Multiple Response Optimization using JMP®

Daniel J. Obermiller, The Dow Chemical Company, Midland, MI

Abstract
Typically in the analysis of industrial data there are many response variables (or physical characteristics of the end product) that are under investigation at the same time. Relationships between these responses are quite common, and the analyst must decide which responses are most important, usually at the expense of other responses. Fortunately, there are several techniques that have been developed to allow the simultaneous optimization of several responses. This paper briefly reviews some of the techniques developed for multi-response optimization. The paper also demonstrates several different ways in which JMP statistical software can solve the problem of optimizing multiple responses.

Introduction

Typically in the analysis of industrial data there are many response variables (or physical characteristics of the end product) that are under investigation at the same time. Relationships between these responses are quite common, and the analyst must decide which responses are most important, usually at the expense of other responses. By evaluating the responses, the analyst can then determine the set of operating conditions for making the product with the overall best response. This set of operating conditions is called the optimum condition for the process.

A wide range of multi-response optimization techniques, also sometimes called multicriteria decision making (MCDM) techniques, can be found in the literature. Two techniques: overlaying contour plots and desirability functions have stood the test of time due to their balance of ease of use and ability to locate an optimum. To demonstrate these two techniques in JMP, a subset of a pharmaceutical dataset published by Hendriks et al. (1992) will be used throughout this paper.

Example

A modified central composite design for three independent variables was used to study the optimization of a coating process of fine granules. The settings for the independent variables (temperature, spray rate of wax coating, and pressure of the atomization air) can be found in Table 1.

Temperature (A)	Spray Rate (B)	Pressure (C)
-1	-1	1
-1	-1	-1
-1	1	1
-1	1	-1
1	-1	1
1	-1	-1
1	1	1
1	1	-1
0	0	0
0	0	0
0	0	0
0	0	0
0	0	1
0	0	-1

Table 1: Modified Centered Central Composite Design

This design allows a second-order polynomial model to be used to describe each response. The form of the second-order polynomial models are

$$Y_i = b_0 + b_1{*}A + b_2{*}B + b_3{*}C + b_{12}{*}A{*}B + b_{13}{*}A{*}C + b_{23}{*}B{*}C + b_{33}{*}C^2.$$

The coefficients from all of these models can be found in Table 2.

Effect	Bulk Density	Particle Size	%age Drug
b_0	0.635	104.08	13.45
b_1	0.004	2.02	-0.02
b_2	-0.009	4.22	0.10
b_3	0.016	-10.64	-0.18
b_{12}	-0.009	-1.40	0.05
b_{13}	-0.001	2.30	0.08
b_{23}	0.001	-3.05	0.05
b_{33}	-0.003	12.44	-0.35

Table 2: Model Coefficients

Overlaying Contour Plots

Perhaps the first method developed for optimizing multiple responses was to overlay contour plots.

For each response, generate a contour plot based on the model. In JMP this can be accomplished by designating each main effect in the model (the A, B, and C terms) as Response Surface Effects (see Figure 1).

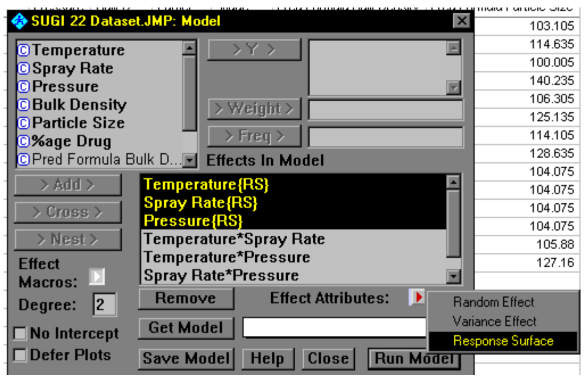


Figure 1

When the model is fit, a Response Surface button appears that allows the plotting of a contour plot. When you see the contour plot, copy and paste the graph into a graphics package or print it on a transparency. Follow these same steps for each response. Then either overlay the transparencies or overlay the plots in the graphics package so that the contours can show through.

The more responses being examined, the busier the overlaid contour plot becomes. For this reason, only a maximum and a minimum contour are typically drawn for each response. This minimizes the clutter and makes the overlaid contour plot easier to interpret.

For our example, contour plots for each response were created with the temperature variable held at 0. The individual contour plots are shown in Figures 2-4. Suppose for this process, we needed bulk density greater than 0.645, particle sizes under 105, and the drug percentage to be over 13. The overlaid contour plot is shown in Figure 5 with an optimum area shaded.

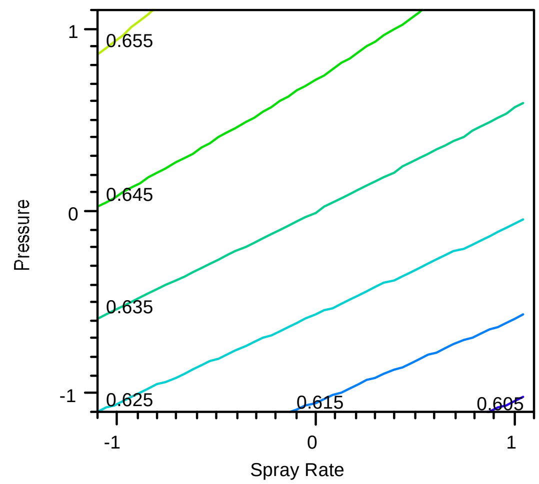


Figure 2: Bulk Density Contour Plot

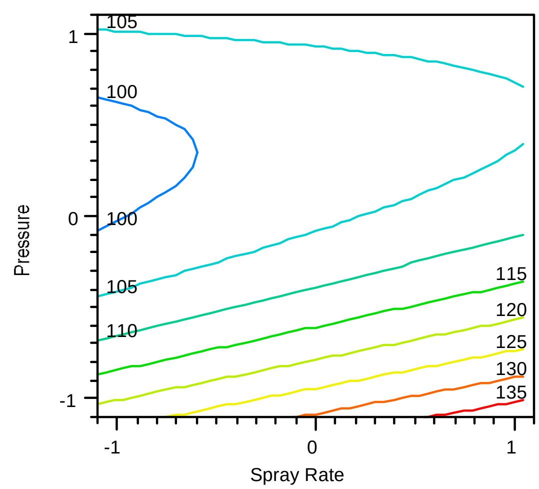


Figure 3: Particle Size Contour Plot

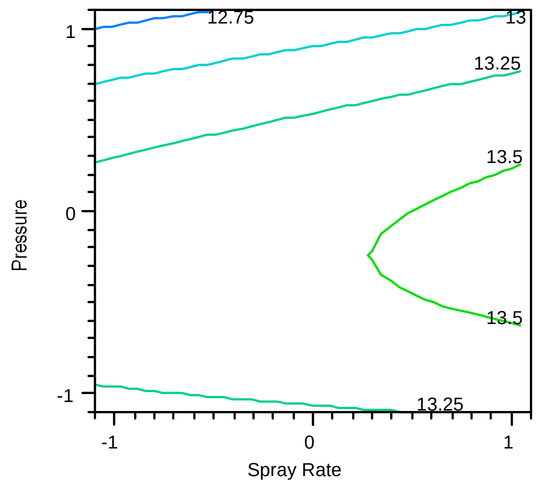


Figure 4: %age Drug Contour Plot

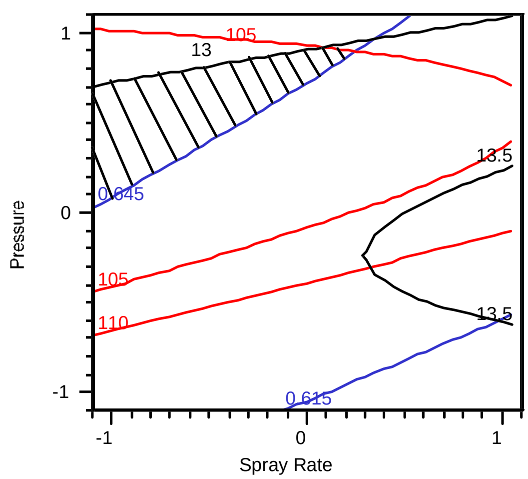


Figure 5: Overlaid Contour Plots.
Optimum Area Shaded

For the overlaid contour plots, the picture may not show the optimum if there are more than 2 independent variables. Any independent variable that is not on the axes of the plot must be held at some value. For this example, the temperature was held at 0.

Overlaid Contour Plots: Another Way

The first method presented for overlaying contour plots requires another software package to do the overlaying or requires the stacking of transparencies. However, JMP offers this functionality within the package as well.

When fitting the model, enter the model to be fit as usual, choose the screening personality and enter ALL of the responses into the response window (Figure 6).

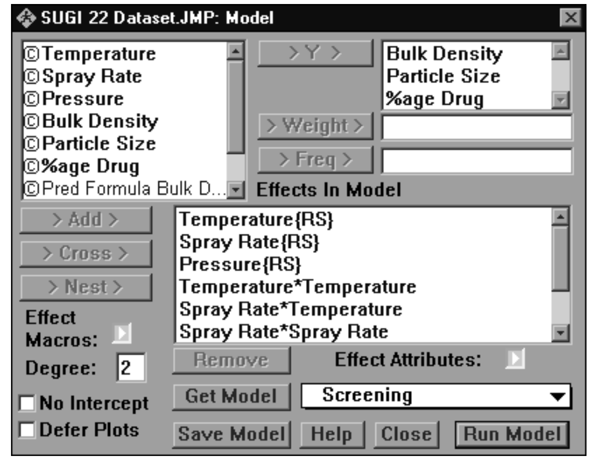


Figure 6: Fit Model Dialog for Overlaying Contours

From the analysis window, choose the checkmark (✓) and select Contour Profiler (Figure 7).

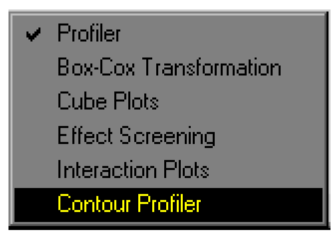


Figure 7: Contour Profiler Choice

The contour profiler will create an overlaid contour plot. This plot will use one contour line for each response. Small dots are placed on one side of the contour line to indicate the direction of a higher response. The contour profiler makes it easier to change settings of any independent variables that cannot be shown on the plot as well as shading out regions of the contour plot that are not wanted.

To change which variables appear on the plot, just check the variables that you want on the horizontal and vertical axes, respectively. Clicking inside the contour plot area will move the "crosshair" which indicates different settings for the independent variables displayed on the plot. For any of the independent variables, especially the one that is not on the plot, you can drag the variable's slider to change the current setting. Alternatively, you can click on the number labeled Current X and type in the desired setting.

There are also a number of options in the response area of this window. The column labeled Contour indicates where the contour line is currently drawn. You can click on the number and type in a desired contour level. To shade out particular regions for each response you can type in a Lo Limit and/or a Hi Limit. Once these numbers are entered, JMP will automatically shade the regions that are not desired. Also notice the slider for the responses has a red circle indicating the predicted response for the current settings of the independent variables. The vertical bar in the slider area represents where the current contour line is drawn.

The previous example is completed using the contour profiler. In this case, the unshaded region shows where the best response is while the "crosshair" on the graph represents the current settings for the independent variables that are shown on the plot (Figure 8).

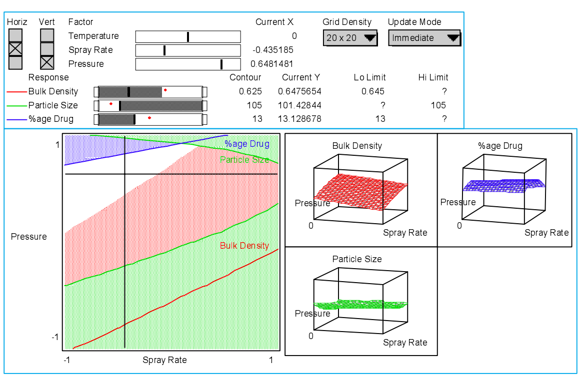


Figure 8: Contour Profiler Output

The contour profiler allows the analyst to make an overlaid contour plot much easier as well as allowing much better exploration of the various response surfaces which are being optimized.

Desirability Function

The second method of multi-response optimization that will be discussed is the desirability function (Harrington, 1965). The desirability function is a transformation of the response variable to a 0 to 1 scale. This transformed response, called d_i, can have many different shapes. Regardless of the shape, a response of 0 represents a completely undesirable response and 1 represents the most desirable response. Creating these desirability functions requires some prior knowledge from the analyst since the shape can be extremely flexible.

In order to simultaneously optimize several responses, each of these d_i are combined using the geometric mean to create the overall desirability (D).

$$D = \sqrt[n]{(d_1 * d_2 * d_3 * \ldots * d_n)}$$

Using the product of the desirability functions insures that if any single desirability is 0 (undesirable), the overall desirability is 0. Thus, the simultaneous optimization of several responses has been reduced to optimizing a single response: the overall desirability, D.

The desirability function has been incorporated into JMP. When fitting the model, be sure to enter all of the responses as the Y's and choose the screening personality. *JMP will fit all of the responses with the same model* (a way around this will be demonstrated later). Under the prediction profile option button, choose Desirability Functions. This will add another row and column to your prediction profile (Figure 9).

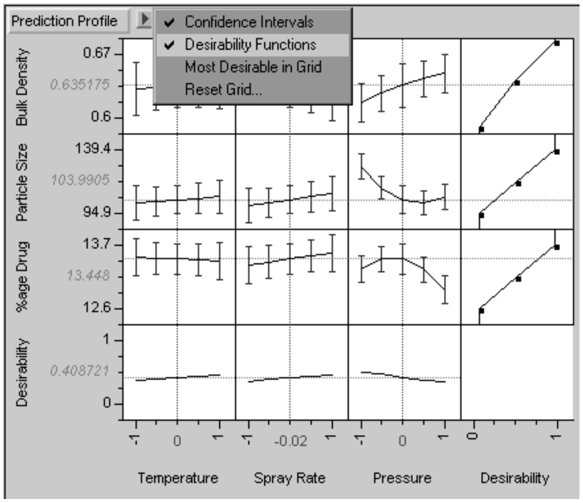


Figure 9: Desirability Option

The right-most column allows the user to specify the desirability function for each response (d_i). JMP allows a piece-wise linear model for the desirability function. The analyst can drag any of the 3 data points to get the shape of the function that is desired, recalling that a desirability of 1 is most desirable. Using an Alt-Click on the graph will bring up a dialog for more precise movement of the points. Table 3 shows some common shapes for the individual desirability functions. Remember that in JMP, the desirability scale is along the X-axis while the response is along the Y-axis.

Now by choosing the operating conditions that achieve the maximum overall desirability (shown in the last row), the analyst has optimized all the responses simultaneously. Alternatively, rather than searching for the maximum overall desirability, the user can simply choose the Most Desirable in Grid option from the pop-up menu. JMP will then find the operating conditions with the highest desirability using the grid of points that has been defined (default of 5 points per independent variable).

One of the problems associated with the desirability function is that each response is weighted equally. Although the overall desirability formula can be revised to allow different weights, JMP cannot do this automatically. One way around this is to put the more heavily weighted response in as a Y variable more than once until you get the weighting that you desire. Other weighting methods are proposed by Derringer and Suich (1980) and DelCastillo, Montgomery, and McCarville (1996).

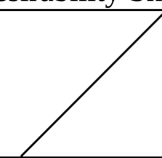
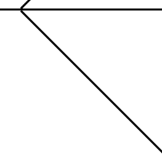
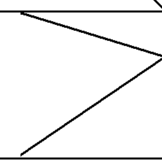
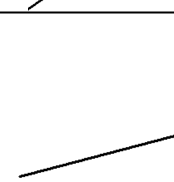
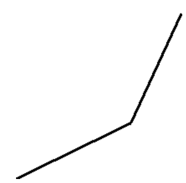
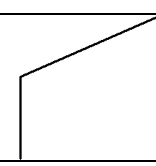
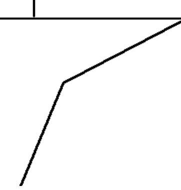
To get:	Desirability Shape:
Maximize (higher is better)	
Minimize (lower is better)	
Target (Specific value is best)	
Maximum Plateau (Improved product to a point, beyond that point is not important)	
Maximum Diminishing Return (Improved product to a point, after that point improvement is seen, but not as steeply.)	
Minimum Plateau (No value up to a point)	
Minimum Diminishing Return (Slow improvement up to a point, then rapid improvement)	 Improved Desirability→

Table 3: Some Desirability Function Shapes

Separate Models

So far the problem of multi-response optimization in JMP has been handled by using the exact same model form for each response. In many real-world applications, the analyst does not want the same model for each response.

Even in this situation, JMP can still be used to optimize all of the responses. The steps are as follows.

1. Create a model for the first response using the Standard Least Squares personality.
2. Using the $, choose to Save Prediction Formula.
3. Repeat steps 1 and 2 for each response.
4. Fit an overall model (a model such that each individual response model is a subset of this overall model) with the Screening personality, specifying the prediction formulas from step 2 as the responses.
5. Ignore all of the model fitting results, but use the contour profiler or the desirability functions as before.

A good example to use is the tire tread experiment from Derringer and Suich (1980). This experiment consisted of a central composite design for three factors (hydrated silica level, silane coupling level, and sulfur level). Four responses were measured: PICO Abrasion Index, 200 percent Modulus, Elongation at break, and Hardness. The objective was to maximize the Abrasion and Modulus, while trying to achieve targets of 500 and 67.5 for the Elongation and Hardness respectively.

Because this design is a central composite design, a second order polynomial can be fit. Following steps 1 and 2 above, each response was fit separately, and variables that were not statistically significant were removed. Table 4 summarizes these reduced models.

Term	Abrasion	Modulus	Elongation	Hardness
A: Silica	X	X	X	X
B: Silane	X	X	X	X
C: Sulfur	X	X	X	X
A*B				X
A*C	X			
B*C	X			
A^2				X
B^2			X	
C^2		X		

Table 4: Statistically significant terms from Model Fitting

The fourth step was to fit an "overall" model, a model such that each individual model is a subset of this overall model. For this example, fitting the full second order polynomial would be the "overall" model since all individual models started with that form. Thus, the "overall" model is:

$$Y = \beta_0 + \beta_1 {*} A + \beta_2 {*} B + \beta_3 {*} C + \beta_{12} {*} A {*} B + \beta_{13} {*} A {*} C + \beta_{23} {*} B {*} C + \beta_{11} {*} A^2 + \beta_{22} {*} B^2 + \beta_{33} {*} C^2$$

Fitting this model with all responses and choosing the screening personality will allow you to optimize all four responses, with separate models, simultaneously. Remember that all statistics for this overall model should be ignored. All of the fits will be perfect. However, you can optimize these four distinct models using either the contour profiler or the desirability functions. The setup for the desirability functions for this problem is shown in Figure 10. Notice that the "optimum" found by the desirability function does not attain the target values for the elongation and hardness.

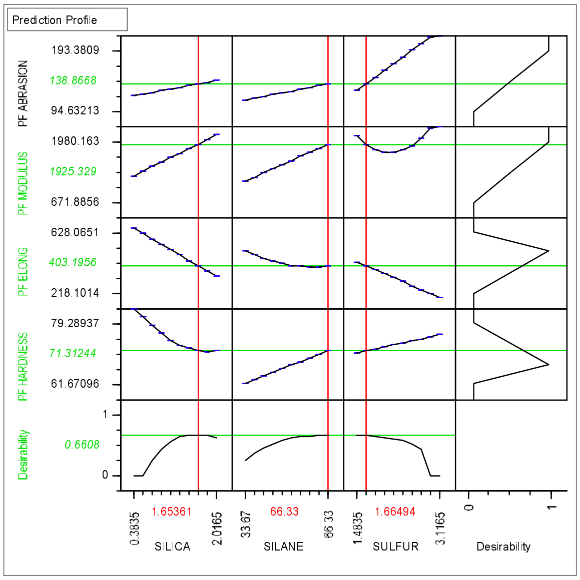


Figure 10: Multiple Response Desirability with Separate Models

Using the Contour Profiler for this same example will yield the results shown in Figure 11.

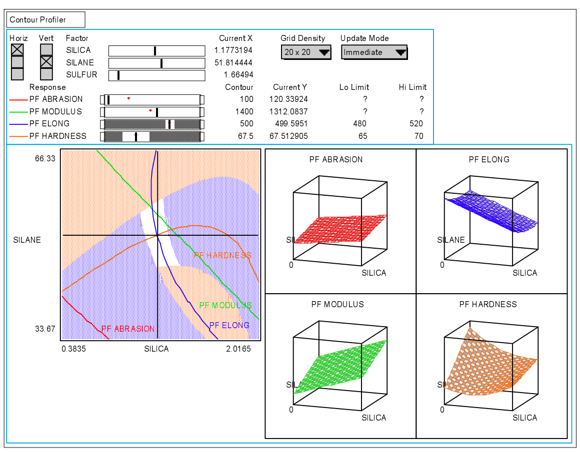


Figure 11: Contour Profiling with Separate Models

Conclusion

The analysis of industrial data often involves the optimization of many response variables. However, relationships between these responses are quite common, and the analyst must decide which responses are most important, usually at the expense of other responses. This paper has demonstrated features in JMP that allow the simultaneous optimization of several responses. JMP also has features that allow the analyst to visually inspect the relationships between the responses as well as the response surfaces.

References

Del Castillo, E.; Montgomery, D. C.; and McCarville, D. R. (1996). "Modified Desirability Functions for Multiresponse Optimization." *Journal of Quality Technology*. Volume 28, No. 3, pp. 337-345.

Derringer, G. and Suich, R. (1980). "Simultaneous Optimization of Several Response Variables." *Journal of Quality Technology*. Volume 12, No. 4, pp. 214-219.

Harrington, Jr. E. C. (1965). "The Desirability Function." *Industrial Quality Control*, Volume 21, No. 10, pp. 494-498.

Hendriks, M. M. W. B.; de Boer, J. H.; Smilde, A. K.; and Doornbos, D. A. (1992). "Multicriteria Decision Making." *Chemometrics and Intelligent Laboratory Systems*, Volume 16, No. 3, pp. 175-191.

Khuri, A. I. And Conlon, M. (1981). "Simultaneous Optimization of Multiple Responses Represented by Polynomial Regression Functions." *Technometrics*, Volume 23, No. 4, pp. 363-383.

Sall, John. "Contour Profiling to Optimize Multiple Responses Across Multiple Factors."

SAS Institute, Inc. (1995). *JMP User's Guide*, Cary, NC.

SAS Institute, Inc. (1995). *JMP Statistics and Graphics Guide*, Cary, NC.

Acknowledgments

I would like to thank Jeff Sweeney of Dow Chemical for his comments and help in preparing this paper.

Dan Obermiller may be reached through the internet at djobermiller@dow.com or by mail at The Dow Chemical Company, 1776 Building, Midland, MI 48674. Phone 517-636-1000. Fax 517-638-9707.