Multifactor RSM Tutorial
(Part 2 – Optimization)

Introduction

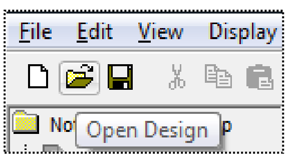
This tutorial shows how to use Design-Expert software for optimization experiments. It's based on the data from Multifactor RSM Tutorial Part 1. You should go back to that tutorial if you've not completed it.

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.

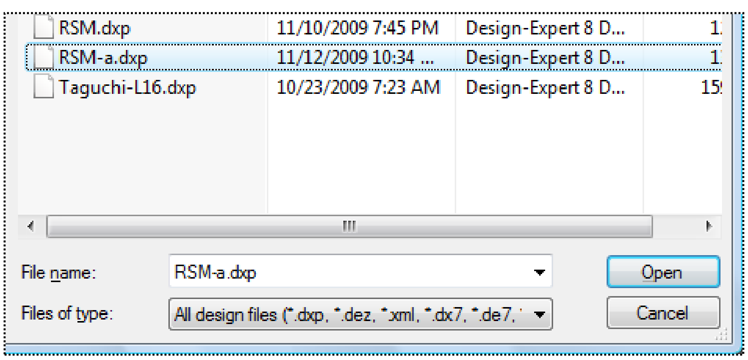
Start the program by finding and double clicking the Design-Expert icon.

You will find the case study data, with the responses already analyzed, stored in a file named **RSM-a.dxp**. Use the **File**, **Open Design** menu or open design icon to load the data file.



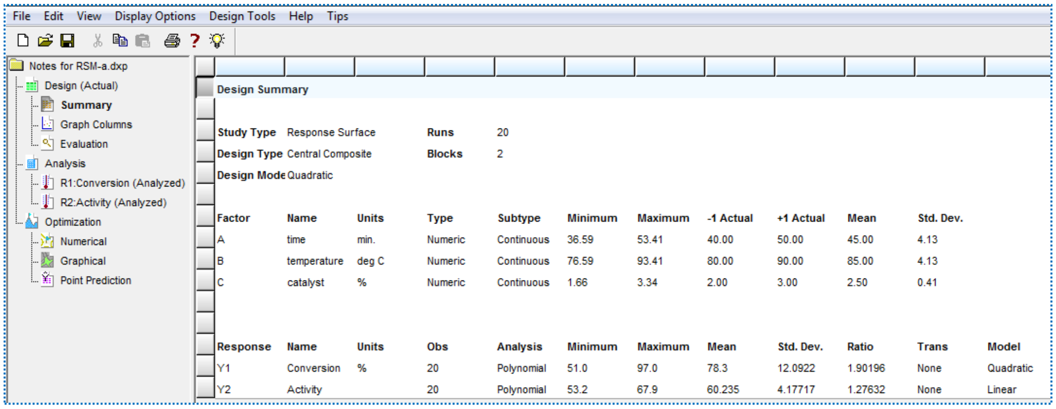
Open design icon

The standard file open dialog box appears.



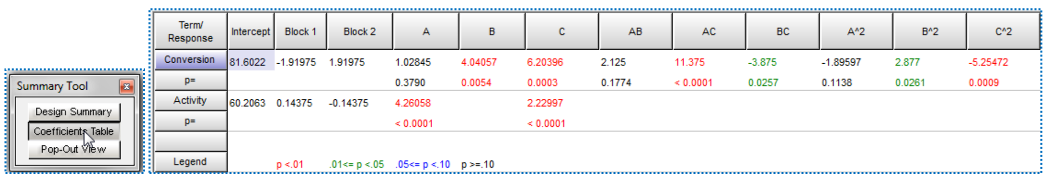
File Open dialog box

Once you have found the proper drive, directory and file name, click **Open** to load the data. To see a description of the file contents, click the **Summary** node under the Design branch at the left of your 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. 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

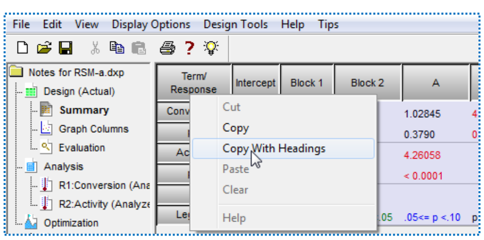
Click on the **Coefficients Table** button on the **Summary Tool** palette. This table provides a convenient comparison of the coefficients for all of the responses. It is done in terms of coded factors. Therefore, you can make inferences about the relative effects. For instance, notice that the coefficient 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.



Term/ Response	Intercept	Block 1	Block 2	A	B	C	AB	AC	BC	A^2	B^2	C^2
Conversion	81.6022	-1.91975	1.91975	1.02845	4.04057	6.20396	2.125	11.375	-3.875	-1.89597	2.877	-5.25472
p=				0.3790	0.0054	0.0003	0.1774	< 0.0001	0.0257	0.1138	0.0261	0.0009
Activity	60.2063	0.14375	-0.14375	4.26058		2.22997						
p=				< 0.0001		< 0.0001						
Legend		p <.01	.01<= p <.05	.05<= p <.10	p >=.10							

Coefficients Table

To copy this table for use in a report, <u>left-click</u> on the upper left header (Term/Response) to highlight the table, then <u>right-click</u> and choose **Copy With Headings** (shown below). Now, you can paste the table into your favorite word processing or spreadsheet program.



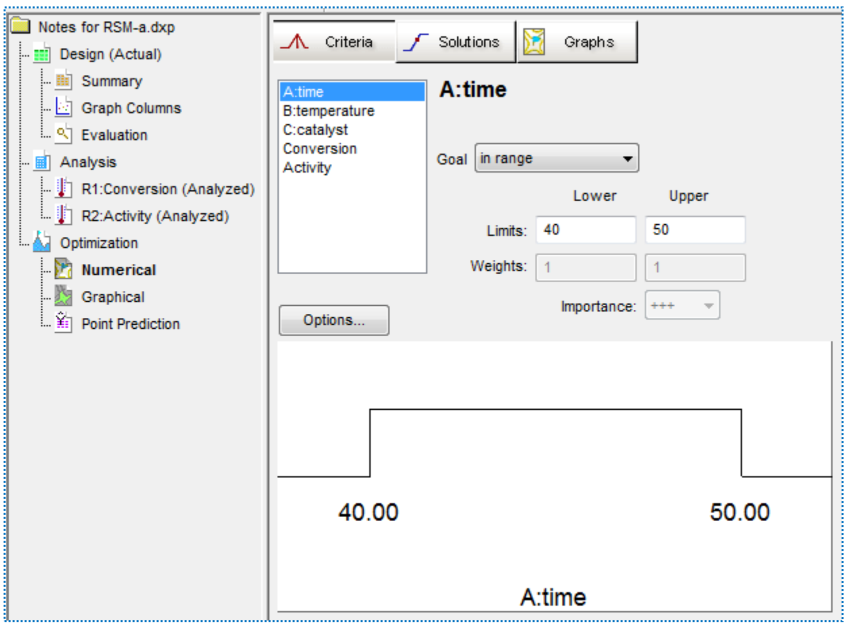
Copying the Coefficients Table

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.

We will lead you through the last case above – a multiple-response optimization. Under the Optimization branch to the left of the screen, click the **Numerical** node to start.



Setting numeric 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 study 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.

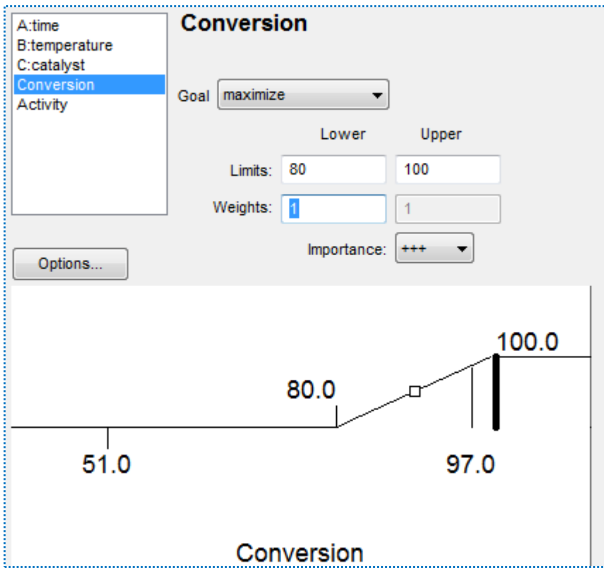
Now you get to the crucial phase of numerical optimization: assigning "Optimization Parameters." The program uses five possibilities as a "Goal" to construct desirability indices (d_i):

- 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.

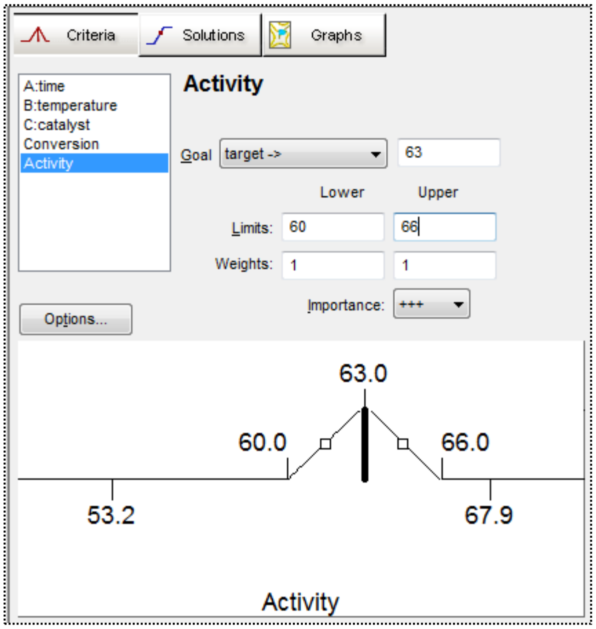
For this tutorial case study, assume you need to increase conversion. Click **Conversion** and set its **Goal** to **maximize**. As shown below, set **Lower Limit** to **80** (the lowest acceptable value, and **Upper Limit** to **100**, the theoretical high.



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.

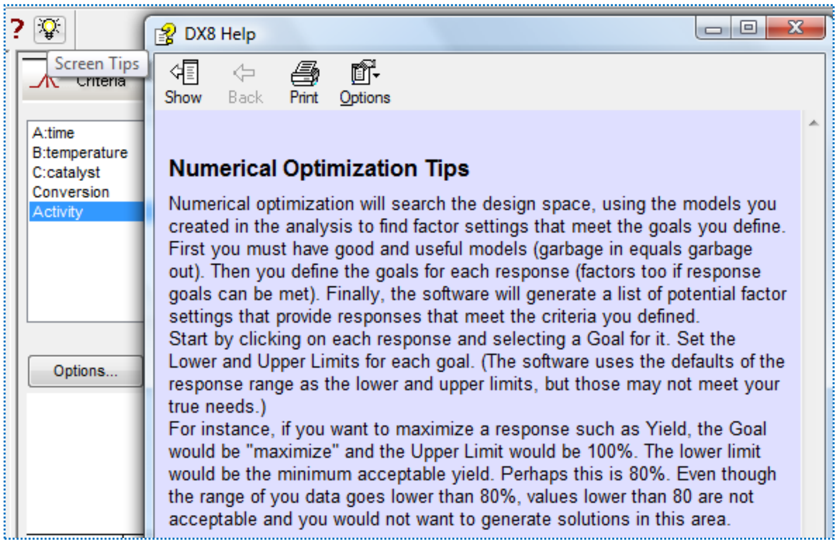


Activity criteria settings

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

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.

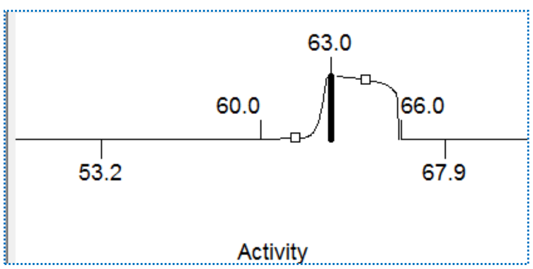


Screen tips

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. 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.

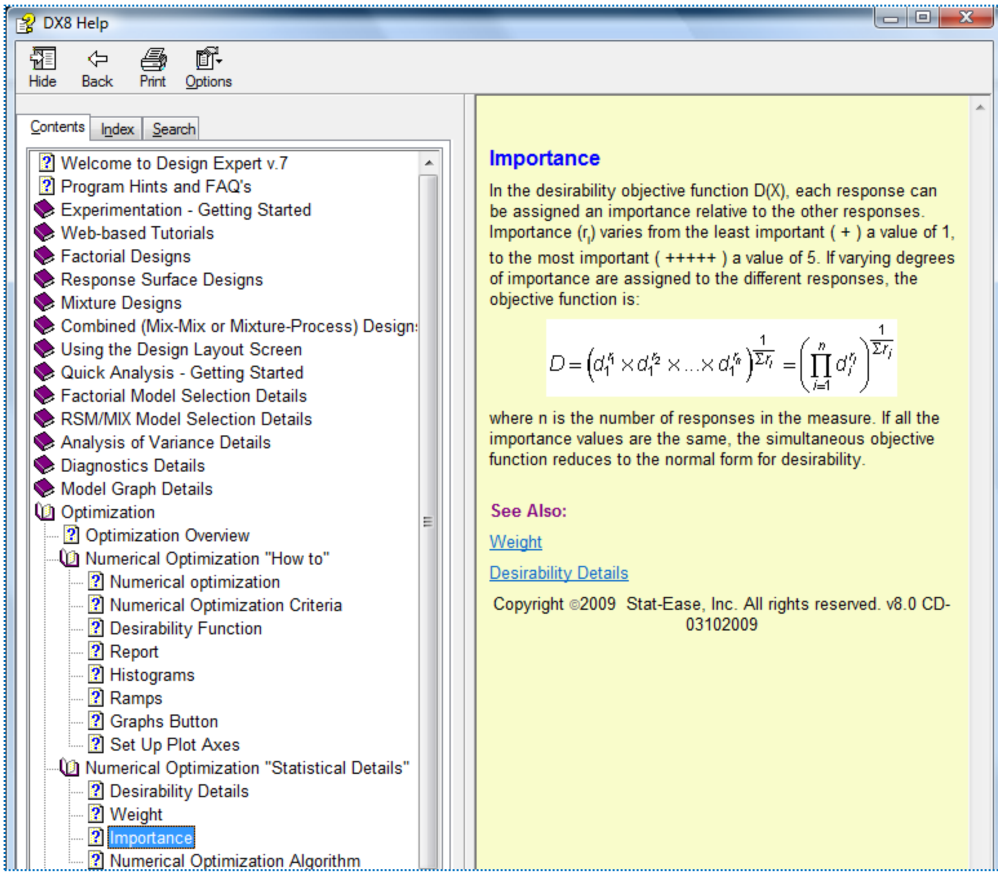


Weights change by grabbing handles with mouse

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.

For statistical details about how desirability functions are constructed – and formulas for weights and importance – select **Help, Topic Help** in the main menu. 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.

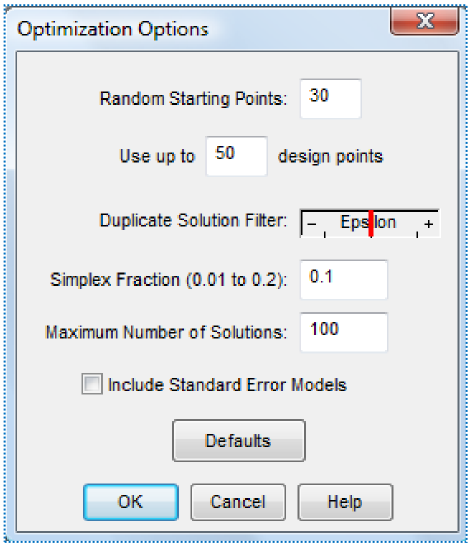


Details about optimization criterion "importance" found in program Help

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 learn how to gain control over how numerical optimization is performed. For example, you can change the number of cycles (searches) per optimization. If you have a very complex combination of response surfaces, increasing the number of cycles gives you more opportunities to find the optimal solution. Duplicate Solution Filter establishes the "epsilon" (minimum difference) for eliminating essentially identical solutions. Simplex Fraction specifies how big the initial steps are relative to factor ranges. ("Simplex" relates to search geometry. For two factors, the simplex is an equilateral triangle. By stepping through the three corners, Design-Expert calculates the path of steepest ascent. For details, go to Help and search "numerical search algorithm.")

Another optimization option, in addition to the random starting points, is to use those set by the design itself. However, these design points are limited to 50 unless you change this default. Leave this and all other options at their default levels shown below. (Note: This screen shot shows underlined letters – the Alt keys for jumping to fields via keystrokes.)

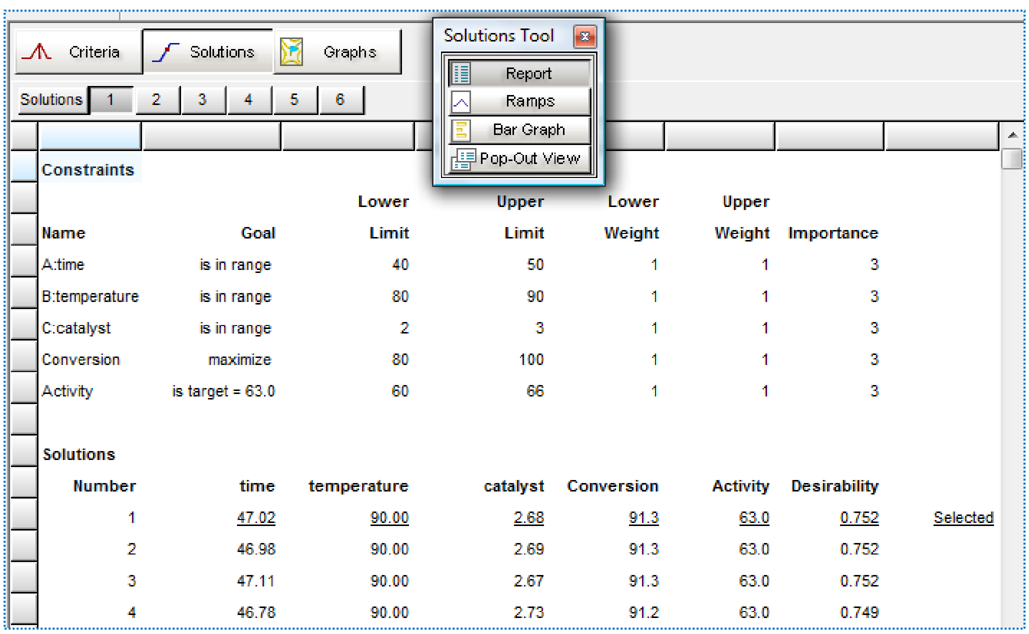
Click **OK** to close Optimization Options.



Optimization Options dialog box

Running the optimization

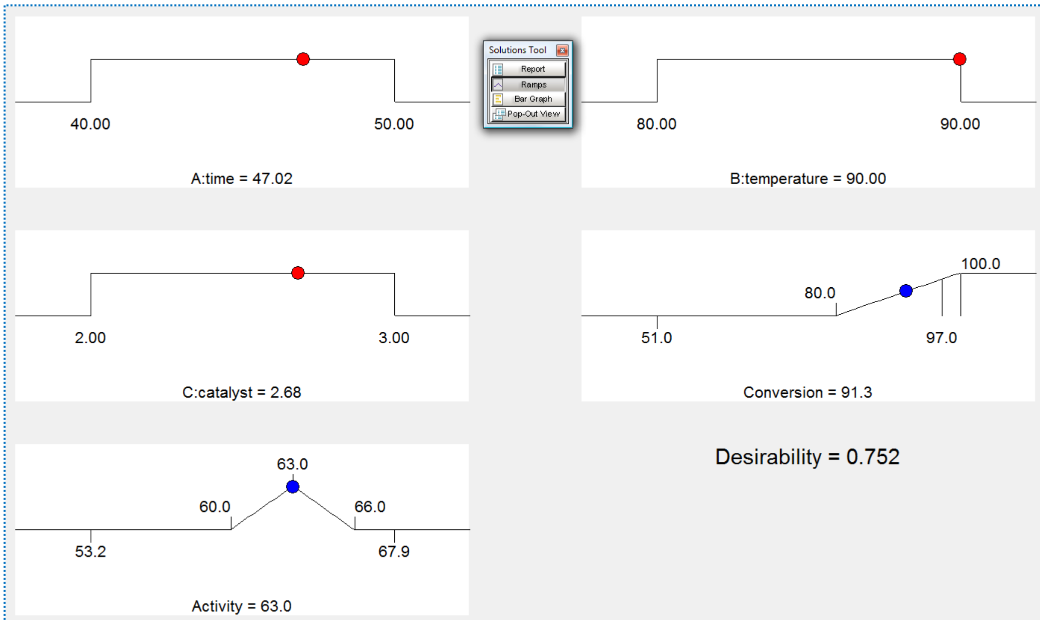
Start the optimization by clicking the ***Solutions*** button.



Numerical Optimization Report on Solutions (Your results may differ)

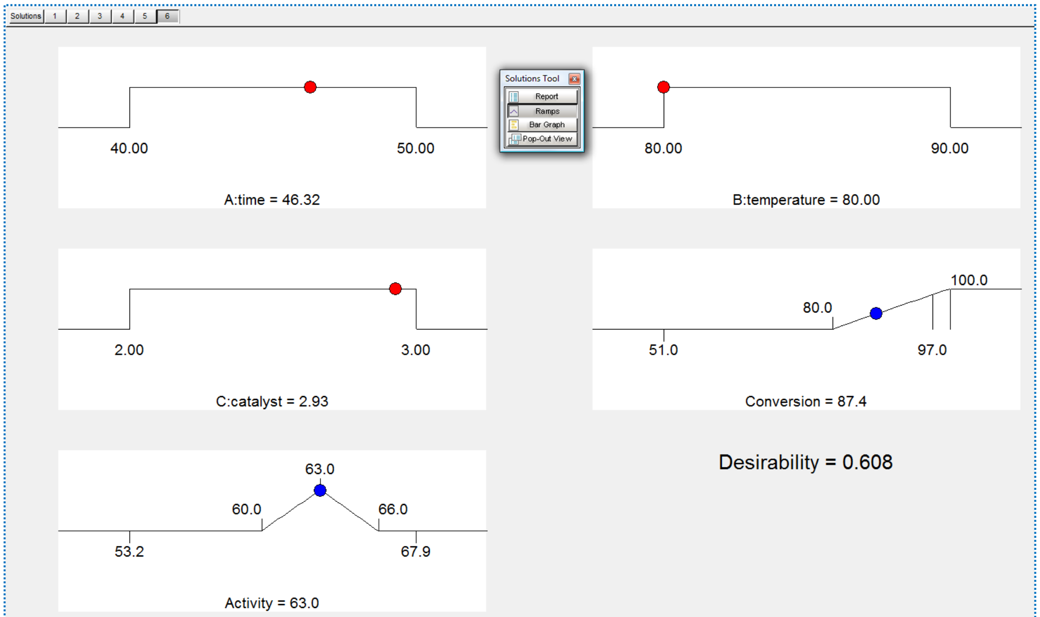
The program randomly picks a set of conditions from which to start its search for desirable results – your results may differ. Multiple cycles improve the odds of finding multiple local optimums, some of which are higher in desirability than others. After grinding through 39 cycles of optimization (30 chosen at random, plus 9 design points found within the factorial region of the central composite design), Design-Expert sorts the results for you in tabular form. Due to random starting conditions, your results are likely to be slightly different from those in the report above. Notice the last solution falls short of the first for conversion. There may be some duplicates in between. These passed through the filter discussed earlier. If you want to adjust the filter, go to the Options button and change the Duplicate Solutions Filter. If you move the Filter bar to the right you decrease the number of solutions shown. Likewise, moving the bar to the left increases the number of solutions.

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 **Ramps**.



Ramps report on numerical optimization

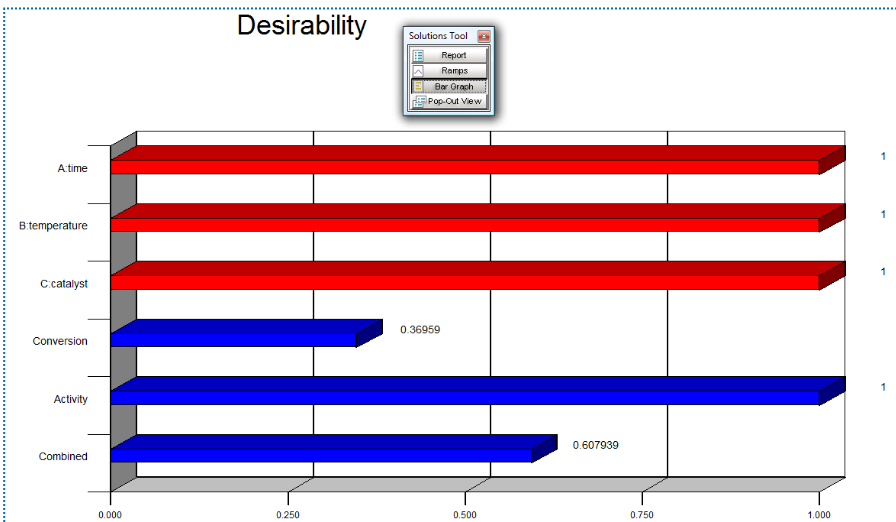
The ramp display combines individual graphs for easier interpretation. The colored dot on each ramp reflects the factor setting or response prediction for that solution. The height of the dot shows how desirable it is. Press the different solution buttons (1, 2, 3,…) and watch the dots. They may move 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.

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

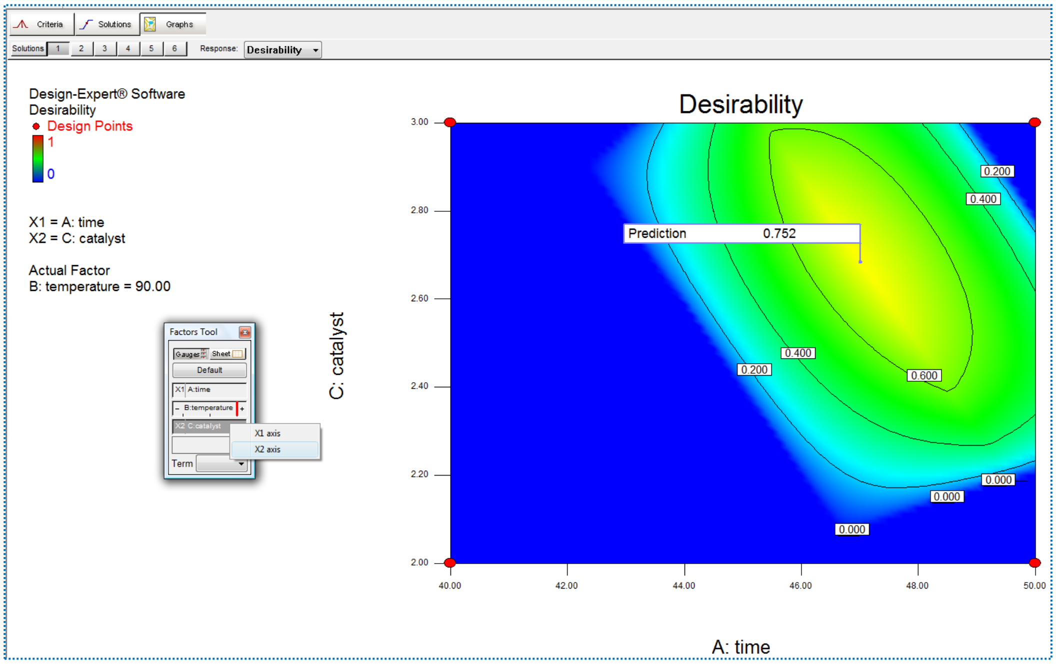


Solution to multiple response optimization - desirability bar graph

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

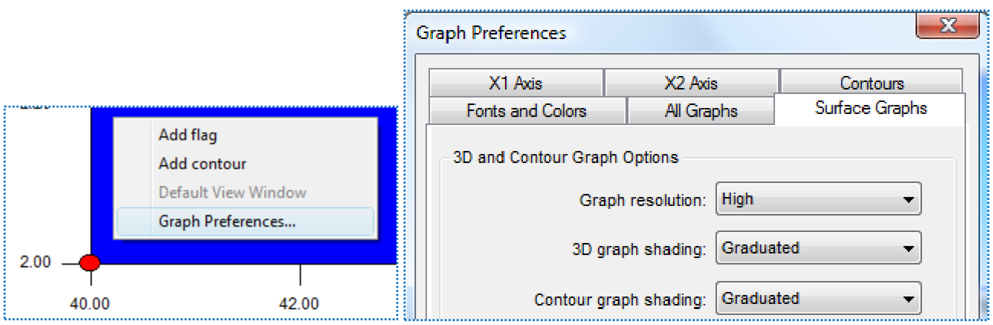
Optimization Graphs

Press ***Graphs*** near the top of your screen to view a contour graph of overall desirability. Click **Solutions** button **1**. On the **Factors Tool** palette, right-click **C:Catalyst**. Make it the **X2 axis**. Temperature then becomes a constant factor at 90 degrees.



Desirability graph (after changing X2 axis to factor C)

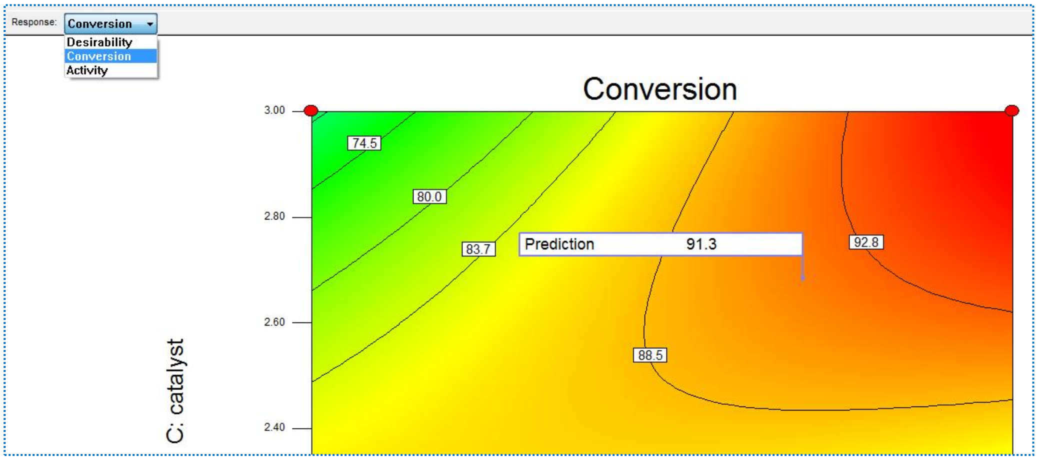
The screen shot above is a graph displaying graduated colors – cool blue for lower desirability and warm yellow for higher. If you just completed part 1 of this tutorial, your graph came up in only one color. This is easily fixed by <u>right-clicking over the graph</u> and selecting **Graph Preferences**.



Graph preferences via right-click menu – Selecting graduated (color) shading

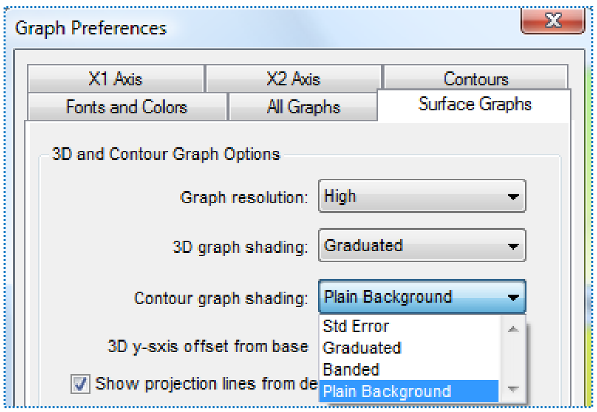
Click the **Surface Graphs** tab and set **Contour graph shading** to **Graduated**. Press **OK**.

Design-Expert software sets a flag at the optimal point. To view the responses associated with the desirability, select the desired **Response** from its droplist. Take a look at the **Conversion** plot.



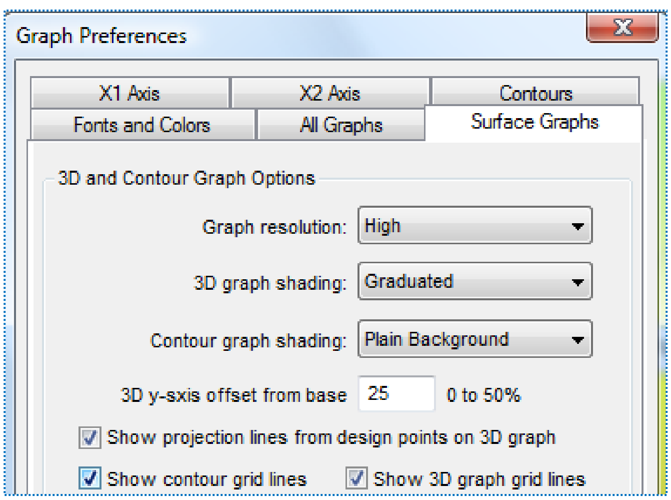
Conversion contour plot (with optimum flagged)

The colors are neat, but what if you must print the graphs in black and white? This is easily accomplished by right-clicking over the graph and selecting **Graph Preferences**. Click **Surface Graphs** and set **Contour graph shading** to **Plain Background**.



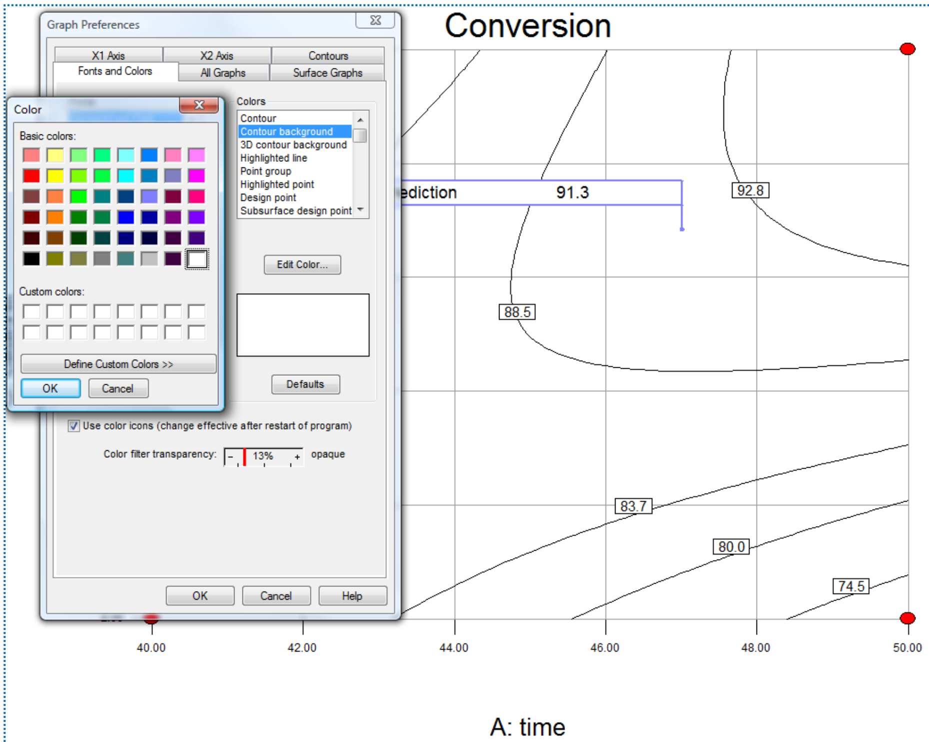
Graph preferences set to plain background

While you're at **Surface Graphs**, also click **Show contour grid lines**.



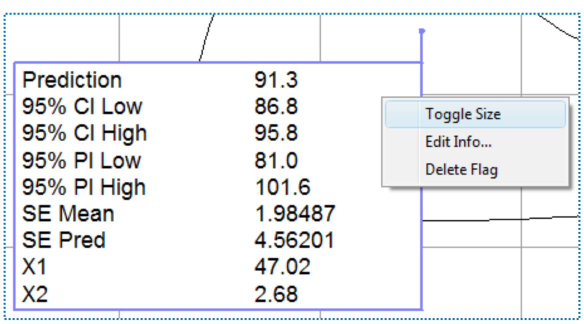
Show contour grid lines option

Finally, to make your graph really plain, click the **Fonts & Colors** tab; under **Colors** choose **Contour Background**, click **Edit Color.** Select white on the grid and press **OK**. Now press **OK** on **Graph Preferences.**



Graph changed to black and white with grid lines

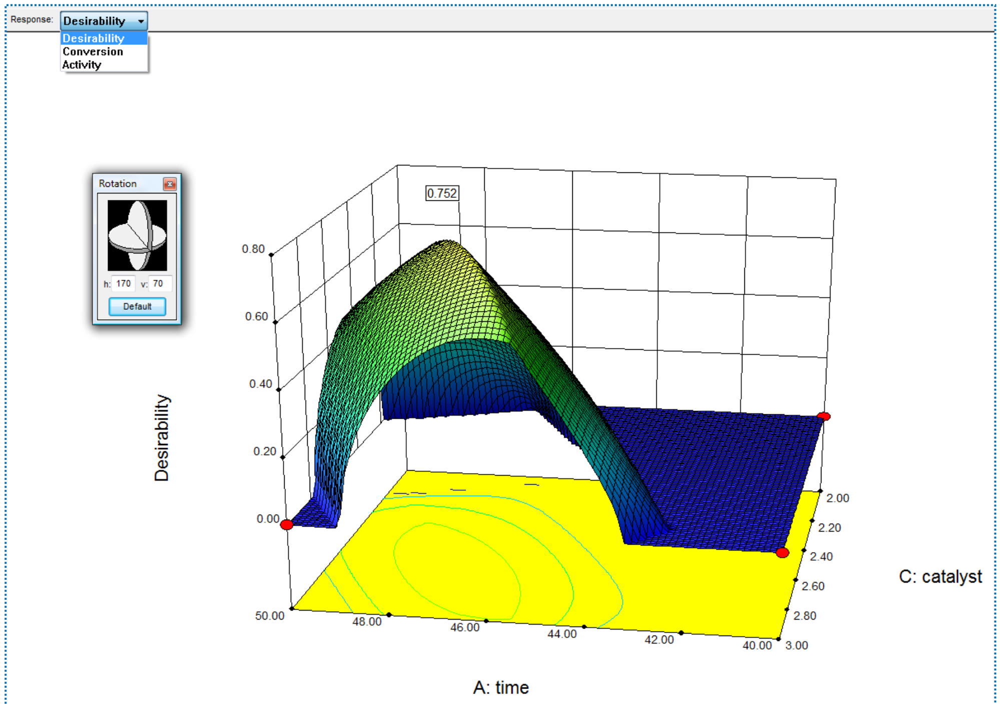
There are many other options on this and other Graph preferences tabs. Look them over if you like and then press **OK** to see what the options specified by this tutorial do for your contour plot. Grid lines help locate the optimum, but for a more precise locator right-click the flag and **Toggle Size** to see the coordinates plus many more predicted outcome details.



Flag size toggled to see more optimum conversion details

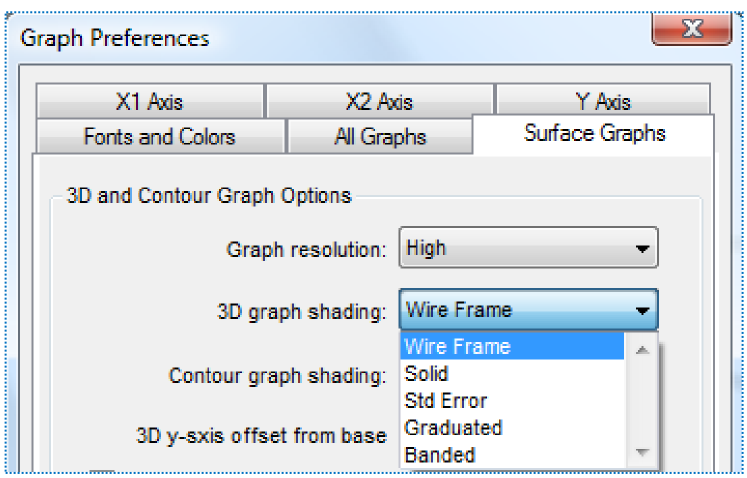
By returning to Toggle size, you can change back to the smaller flag. If you like, view optimal activity response as well.

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!



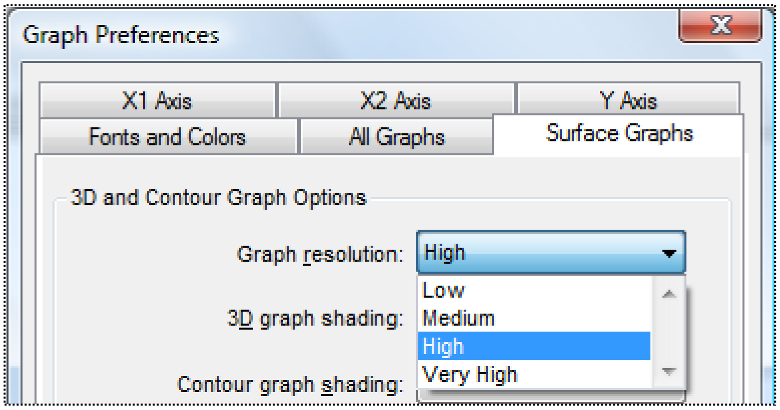
3D desirability plot

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. Go to the floating Factors Tool palette and move the slide bar on B: Temperature. How does this affect desirability? If you have a color printer attached, print a hard copy via File, Print. For black and white printing, right-click over your graph to re-summon **Graph preferences.** Select the **Surface Graphs** tab (if necessary) and change the **3D graph shading** option to **Wire Frame**.



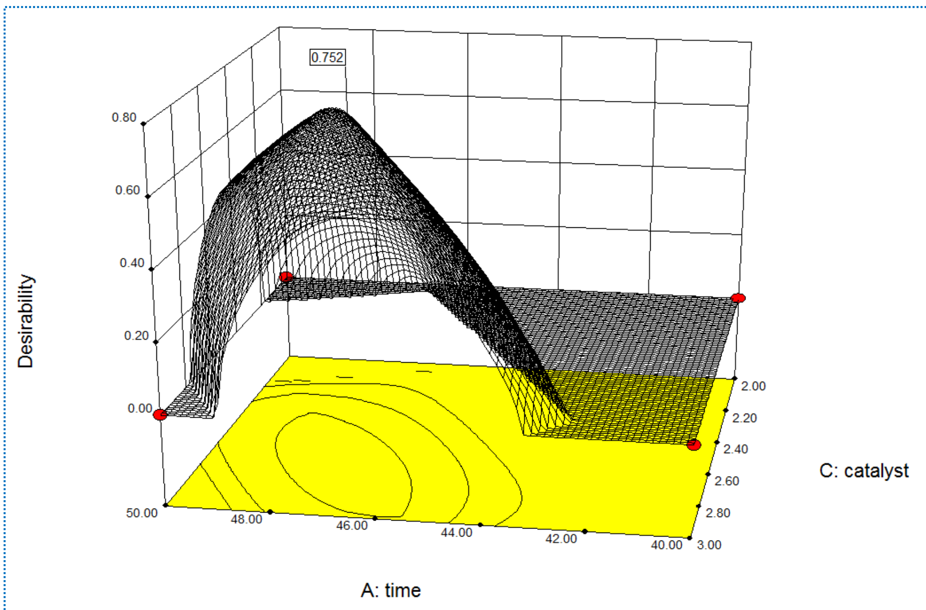
3D graph shading changed to wire frame (for black and white printing)

Before leaving this dialog box note that Design-Expert offers a very high 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.



Very high resolution available as an option

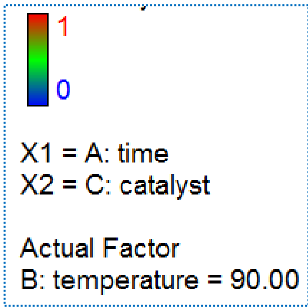
Press **OK** and see what you get. (To make the graph really plain – not shown here – go to **Graph Preferences,** click the **Fonts & Colors** tab; under **Colors** choose **3D Contour Background**, click **Edit Color.** Select white on the grid and press **OK**. Now press **OK** on **Graph Preferences.**)



Wire frame view of 3D desirability graph

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 right-clicking and selecting **Graph Preferences,** then pressing the **Default** buttons for **Fonts and Colors** (Colors side only), **All Graphs**, and **Surface Graphs**.

Before moving on to graphical optimization, here is a postscript on the chromatic shading options offered in the All Graphs dialog box – a very esoteric feature that you may be wondering about.



Trichromatic shading option

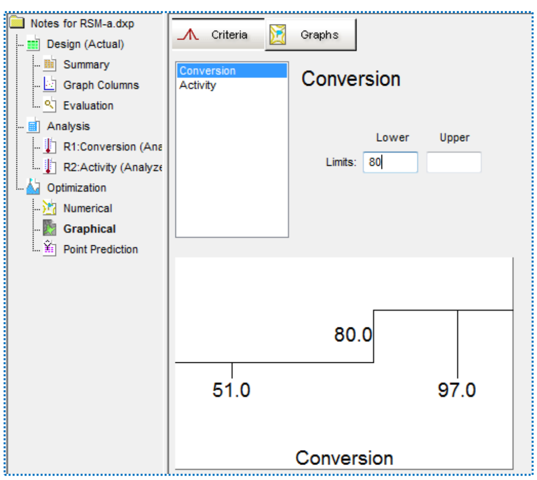
For your information, monochromatic ("mono") shading comes out flat like a gray scale, only instead of moving from black to white it changes from one color to another – the end colors are brighter and the middle ones darker. Dichromatic ("di") shading improves the appearance by using a midpoint color that has the maximum RGB values of both end colors. However, in order to get the full range of colors, you have to use a completely different third color for the midpoint, which is what trichromatic ("tri") shading does. The particular colors used (shading for Low, Middle, and High) can be selected from the Fonts & Colors tab under Colors (scroll down to see them). Feel free to mess around with these color options at this point, but if you are pressed for time, move on!

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:

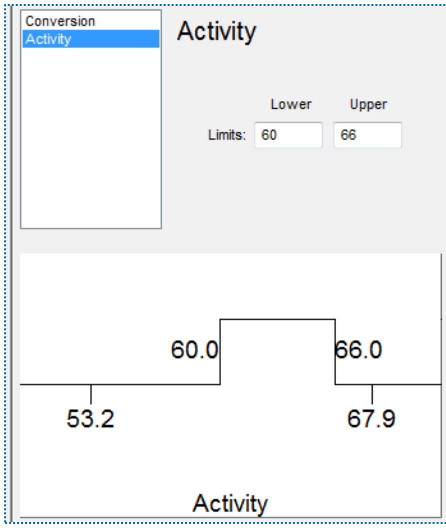
- 80 < Conversion
- 60 < Activity < 66

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

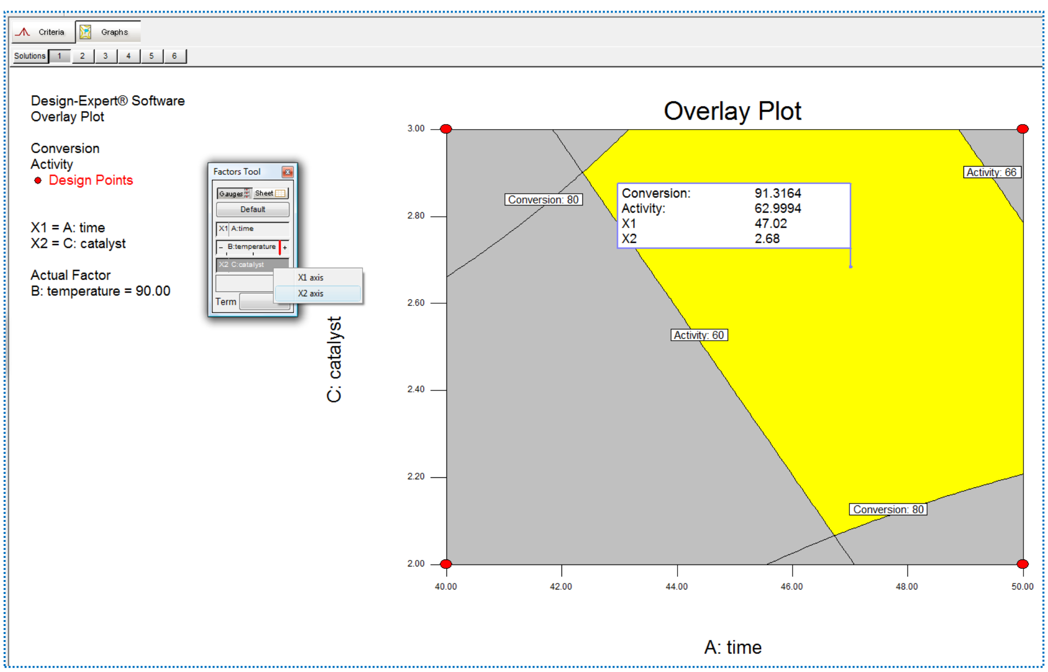
Click **Activity** response. If not already entered, type in **60** for the **Lower Limit** and **66** for the **Upper Limit**.



Activity limits

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." (If you still see the grid lines you added earlier, right-click over the graph, select Graph Preferences and go to the Surface Graphs tab. Uncheck Show contour grid lines to avoid cluttering the graph.)

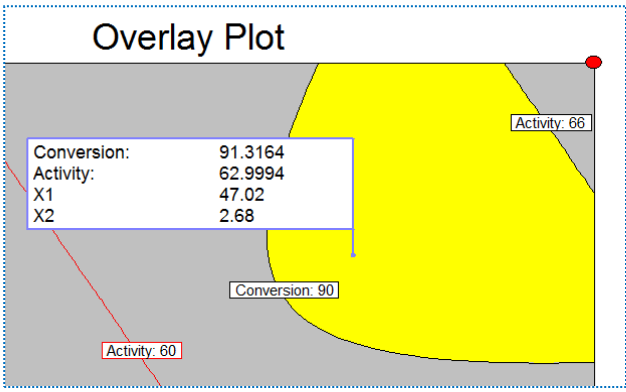
Now go to the **Factors Tool** palette and <u>right-click</u> **C:Catalyst**. Make it the **X2 axis**. Temperature then becomes a constant factor at 90 degrees as before for Solution 1.



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 not meet the selection criteria. The clear "window" shows where you can set factors that satisfy requirements for both responses. (If you are subject to FDA regulation and participate in their quality by design (QBD) initiative, this might be your "design space.") Lines marking high or low boundaries on the responses can be identified via a mouse-click. Notice that the contour and its label change color for easy identification.

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 of **90**. Then click the Activity 60 contour to see it more easily in the highlighted color.



Changing the conversion specification to 90 minimum

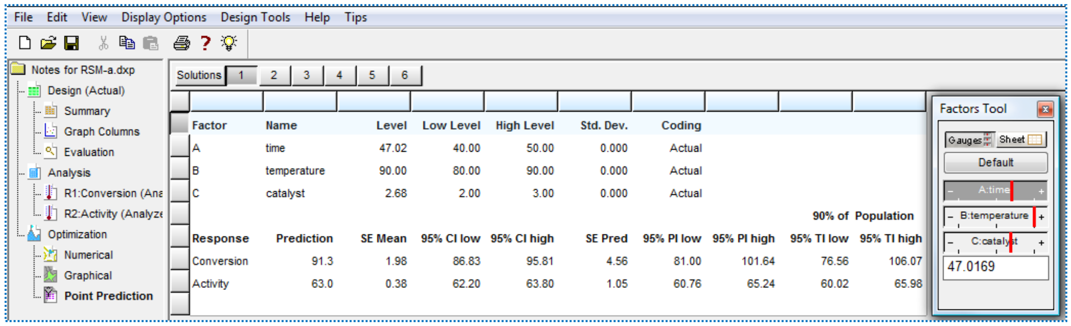
Caution: Having changed criteria, the flagged optimum is no longer valid. To get it right you would have to go back to the Numerical optimization option and enter any new response criteria there.

It appears that the more ambitious goal of 90 percent conversion is feasible. This requirement change would make the lower activity specification superfluous.

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 for presentation purposes.

Response Prediction at the Optimum

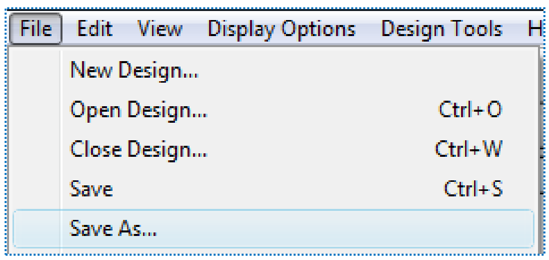
Click the **Point Prediction** node (left on your screen). Notice it now defaults to the first solution. (Be thankful Design-Expert programmers thought of this, because it saves you the trouble of dialing it up on the Factors Tool.)



Point prediction set to solution #1

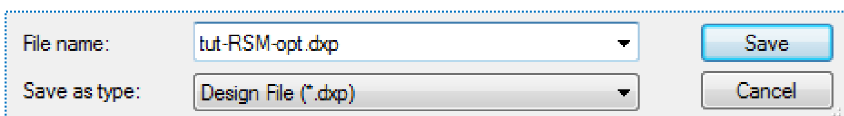
Save the Data to a File

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**.



Save As selection

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



File Save As dialog box

You will need this file in Part 3 of this series of tutorials.

Final Comments

We feel that numerical optimization provides powerful insights when combined with graphical analysis. Numerical optimization becomes essential when you investigate many factors with many responses. However, computerized optimization will not work very well in the absence of subject-matter knowledge. For example, a naive user may define impossible optimization criteria. The result will be 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 Response Surface optimization tutorial completes the basic introduction to doing RSM with Design-Expert software. Move on to the next tutorial on advanced topics for multifactor RSM for more detail on 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. Call us, send an annotated fax of output, write us a letter, or send us an e-mail. You will find our contact information and email links at www.statease.com.