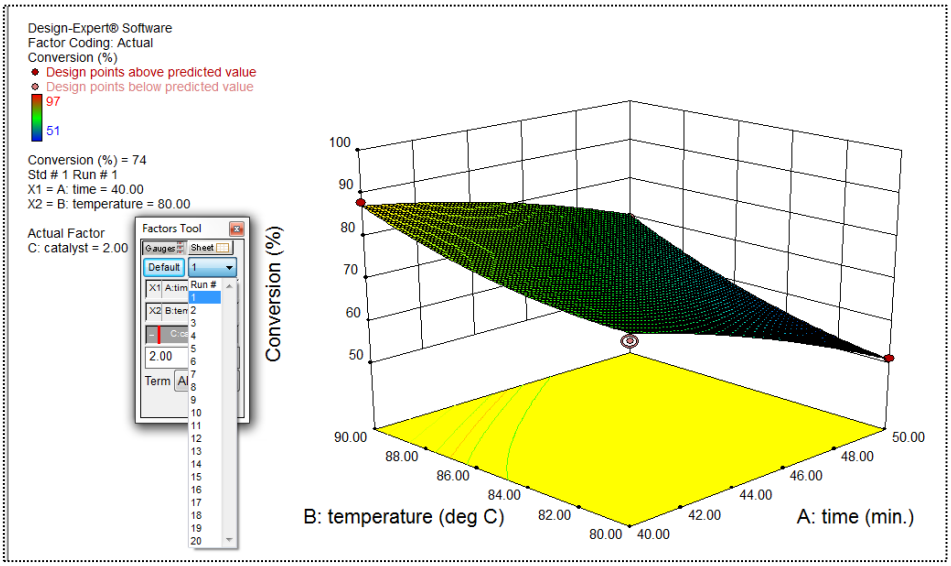
Edit Legend dialog box to change the color gradient

Now click the design point sticking up in the middle. See how this is identified in the legend at the left by run number and conditions.



3D graph enhanced for color gradient with point click and identified

Now try a handy feature for pulling up the right plot for any given run. On the **Factors Tool** select off the **Run #** dropdown-list number **1**. The 3D view now shifts to the correct 'slice' on factor C (catalyst). However the colors are not ideal now. So right-click over the gradient and in the **Edit Legend** dialog box press the **Defaults** button. Your graph should now match the one shown below.



Jump to run feature demonstrated

By the way, if you put in any comments on a particular run, it will show in this view with the point having been selected.

☒ ***Explore adding a comment***: Hearken back to the General One-Factor tutorial where we demonstrated how to add a comment using tools in the Design layout. This can be very useful to document unusual happenings during any given run.

Much more can be done for your show-and-tell. Spend time beforehand to try different things that Design-Expert can do. Take advantage of default buttons to put things back the way they were.

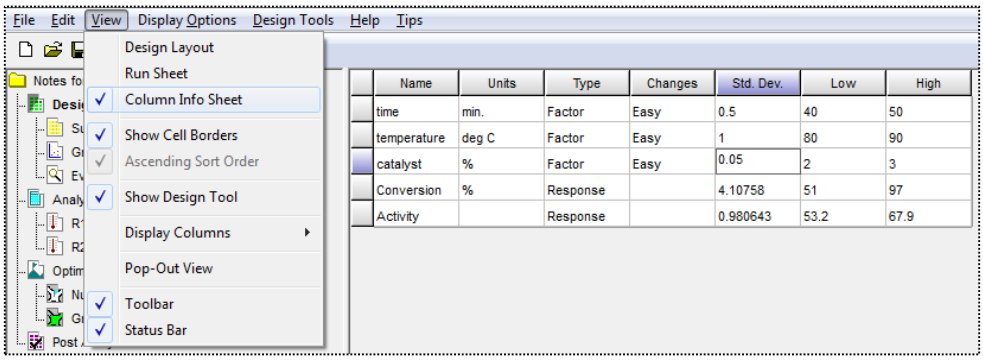
Adding Propagation of Error (POE) to the Optimization

Details about the variation in your input factors can be fed into Design-Expert® software. Then you can generate propagation of error (POE) plots showing how that error is transmitted to the response. Look for conditions that minimize transmitted variation, thus creating a process that's robust to factor settings. This tutorial shows how to generate POE from an experiment designed by response surface methods (RSM).

☒ ***Explore simpler case for application of POE***: Propagation of error is covered in the One Factor RSM tutorial in a way that is far easier to see, so be sure to review this if you want to develop a fuller understanding of this mathematical tool.

To be sure we start from the same stage of analysis, re-open the file named **RSM-a.dxpx**. Then click the **Design** node on the left side of the screen to get back to the design layout. Next select **View**, **Column Info Sheet**. Enter the following

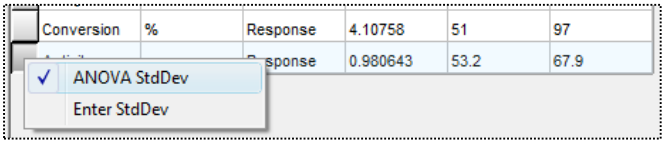
information into the Std. Dev. column: time: **0.5**, temperature: **1.0**, catalyst: **0.05**, as shown below.



Column Info Sheet with factor standard deviations filled in

Notice the software already entered the standard deviation for the analyzed response, Conversion (4.1…). Because you haven't changed any other data, Design-Expert remembers your previous analysis choices — you can simply click through the analysis buttons.

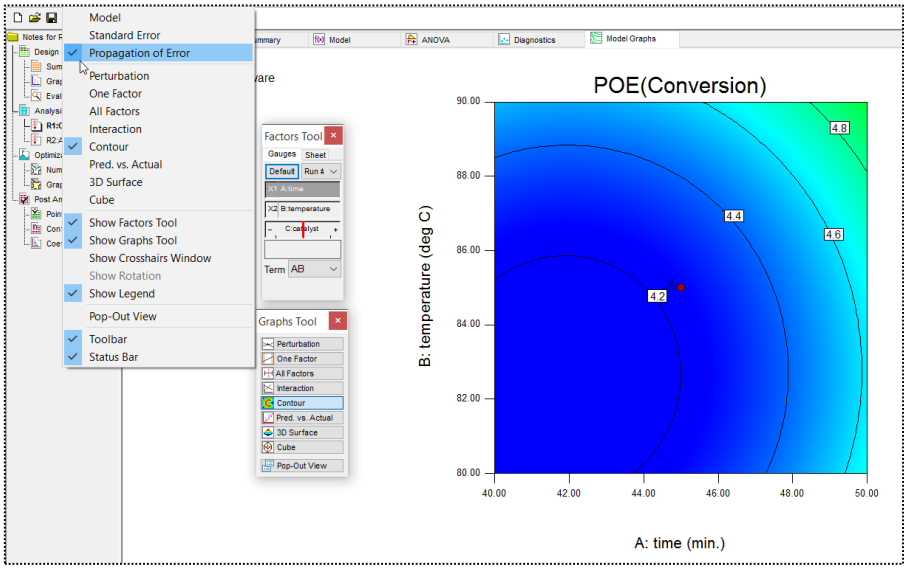
☒ ***Explore another way to specify variation in response***: For your information, right-clicking the buttons to the left of response names allows you to specify a different standard deviation.



Option to enter a different standard deviation for response

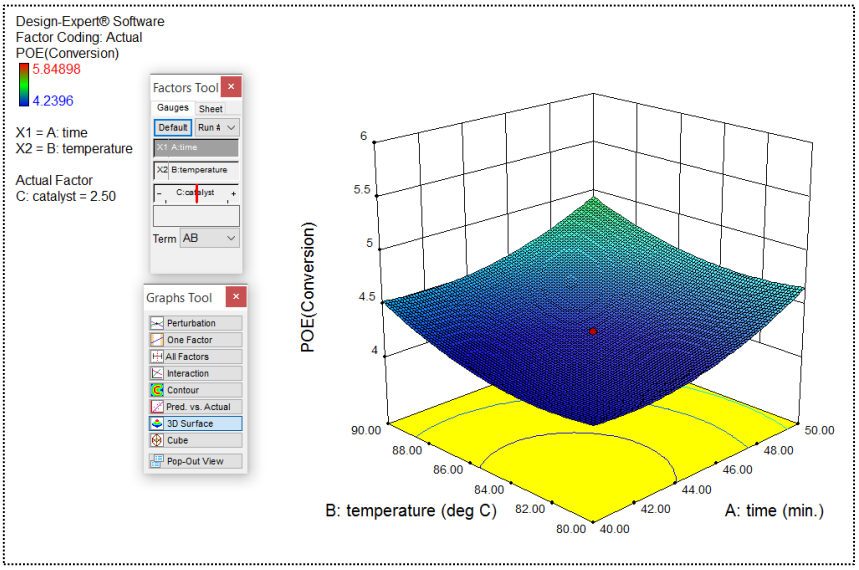
Otherwise the field will be protected, that is, you cannot alter it.

Under the **Analysis** branch click the **Conversion** node. Then jump past the intermediate buttons for analysis and click the **Model Graphs** tab. Select **View**, **Propagation of Error**. (This option was previously grayed out — unavailable — because the standard deviations for the factors had not yet been entered.)



Contour graph for POE

Now on the floating **Graphs Tool** select **3D Surface**.

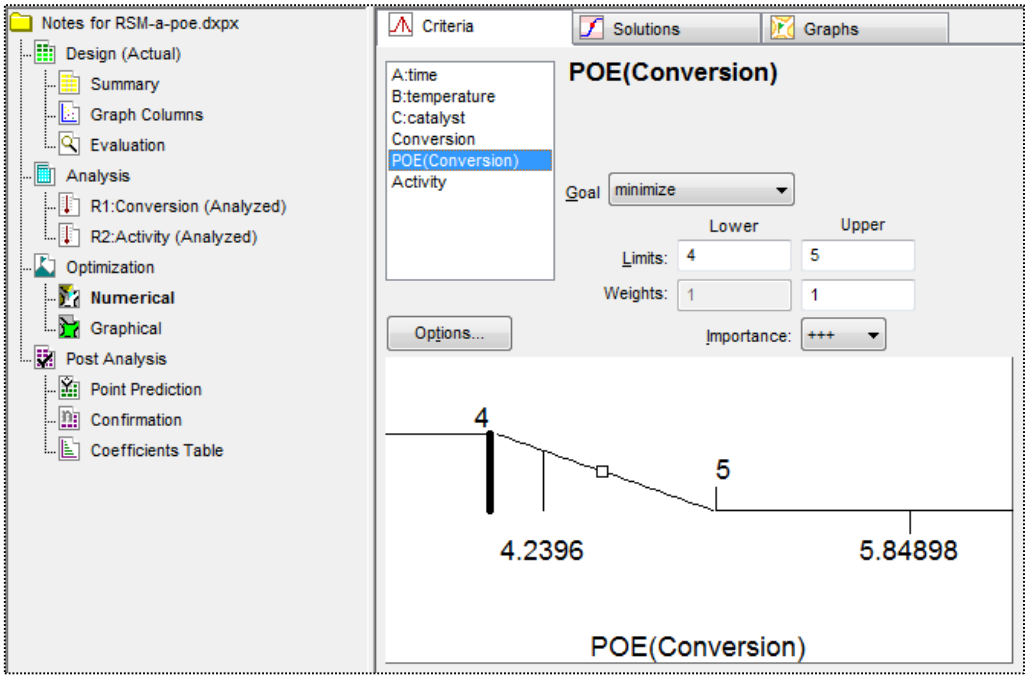


3D Surface view of the POE Graph

The lower the POE the better, because less of the error in control factors will be transmitted to the selected response, which results in a more robust process.

☒ ***Explore what happens if you try to generate POE on a response that's fitted to a linear model***: When the surface is linear, such as that for Activity, error is transmitted equally throughout the region. Therefore, Design-Expert software 'grays out' the option for propagation of error. See this for yourself by trying it.

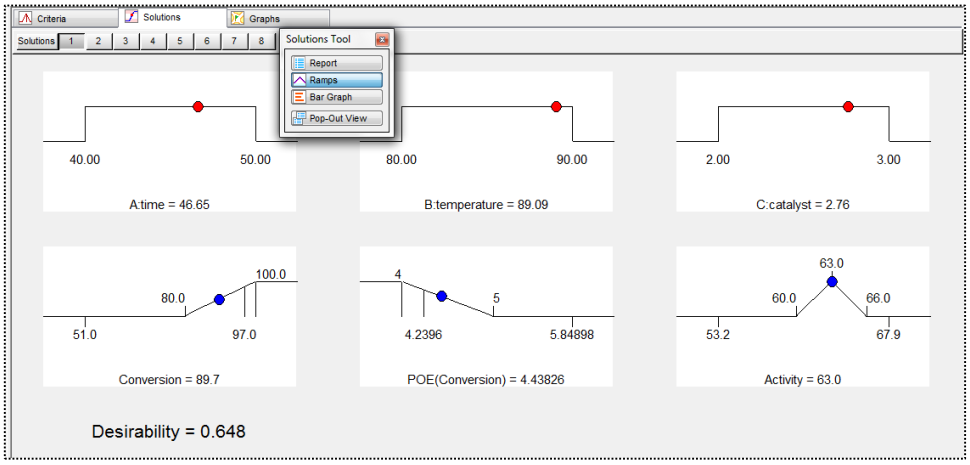
Now that you've generated POE for Conversion, let's go back and add it to the optimization criteria. Under the **Optimization** branch click the **Numerical** node. For the **POE (Conversion)** set the **Goal** to **minimize** with a **Lower Limit** of **4** and an **Upper Limit** of **5** as shown below.



Set Goal and Limits for POE (Conversion)

You may also have to go back and set the goalf for Conversion (maximize; LL 80-UL 100) and Activity (Target->63; LL 60-UL 66).

Now click the **Solutions** button atop the screen to generate new solutions with additional criteria. On the floating **Solutions Tool** click **Ramps**. (Note: Due to random starting points for the searches, you may see slight differences on your screen versus the shot below.)



Ramps view for optimization with POE (Your results may differ)

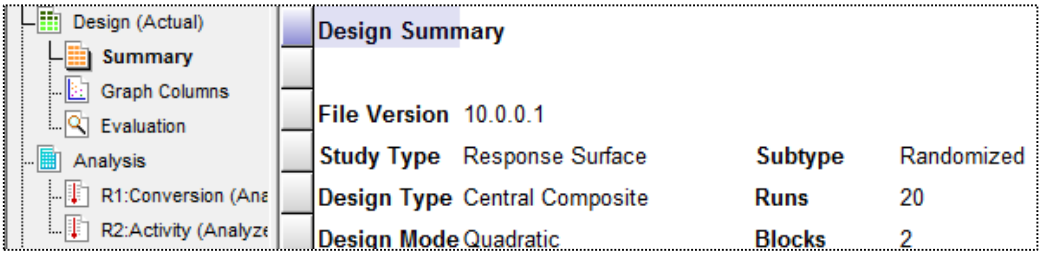
The above optimal solution represents the formulation that best maximizes conversion and achieves a target value of 63 for activity, while at the same time finds the spot with the minimum error transmitted to the responses. So, this should represent process conditions that are robust to slight variations in factor settings. In this case it does not make much of a difference whether POE is

accounted for or not (go back and check this out for yourself). However, in some situations it may matter, so do not overlook the angle of POE.

Design Evaluation

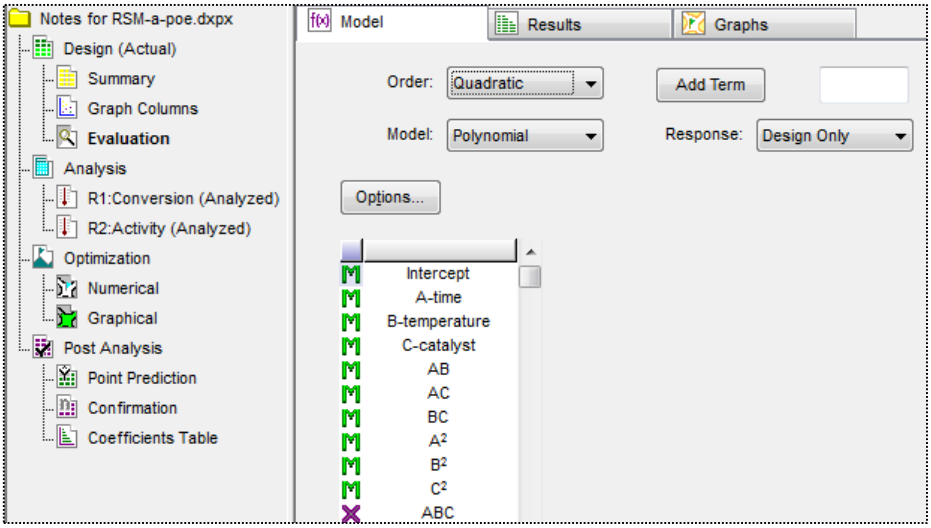
Design-Expert offers powerful tools to evaluate RSM designs. Design evaluation ought to be accomplished prior to collecting response data, but it can be done after the fact. For example, you may find it necessary to change some factor levels to reflect significant deviations from the planned set point. Or you may miss runs entirely – at least for some responses. Then it would be well worthwhile to re-evaluate your design to see the damage.

For a re-cap of what's been done so far, go to the **Design** branch and click the **Summary** node.



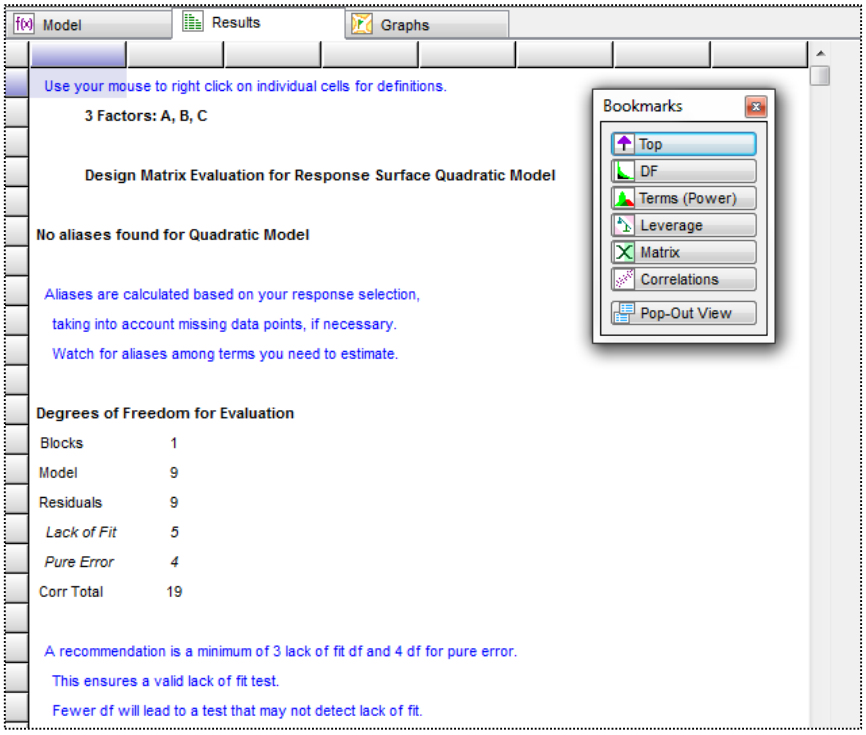
Design summary

The summary reports that the experimenter planned a central composite design (CCD) in two blocks, which was geared to fit a quadratic model. Click the **Evaluation** node and notice Design-Expert assumes you want details on this designed-for order of model.



Design evaluation – model choice

Click the **Results** tab for an initial report showing annotations on by default.

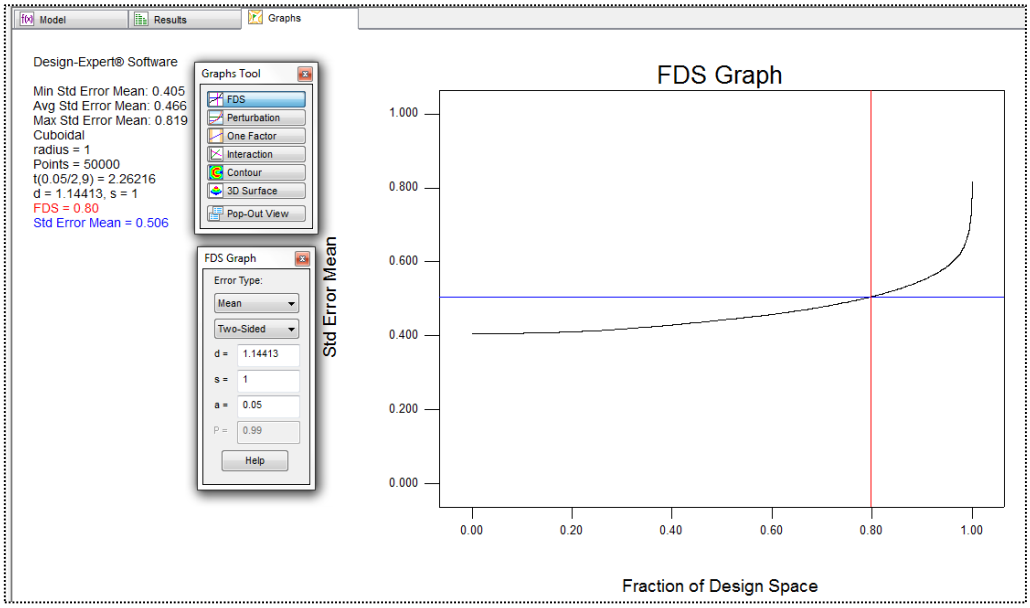


Design evaluation results

Scroll through the results or use the handy Bookmarks palette and note the results look very good – as you'd expect from a standard design for RSM.

☒ ***Explore a really bad factor matrix***: For a design that produces a far worse evaluation, take a look at the Historical Data RSM Tutorial.

Press ahead to the **Graphs** tab atop the screen. It defaults to the FDS Graph that depicts standard error versus the fraction of design space. Click the curve you see depicted. Design-Expert now provides coordinate lines for easy reading.

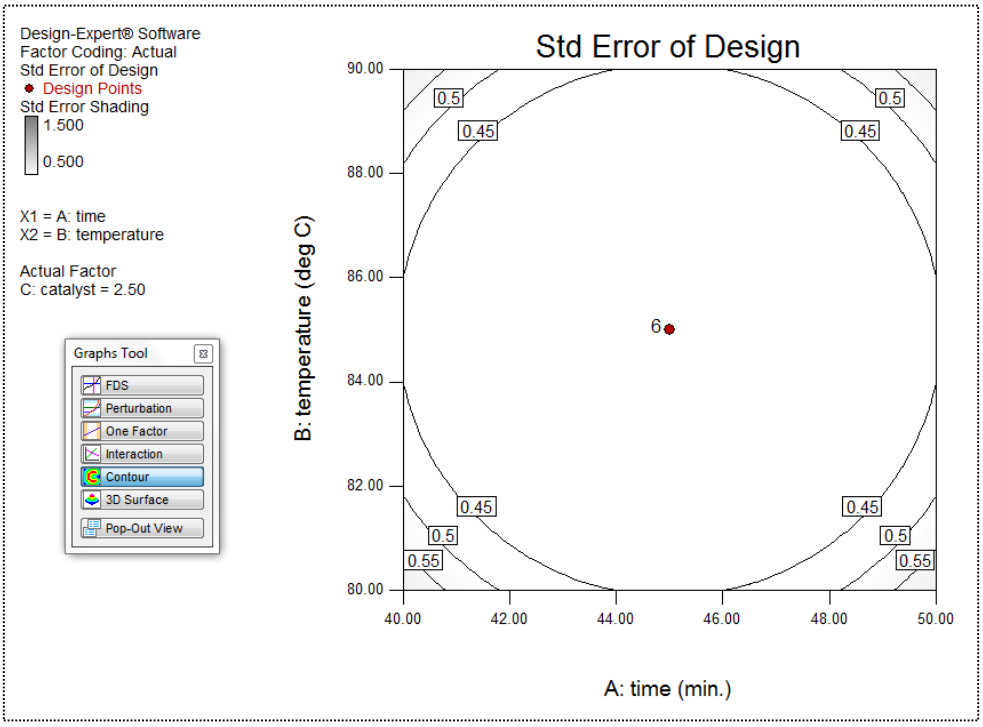


FDS (fraction of design space) graph with coordinates clicked on

Based on extensive sampling of the experimental region (50,000 points by default as noted in the legend), the "y" axis on the FDS graph quantifies the maximum prediction variability at any given fraction of the total space. For example, as noted in the legend at the left of the screen, 80 percent of this response surface method (RSM) design falls at or below ~0.5 units of standard error (SE). Due to the random sampling algorithm, your FDS may vary a bit. When you evaluate alternative designs, favor those with lower and flatter FDS curves.

☒ ***Explore FDS for sizing designs***: FDS provides the mechanism for sizing RSM designs based on how precisely you need to predict your response. Stat-Ease teaches how to do this in its workshop on RSM. For statistical details, see the pdf of the talk on "Practical Aspects of Algorithmic Design of Physical Experiments" posted to the webinar page at our website, or just click the link above.

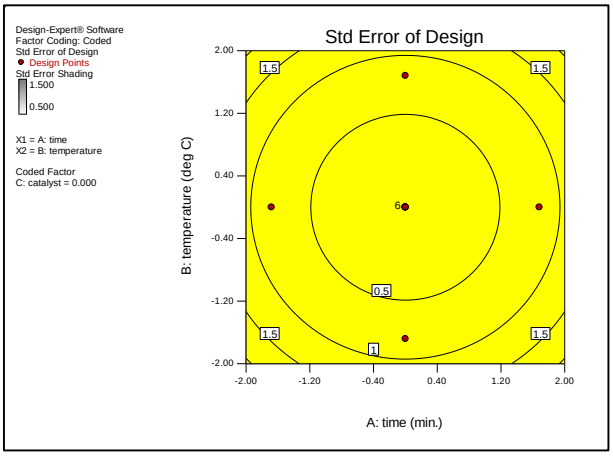
The FDS provides insights on prediction capabilities. To view design 'rotatability' criteria, select **View**, **Contour**. Design-Expert then displays the standard error plot, which shows how variance associated with prediction changes over your design space.



Standard error contour plot

You can see the central composite design (CCD) provides relatively precise predictions over a broad area around the 6 center points. Also, notice the circular contours. This indicates the desirable property of rotatability – equally precise predictive power at equal distances from the center point of this RSM design. For standard error plots, Design-Expert defaults to black and white shading. The graduated shading that makes normal response contour plots so colorful will not work when displaying standard error. Look closely at the corners of this graph and notice they are gray, thus indicating regions where the response cannot be predicted as precisely.

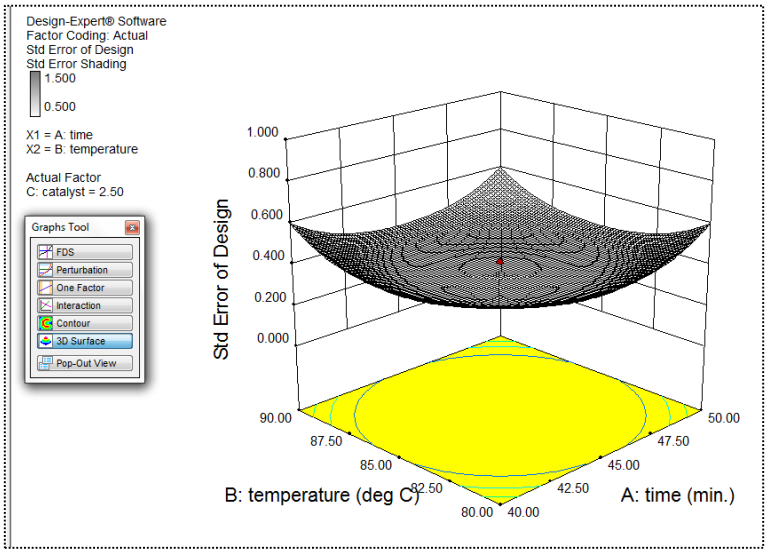
☒ ***Explore the outer regions of a central composite design***: See what happens when you extrapolate beyond experimentation regions by following these steps. First select **Display Options**, **Process Factors**, **Coded**. Then right-click over the graph and select **Graph Preferences**. Change the default **X1 Axis** values for **Low** to **-2** and **High** to **2**. Next, click the **X2 Axis** tab and change **Low** value to **-2** and **High** value to **2**. After completing these changes, press **OK**. You now should see a plot like that shown below.



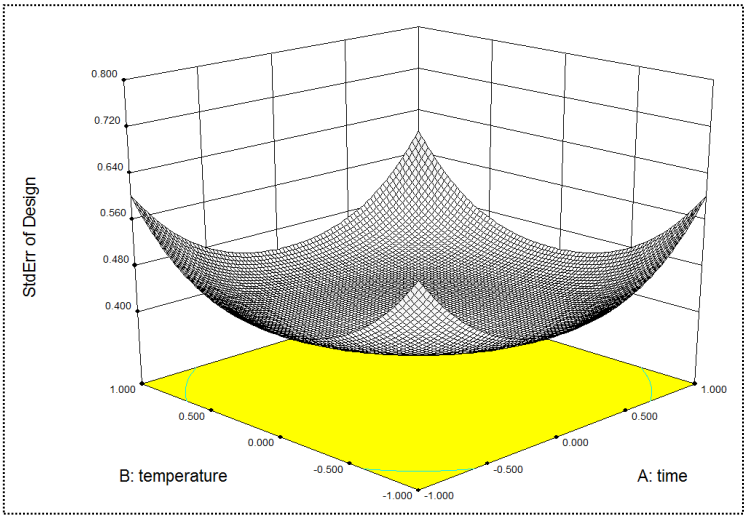
Contour plot of standard error with expanded axes, extrapolated area shaded

As shown in the key, shading begins at one-half standard deviation and increases linearly up to 1.5 times standard deviation. So long as you stay within specified factorial ranges (plus/minus 1), shading remains relatively light — beyond that the plot darkens. Be wary of predictions in these nether regions! Before leaving this sidebar exploration, go back to Graph Preferences and reset both axes to their defaults. Also, change factor back to their actual levels.

Now on the floating **Graphs Tool** click **3D Surface**.



3D view of standard error



3D plot of standard error

Notice the flat bottom in this bowl-shaped surface of standard error (this bottom plot was created by changing the Y-axis low to 0.4 and high to 0.8). That's very desirable for an RSM design. It doesn't get any better than this!