RESPONSE SURFACE OPTIMIZATION USING JMP® SOFTWARE

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ABSTRACT

Response Surface Methodology (RSM) is a sequential form of experimentation used to help predict or optimize response (dependent, outcome) variables made up of a mathematical-statistical model of several input (independent, predictor) factors.

This paper will review the RSM strategy, demonstrate the use of JMP® Software to construct the experimental design matrix (or layout of treatment combinations), and analyze results to two applications. One application involves optimizing a single response to a bag-sealing problem. The other application involves the simultaneous optimization of dual responses that have "larger-the-better" and "target-the-best" objectives. The combined experimental design, analysis, and data visualization features of JMP® assist the process engineer, quality analyst, or statistician's selection of the most appropriate levels of input factors that will optimize responses.

INTRODUCTION

Response Surface Methodology (RSM), introduced by Box and Wilson (1951), is a collection of techniques that were developed as a means to find optimal settings of input (predictor, independent) factors or design variables that maximize, minimize, or target measured responses or outcome variables.

The mathematical representations of RSM Models are the following:

first-order (linear) model without interaction/cross-product terms:

$$Y(x) = b_0 + \sum_{i=1}^{k} b_i x_i + e \qquad [1];$$

the first-order (linear) model with interaction/cross-product terms

$$Y(x) = b_0 + \sum_{i=1}^{k} b_i x_i + \sum_{j=2}^{k}\sum_{i=1}^{j-1} b_{ij} x_i x_j + e \quad [2];$$

the second-order (quadratic) model

$$Y(x) = b_0 + \sum_{i=1}^{k} b_i x_i + \sum_{j=2}^{k}\sum_{i=1}^{j-1} b_{ij} x_i x_j + \sum_{i=1}^{k} b_{ii} x^2 + e \qquad [3].$$

Cornell (1990, pp. 39-40) indicated that models can be fitted with RSM to: (I) Screen for the most important factors influencing the response (Most screening designs stop at this point); (ii) Find the region of the factor space that can be approximated reasonably well by the RSM model (This is sometimes referred to as parsimonious empirical model building); (iii) Obtain an initial approximation of the surface in as simple a model as possible to hold the time and costs of experimentation to a minimum; (iv) Develop a sequential procedure that attempts to locate more desirable values of the response.

Box and Draper (1975) listed 14 design properties of RSM. Cornell (1990, pp. 39-40) cited seven of these key properties as: (i) produce satisfactory distributions of information throughout the region of interest; (ii) ensure the predicted responses of the fitted model closely approximate the "true" response values; (iii) closely fit the model to the data; (iv) provide the ability to perform the experiment in blocks; (v) build RSM models in increasing order sequentially, from first-order up to second-order (or higher-order) models; (vi) provide internal estimates of error variance (or standard deviation); and (vii) ensure simple calculation of parameter coefficients.

DISADVANTAGES OF OTHER EXPERIMENTAL DESIGNS VS. ADVANTAGES OF RSM MODELS

Screening designs have the objective of finding the "vital few" number of factors (from a larger set of possible candidates) believed to affect the outcome response variables of interest. Their drawback is that they do not tell the best values of the key factors that will produce the desired responses.

Plackett-Burman (P-B) designs are among the commonly used screening designs. Two disadvantages of (P-B) designs are: First, P-B designs are Resolution III, meaning that some main effects are confounded with certain two-factor interactions. This results in biased estimates of some main effects, unless they are augmented by additional runs to raise the Resolution, remove the confounding and allow enough degrees of freedom for experimental error. The second disadvantage of

screening designs is that they do not have enough runs to detect important effects (see Lucas, 1994).

Orthogonal Arrays (OA) are part of Taguchi's robust tolerance design strategy. OAs attempt to find optimum values for the response, but they confine the optimum within the regions of the factor settings. They tend to add more cost because more experimental trials are needed to find the optimum outside the experimental region. OAs do not easily find the optimum whenever more than one response variable is involved, especially when the objectives for the responses conflict. For instance, one objective maximizes the response while the other objective minimizes or has target-the-best responses. OAs do not guide what direction to take to achieve desired response levels beyond those considered in the regions of the input factors tested. To get this direction, investigators must rely on subject matter or engineering expertise.

Schmidt and Launsby (1991) listed major weaknesses of Taguchi and the One-Factor-At-a-Time (OFAT) approaches as follows: (i) they use excessive amounts of resources; (ii) the results are confined to the factor ranges tested in the experiment; and (iii) they offer no efficient means of searching the direction of the optimum response outside the localized experimental region of the factor ranges.

Lucas (1994) pointed out ways that RSM could produce Taguchi analyses. Yet he showed how certain classes of RSM designs were more efficient and economical than Taguchi's Inner and Outer Arrays. Furthermore, Taguchi's methods lack provisions for examining goodness-of-fit. Also, no settlement has been reached over the controversy of how to handle interactions that were argued by the statistical community and Taguchi advocates.

Lawson and Madrigal (1994) also pointed out that RSM models were as efficient in optimizing the relationship between input design factors and outcome preformance characteristics as other optimizing techniques such as nonlinear optimization, dynamic programming, and Monte Carlo simulation.

RSM provides an additional advantage because the investigator has the ability to select input values that move closer to the direction of the desirable outcome response values.

KINDS OF RSM MODELS (FIRST-ORDER LINEAR AND SECOND-ORDER BOX-BEHNKEN & CENTRAL COMPOSITE)

The most common RSM models are the Central Composite Design (CCD) and Box-Behnken (B-B) designs. CCD, Box-Wilson (1951), combine two-level

fractional factorials (vertex corners of cubes) with Center and Axial points. Center points are set to the zero (mid-range) for all factor values. Axial points are determined such that all but one factor value is set to zero (mid-range) and one factor is set at the outer values (cube-face centers).

B-B designs envelope a factor space with three-levels for each factor, avoiding the corners of the face, and filling the combinations of the center and extreme levels. B-B designs combine fractional factorials with incomplete block designs such that the extreme vertices of cubes (or hypercubes) are avoided to produce rotatable designs with three levels for each factor.

IMPORTANT RSM PROPERTIES AND FEATURES (ORTHOGONALITY, ROTATABILITY, UNIFORMITY)

Orthogonality: The property that allows individual effects of the k-factors to be estimated independently without (or with minimal) confounding. Also orthogonality provides minimum variance estimates of the model coefficients so that they are uncorrelated.

For first-order models, equation [1] gives the basic model representation.

For second-order models, orthogonality is somewhat more complex because the individual effects are redefined as orthogonal polynomial terms. This is beyond the scope of this paper but is discussed by Khuri and Cornell (1987). Orthogonal CCDs can be run as blocked experiments, see Cornell (1990, pp. 54-55) for more information.

Rotatability: The property of rotating points of the design about the center of the factor space. The moments of the distribution of the design points are constant. The variance (or standard deviation) of the predicted response Y(x) is equidistant at all points from the center of the design. Therefore, the variance contours of Y(x) are concentric circles (for k = 2 dimensions), concentric spheres (for k = 3 dimensions) or concentric hyperspheres (for k ≥ 4 dimensions).

Uniformity: A third property of CCD designs used to control the number of center points is uniform precision (or uniformity). Uniformity means that the estimated response Y(x) at the origin is approximately equal to the estimated response variances at the design vertices, one unit distance in any direction from the origin (analogous to the radius of a sphere). Uniformity helps protect against biased regression coefficients that orthogonal designs lack, especially when there are third or higher-order terms in the "true" surface, see Montgomery (1991, p. 546) for more information.

HOW TO CONSTRUCT AND ANALYZE RSM MODELS WITH JMP

The general steps in performing RSM are as follows:

1. Select a model for the data, either first-order or second-order. Start with a first-order model if the form of the model is known from past experience or if it is to be determined.

2. Estimate parameters of the model from the data after the responses have been collected. One can create response values using random number generators until all the data for the factor levels and replicates have been collected. This usually is a good preliminary step to get practice in the analysis. The random numbers can be generated in JMP by using the "?normal" or "?shuffle" calculator functions.

3. Check the fitness of the model to the data. If a first-order model does not fit, try adding cross-product (interaction) terms. If the fit does not improve, then add the second-order (quadratic) terms. If fitness is still not achieved, the alternatives are to (i) pool the estimates of variance; (ii) apply transformations to either the responses or the factors; or (iii) consider a different model form. For more information, see Box, Hunter, and Hunter (1978).

    Cornell (1990, pp. 25-26) described criterion when alternative (i) was appropriate (e.g., if the error variation was believed to be constant from one set of experiments to another). Alternative (ii) involves deciding which transformation to use. Using coded values to establish new centers for the experimental region helps to avoid multi-collinearity effects. Using Stepwise regression in JMP is another simple way to avoid multi-collinearity and improve the fit without extensive effort. Alternative (iii) involves additional computational work when higher-order models such as cubic forms are considered.

4. Determine the response surface from the fitted model with a "map" of the surface contours. Study the contour lines of factor pairs X_1, X_2 and the response Y. Follow the directions of movement along the paths towards the optimum response from a reference point. This movement starts the path of steepest ascent (descent, ridge or saddle point).

5. Examine the response surface to determine if the optimum operating conditions (values of input factors) reaches the maximum, minimum, ridge, or saddle point region for the response variable. Eigenvalues and eigenvectors help identify the shape and curvature orientation of the response surface. If the optimum response region is not reached, exploration continues in the direction towards the maximum (if there are negative eigenvalue signs associated with the stationary point), towards the minimum (if there are positive eigenvalue signs associated with the stationary point), or towards the saddle point (if there are different eigenvalue signs). Zero eigenvalues indicate a flat fitted surface.

Typically, these values are obtained by differentiating the fitted Response Surface model with respect to each factor, equating the derivatives to zero, and simultaneously solving the equations for each factor. This result forms a gradient vector. The next step is to move along the gradient direction in increments by setting the coordinates of the stationary point to the center (origin). Gradient movement continues about the vicinity of the stationary point until the optimum point (maximum, minimum, or minimax/saddle point) is found.

With JMP, the values are displayed by holding the (left) mouse button down as the pointer moves along the contour surfaces. Clicking on the rotated triangles allows you to flip through various frames, change the values of the factors and display the surface changes.

JMP Design Menus, Steps, and Windows

The **Design Experiment** command in the **Tables** menu is used to construct RSM models in JMP. RSM models are built by completing the **Response Surface** dialog:

1. Enter the **Number of Factors** (up to eight).
2. Click the **Search for Designs** to get a list of design choices, then highlight and click to choose.
3. When selecting a central composite design, click an **Axial Scaling** option.
4. Click the **Generate Selected Design** box to create a JMP data table for the specified design. A new JMP table is created having a row for each run, and a column **Y** for recording the results. If the **Make Model** box is checked, JMP opens the **Fit Model** dialog window listing the effects for the model selected. The model can also be built using terms for a complete quadratic model, selected linear, and squared terms for each factor and cross-products between factors.

JMP Analysis Menu and Commands

To Analyze RSM models in JMP

1. Choose the **Fit Model** command in the **Analyze** menu.

2. Click the variables to enter specific model effects and error terms.
3. Select one or more columns in the column selector list.
4. Choose **Response Surface** from the Effect Macros pop-up menu. The **Response Surface** effect attribute **{RS}** may be selected for each main effect.
5. Choose **Screening Fit** from the fitting pop-up menu, and click **Run Model**. You can optionally select **Standard Least Squares** to solve for the critical surface values or zero slope point. The **Contour Plot Specification** lets you see the structure of the two-factor response surface. For more than two factors you can sequence through **Contour Plot** frames by editing the **From**, **To**, and **By** fields.
6. Review and interpret the output from the **Screening Fit** menu. Contour profiling is a new feature in JMP version 3.1.5 that is useful for optimizing one or more responses graphically and interactively. After fitting the data to the response surface model, the **Contour Profiler** panel may be called to change the factor and contour variables by editing value fields and moving slider controls. **Contour Profile** plots allow for the interactive exploration of the factor space. That way, the expected effects on the responses variables can be examined. This exploration helps to establish the tradeoffs that may need to be made.

Dual Response Example

Montgomery and Runger (1994) described an experiment to investigate the effect of reaction time and temperature on two chemical process response variables, percent conversion/yield and viscosity. A central composite design (Table 1) provided the experimental design layout for the analysis. The objective was to maximize Conversion % and sustain a target Viscosity within a tolerance range of 40 ± 2 mPA-secs.

Table 2 showed that the fitted models accounted for over 91 percent and 83 percent of the variation in Conversion % and Viscosity, respectively. The Parameter Estimates showed the coefficients and significance of the linear, cross-product, and quadratic terms on each response. A second-order (quadratic) model without the cross-product term seemed to fit Conversion %. Whereas, a first-order (linear) model was adequate for Viscosity.

Table 1. Montgomery and Runger's (1994) Central Composite Design

Time (mins.)	Temperature (°F)	X1	X2	Conversion %	Viscosity (mPa-sec)
50	160	-1	-1	65.3	35
60	160	1	-1	68.2	39
50	170	-1	1	66	36
60	170	1	1	69.8	43
48	165	-1.4142	0	64.5	30
62	165	1.4142	0	69	44
55	158	0	-1.4142	64	31
55	172	0	1.4142	68.5	42
55	165	0	0	68.9	37
55	165	0	0	69.7	34
55	165	0	0	68.5	35
55	165	0	0	69.4	36
55	165	0	0	69	37

Table 2. JMP's Summary of Fit and Parameter Estimates for Conversion % and Viscosity

Conversion%	

Summary of Fit	
RSquare	0.914333
RSquare Adj	0.853142
Root Mean Square Error	0.783749
Mean of Response	67.75385
Observations (or Sum Wgts)	13

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	69.1	0.350503	197.15	<.0001
X1	1.6329951	0.277097	5.89	0.0006
X2	1.0829951	0.277097	3.91	0.0058
X1*X1	-0.96875	0.297154	-3.26	0.0139
X2*X1	0.225	0.391875	0.57	0.5838
X2*X2	-1.21875	0.297154	-4.10	0.0046

Viscosity (mPa-sec)	

Summary of Fit	
RSquare	0.839648
RSquare Adj	0.725111
Root Mean Square Error	2.233106
Mean of Response	36.84615
Observations (or Sum Wgts)	13

Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	35.8	0.998675	35.85	<.0001
X1	3.8498737	0.789522	4.88	0.0018
X2	2.5695436	0.789522	3.25	0.0140
X1*X1	0.975	0.846668	1.15	0.2873
X2*X1	0.75	1.116553	0.67	0.5233
X2*X2	0.725	0.846668	0.86	0.4202

The Contour plots for Conversion % and Viscosity are shown in Figures 1a and 1b.
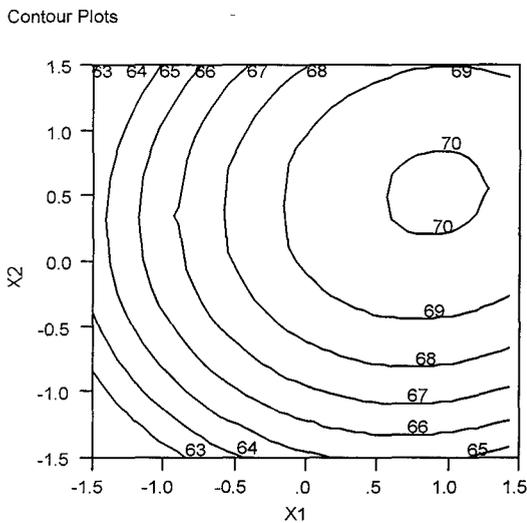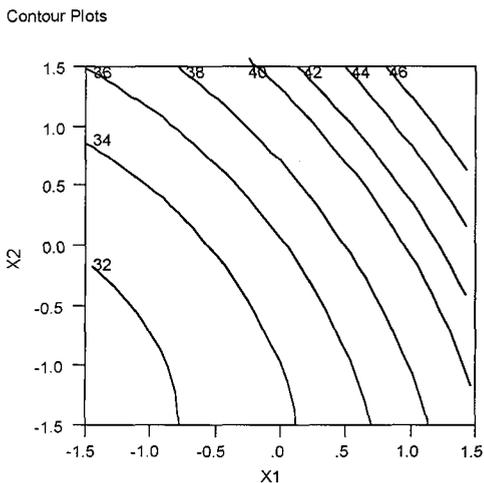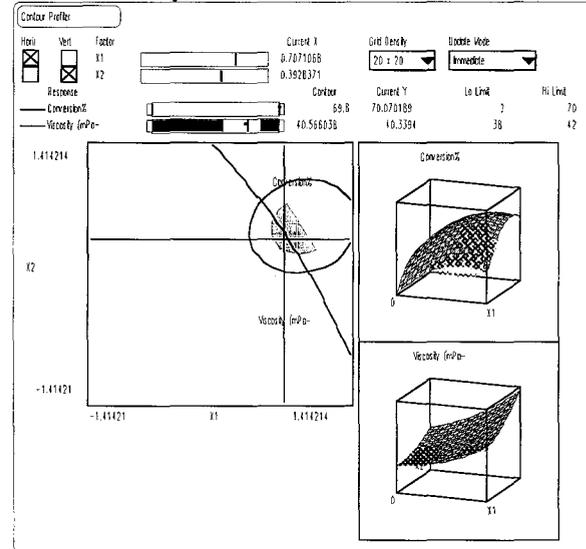
Figure 1a. Contour plot for Conversion %

Contour Plots

Figure 1b. Contour plot of Viscosity

Contour Plots

These two plots were combined using JMP's Contour Profiler as shown in Figure 2.

Figure 2. Contour Profile Plot Overlaying Conversion % and Viscosity

The optimal values of the coded (Current X) values, X1=0.7071068 and X2=0.3928371, produced the two response values (Current Y) of 70.070 and 40.339 for Conversion % and Viscosity, respectively.

These coded values were converted into the scales of the original Time and Temperature uncoded values using the formula below found on page 471 of the *JMP Statistics and Graphics Guide, Version 3.1*:

actual = low + 0.5 x (coded + 1)x(high-low).

Thus,
Time = 48 + 0.5 (X1+1) (62-48)
     = 48 +.0.5 (1.7071068)(14)
     = 59.94974 or about 60 sec.

Temperature = 160 + 0.5 (X2+1)(172-160)
            = 160 +0.5(1.3928371)(12)
            = 168.35704 or about 168°F.

Both values closely agreed with the optimum time (60 sec.) and temperature (167°F) values Montgomery and Runger found. Other time and temperature settings satisfying the response constraints were examined by moving the slider controls. Aligning the slider bars with the red dots (Current Y values) allows interactive exploration of the factor space. This can also be accomplished by positioning the cross-hair lines on the graphs or by editing the fields of the Current X and Contour values. The Mesh (Surface) plots next to the Contour graph showed the grid of response values for the factor pairs checked in the

boxes of the Control Panel. These plots were rotated to give different points of view.

Barrier-Bag Sealing Example

Barrier bags help protect microcircuits, semiconductor devices, and associated higher electronic assemblies. Materials sealed in these bags maybe stored for long periods of time and must not allow vacuum air to enter inside the bags after sealing has occurred. A problem existed with bags' seams separating, causing air and contaminants to enter and form on the sealed materials.

One of the tests of strength of barrier bags is the heat-sealed seam test. Test strips are cut from a sample of bags in stock. The ends of the strips are sealed with heat-sealing equipment and spread across a test frame. Weights suspend from the lower ends of the strips. If the seams hold together without separations from the suspended weights for at least five minutes, then the barrier bag seams pass the test. The objective was to find optimum sealing conditions (heat sealing settings and bag age) that ensured strong seams of barrier bag pull strengths.

The variables in this example were:

Months - The number of months between the lot manufacturing. date (printed on the bag) and the date bags were sampled for testing in this study. The bag age dates ranged from 7 months to 75 months.

Temperature - Temperature setting (°F) of the sealer (250°F, 255°F, 280°F, and 330°F)

Pressure - Pressure setting of the sealer (psi) (50, 60, and 70 psi).

Dwell - Dwell time, the number of seconds (sec.) the jaw sealer held down on the bag (2, 3, 4 sec.)

The RSquare in the Summary of Fit below showed that about 86.7 percent of the test time variation was explained by the fitted model

Summary of Fit	
RSquare	0.866963
RSquare Adj	0.829439
Root Mean Square Error	0.854926
Mean of Response	4.484902
Observations (or Sum Wgts)	51

The Prob > F = 0.3789 in the Lack of Fit table below suggested that the fitted model was adequate. Therefore, the search for the optimum values could continue.

Lack of Fit				
Source	DF	Sum of Squares	Mean Square	F Ratio
Lack of Fit	5	3.966752	0.793350	1.0993
Pure Error	34	24.538267	0.721714	Prob>F
Total Error	39	28.505018		0.3789
				Max RSq
				0.8855

All of the main effects, except dwell, were statistically significant. The significant interactions of factors terms were temperature * months, pressure * temperature, dwell * month, and dwell * pressure from the Parameter Estimates table below.

Parameter Estimates				
Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	100.32556	25.1816	3.98	0.0003
months	0.6750373	0.234688	2.88	0.0065
temperature	-0.595184	0.149233	-3.99	0.0003
pressure	-0.452846	0.192209	-2.36	0.0236
dwell	1.3922942	2.178532	0.64	0.5265
months*months	-0.004395	0.00063	-6.98	<.0001
temperat*months	-0.00167	0.000769	-2.17	0.0361
temperat*temperat	0.0007608	0.00025	3.04	0.0042
pressure*temperat	0.0022594	0.000602	3.75	0.0006
dwell*months	0.0206098	0.008901	2.32	0.0259
dwell*temperat	0.0117228	0.008634	1.36	0.1823
dwell*pressure	-0.092956	0.027373	-3.40	0.0016

The next four graphs, produced with JMP's Contour Profiler, provided further exploration of the significant interactions.

There were two optimal temperature values for the temperature by month interaction. Moving the crosshairs to the higher temperature setting of 324.4°F and 24.12963 months provided satisfactory test times as shown by the connecting arrow below.
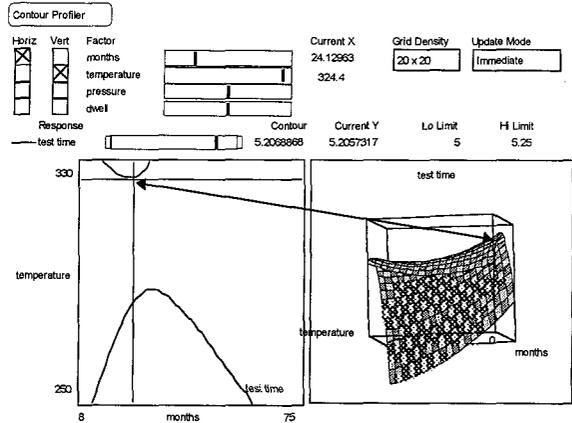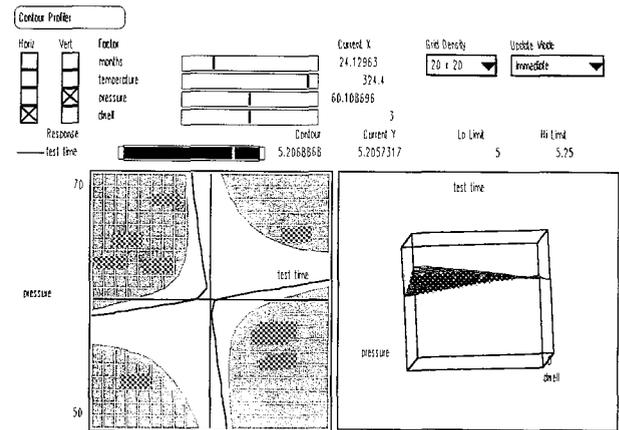
The 324.4°F temperature and pressure of 60 psi also satisfied the test time requirement.
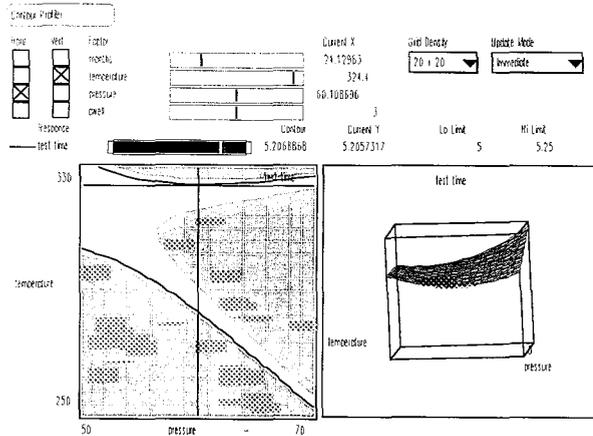
Next, a three second dwell time was chosen to examine the month by dwell interaction.
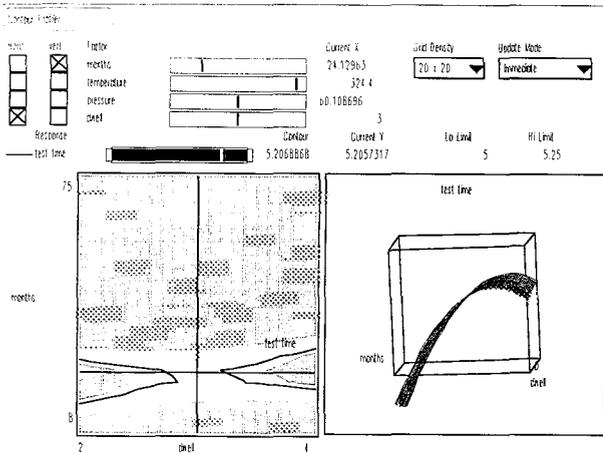
Finally, the 60 psi pressure by three second dwell time completed the pressure by dwell interaction.

The optimal settings for the input factors were: bag age of approximately 24 months, a temperature setting of 324°F, a pressure setting of 60 psi, and a dwell time of three seconds to yield test times over five minutes.

Eighteen confirmation runs were successful on subsequent trials. The test times exceeded five minutes on all combinations of factor settings (i.e., 18 out of 18 trials had 100% success). The results led to recommended settings for the jaw sealers that the manufacturing engineers and operators could follow. To date, no barrier bags failed the pull test since using the recommended settings for the sealers.

CONCLUSIONS

The combined experimental design, analysis, and data visualization features of JMP assist process engineers, quality analysts, and statisticians' selection of the most appropriate levels of input factors that will optimize the critical variables from Response Surface models.

The interactive exploration of the factor space that JMP offers provides valuable opportunities to learn and to understand the complex surfaces, shapes, and feasible regions that will satisfy the factor constraints so that tradeoffs can be made interactively, in a matter of minutes, no matter how complex the problem.

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