NHG
North Haven Group, LLC

Multiple Optimization Using the JMP® Statistical Software

Kodak Research Conference
May 9, 2005

Philip J. Ramsey, Ph.D., Mia L. Stephens, MS, Marie Gaudard, Ph.D.

North Haven Group, http://www.northhavengroup.com/

pramsey@northhavengroup.com, 603-672-5651

mstephens@northhavengroup.com, 207-363-5739

mgaudard@northhavengroup.com, 352-560-0312

Talk Outline

- Introduction
- Desirability Functions
- Multiple Response Optimization
- Desirability Optimization in JMP
- Optimizing an Anodizing Process
- Using Importance Values
- Constrained Mixture Example

Introduction

The challenge in multiple response optimization is to find settings for multiple input variables that achieve desirable performance levels for one or more responses.

Designed experiments are often used to model each response as a function of the input variables.

Each response of interest has its unique predictive model.

These predictive models then form the basis for optimization.

Often, settings that optimize one response will degrade another response.

Introduction

Sometimes, predictive models for each response are derived from observational studies.

The JMP software allows multiple optimization using models derived either from designed experiments or observational studies.

JMP's approach to optimization for multiple responses is based upon the concept of **desirability**.

NHG
North Haven Group, LLC

Desirability Functions

Desirability appears to have been first proposed as a criterion for response optimization by Harrington (1965) and popularized by Derringer and Suich (1980).

The first step in defining a desirability function is to assign values to the response that reflect their desirability.

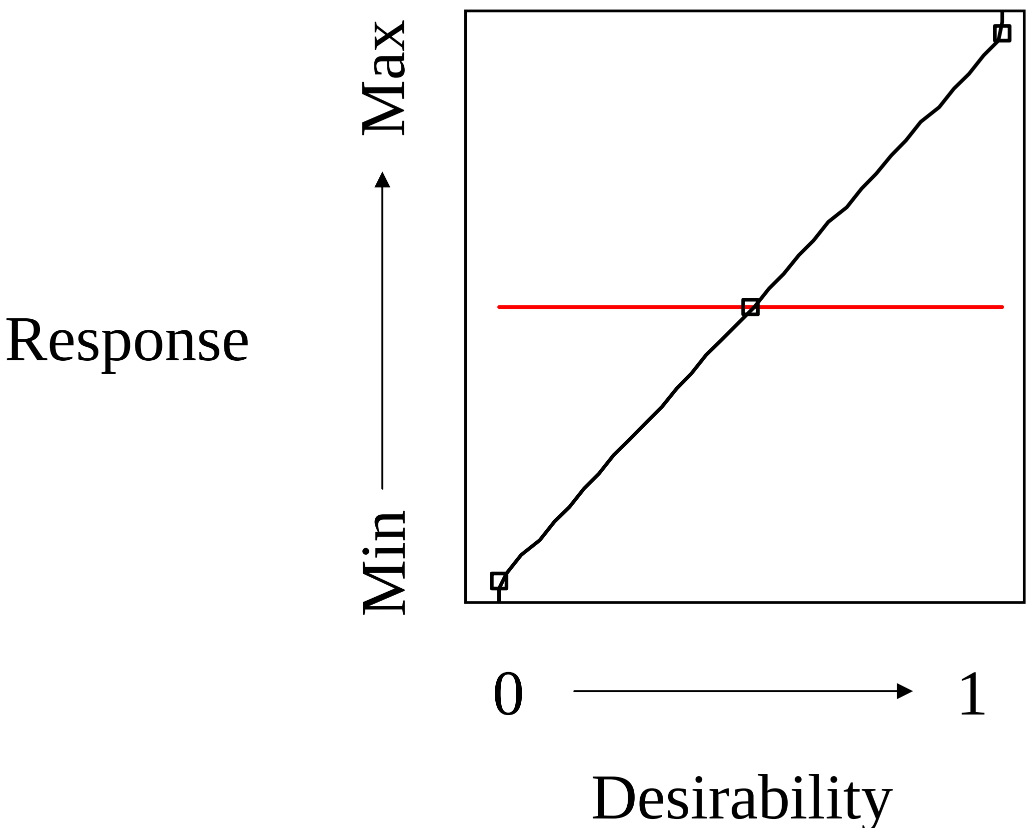
For the i^{th} response, we define a function d_i , that assumes values between 0 and 1, where:

- 0 indicates a value of the response that is least desirable,
- 1 indicates a value that is most desirable, and
- a value between 0 and 1 indicates the desirability of the associated response.

North Haven Group, LLC

Desirability Functions

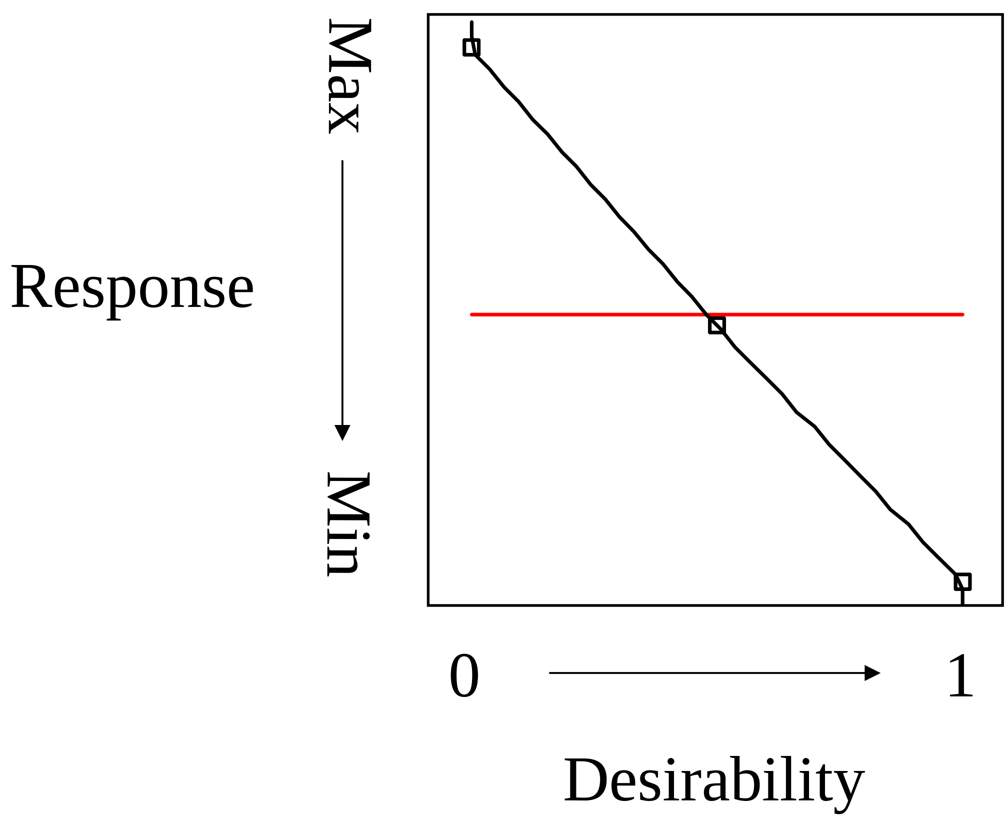
If the objective is to maximize a response, the desirability function might have the following shape (the specific shape depends upon the response optimization goals):



NHG
North Haven Group, LLC

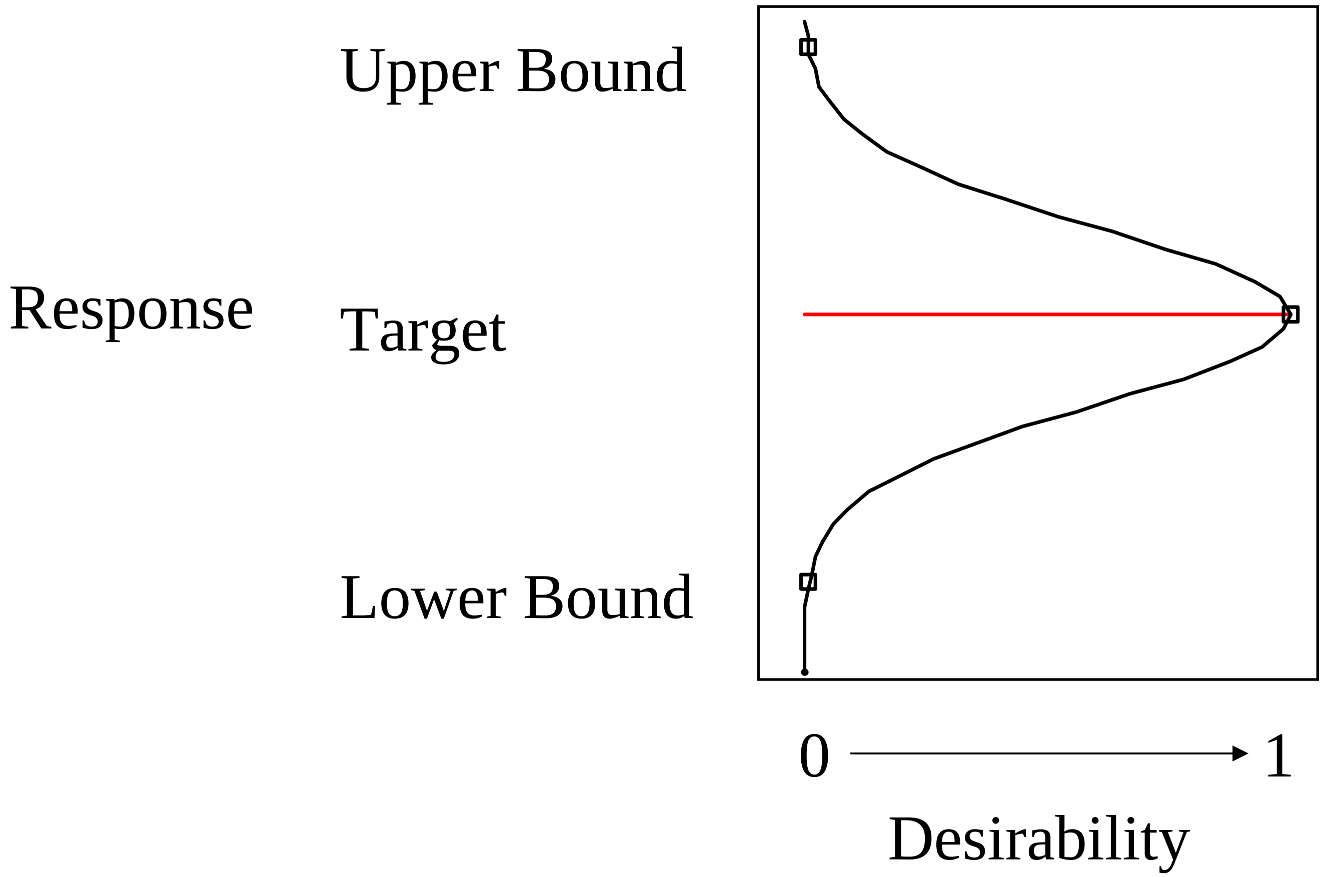
Desirability Functions

If the objective is to minimize the response, the desirability function may have this shape (again, the exact shape depends upon the response optimization goals):



Desirability Functions

If the objective is to match a target, the desirability function might have the following shape:

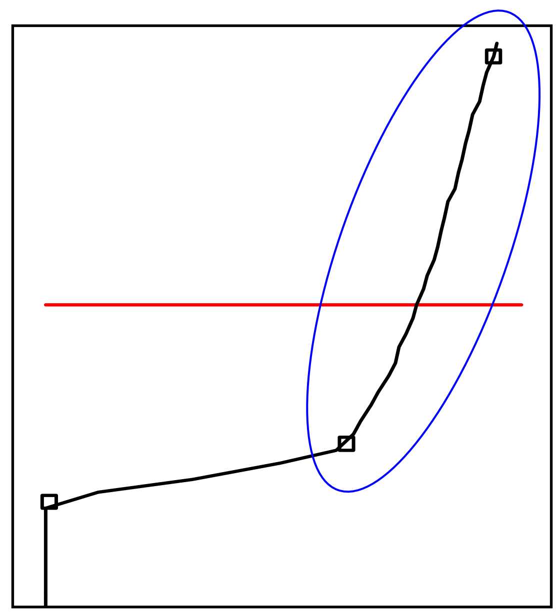


Desirability Functions

Suppose one wants to **maximize the response**, where a specified lower bound exists and the specified desirability control points are not linear over the range of the response. Below is a possible desirability function

Desired Maximum

Lowest Acceptable Level



Most Desirable Region

0 0.6 1

Desirability

Desirability Functions

Derringer and Suich (1980) proposed forms for the desirability function, based on the particular desirability goal.

These equations are not smooth functions - the possible shapes of the desirability functions are limited.

In contrast, JMP defines the desirability function based upon control points determined by the user, using piecewise smooth functions.

These piecewise smooth functions allow greater flexibility in the shapes of the desirability functions and ensure good behavior of the desirability function over the three basic types of optimization.

Multiple Response Optimization

A typical desirability objective function for multiple optimization is based on the geometric mean of the transformed responses d_i (or the average of the natural logs of the desirabilities).

For k responses:

$$D^* = \sqrt[K]{d_1 * d_2 * \ldots * d_k} \quad \text{, or equivalently,}$$

$$D = \ln(D^*) = \frac{1}{k}\left[Ln\left(d_1\right) + Ln\left(d_2\right) + \ldots + Ln\left(d_k\right) \right].$$

Notice this form of the objective function treats all k responses with equal weight or importance.

Multiple Response Optimization

We define the **weight** or **importance** level of the i^{th} response as w_i.

We impose the following constraints on the weights:

$$0 \leq w_i \leq 1 \quad \text{where } i = 1, 2, \ldots, k$$

$$\sum_{i=1}^{k} w_i = 1.0.$$

The objective functions, incorporating differential weighting, have the form

$$D = \left[w_1 Ln(d_1) + w_2 Ln(d_2) + \ldots + w_K Ln(d_k) \right] \text{ or}$$

$$D^* = Exp[D].$$

Desirability Optimization in JMP

The JMP Prediction Profiler is a powerful tool for finding optimum settings for one or more responses of interest.

The optimum settings may be minima, maxima, target values, or a combination of these.

The user may also specify upper or lower bounds on the responses.

The Prediction Profiler may be accessed through the Fit Model platform or it may be accessed directly from the Graph menu.

To access the Prediction Profiler directly from the Graph Menu, the user must save the prediction formulas for the responses to the spreadsheet from within the Fit Model platform.

Desirability Optimization in JMP

The Prediction Profiler allows **simultaneous optimization on multiple responses** employing a different model for each of the responses.

The ability to optimize multiple responses based on a different model for each response is a powerful capability of the JMP software.

To perform multiple optimization with the Prediction Profiler:

- Use Fit Model to fit a best model for each of the responses,
- Save each of the Prediction Formulas to the data table, and
- Open the Prediction Profiler from the Graph menu and enter the prediction formulas as the responses to be optimized.

Desirability Optimization in JMP

The models used to perform the optimization can be estimated from observational data or from a designed experiment.

The Fit Model platform of JMP, where the predictive models are estimated, does not place any requirements on the source of the data.

Therefore, one can develop the predictive models from observational data and then use the Prediction Profiler in JMP to perform the optimization on the responses.

However, keep in mind that experimental design data is always preferable to observational data for deriving cause and effect models.

Optimizing an Anodizing Process

A Six Sigma project team is attempting to optimize an anodizing process (oxide surface coating) for an aluminum substrate.

For aesthetics, the customer requires that the anodized surfaces be black in color.

The process has two stages: anodize (A) and dye (D).

Five factors are selected for an experiment:

- Bath Temp (A),
- Anodizing Time (A),
- Acid Concentration (A),
- Dye tank concentration (D), and
- Dye tank pH (D).

Optimizing an Anodizing Process

Due to production requirements, only enough anodizing equipment time is available to perform eight to ten runs.

The team elects to perform a resolution III, 2^{5-2} fractional factorial with two center points (10 runs).

Some of the potential two-way interactions were discounted for technical reasons, reducing the amount of aliasing.

The four primary responses are:

- Anodize Thickness,
- L* (lightness of the color),
- a* (redness/greenness of the color), and
- b* (yellowness/blueness of the color).

Optimizing an Anodizing Process

To meet customer requirements, the following specifications are set by the engineers (the color parameter targets and ranges were empirically determined from production data):

- **Anodize Thickness**: 0.9 ± 0.2 microns.
- **L*:** 10 ± 2.
- **a*:** 2 ± 2.
- **b*:** 0 ± 2.

We will use the Prediction Profiler to find anodizing process conditions that simultaneously achieve the four response targets (or at least stay within the specification ranges).

Optimizing an Anodizing Process

Using Fit Model, a separate model was fit to each of the four responses and the Prediction Formulas saved to the spreadsheet. We recommend saving the Fit Model Script to the data table for each model.

Recall, to save the Prediction Formula to the spreadsheet:

- Click on the red diamond at the top of the Fit Model analysis output,
- Select the menu option ‘Save Columns’, and
- From ‘Save Columns’, select ‘Prediction Formula’.

The next slide shows the Fit Model output for the best model for Thickness. Each of the four responses had a separate model.

NHG
North Haven Group, LLC

Optimizing an Anodizing Process

For Anodize Thickness, only factors for the anodize stage could have an influence.

This allowed the team to estimate a model with no aliasing.

To the right is the Fit Model report for the predictive model.

Notice that the lack of fit test (based on center points) is not significant.

Summary of Fit

RSquare	0.993264
RSquare Adj	0.984844
Root Mean Square Error	0.034912
Mean of Response	0.73815
Observations (or Sum Wgts)	10

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	5	0.71889166	0.143778	117.9630
Error	4	0.00487537	0.001219	Prob > F
C. Total	9	0.72376702		0.0002*

Lack Of Fit

Source	DF	Sum of Squares	Mean Square	F Ratio
Lack Of Fit	3	0.00372337	0.001241	1.0774
Pure Error	1	0.00115200	0.001152	Prob > F
Total Error	4	0.00487537		0.5936
				Max RSq
				0.9984

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	-1.16418	0.150969	-7.71	0.0015*
Anodize Temp	0.0164458	0.000823	19.99	<.0001*
Anodize Time	0.0098187	0.001234	7.95	0.0014*
Acid Conc	0.0019964	0.000705	2.83	0.0473*
(Anodize Temp-75)*(Acid Conc-187.5)	-0.000364	0.000047	-7.74	0.0015*
(Anodize Time-30)*(Acid Conc-187.5)	0.0005425	7.053e-5	7.69	0.0015*

Optimizing an Anodizing Process

The four columns furthest to the right in the data table contain the **Prediction Formulas** saved in the Fit Model platform.

In the table to the left are the saved scripts for the models.

These Prediction Formula columns can now be used by the Prediction Profiler to perform multiple optimization.

AnodizeDOE

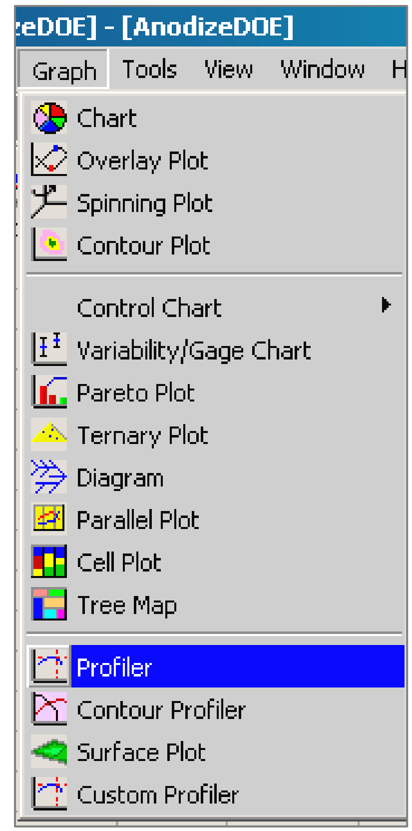
- AnodizeDOE
- Source
- Full Model
- Thickness Model
- L* Model
- a* Model
- b* Model

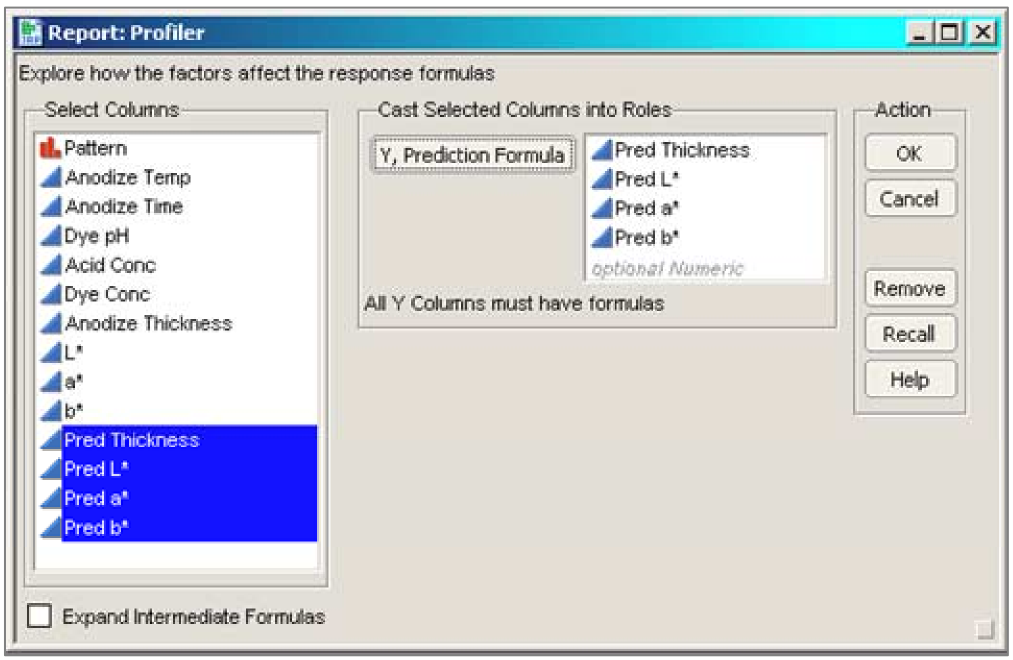
13/0 Cols	Anodize Temp	Anodize Time	Dye pH	Acid Conc	Dye Conc	Anodize Thickness	L*	a*	b*	Pred Thickness	Pred L*	Pred a*	Pred b*
1	90	20	5.00	170.00	15.00	1.03	5.75	2.23	-4.34	1.04	5.78	2.63	-4.34
2	75	30	5.75	187.50	12.50	0.69	11.33	3.02	-2.84	0.74	10.83	3.53	-2.77
3	90	20	5.00	205.00	10.00	0.73	4.30	1.17	0.91	0.73	4.33	0.56	0.91
4	75	30	5.75	187.50	12.50	0.73	10.58	3.23	-2.68	0.74	10.83	3.53	-2.77
5	60	20	6.50	205.00	15.00	0.45	19.10	7.85	-5.57	0.43	19.13	7.86	-5.57
6	60	20	6.50	170.00	10.00	0.38	15.05	8.04	-5.42	0.36	15.08	7.84	-5.41
7	90	40	6.50	205.00	15.00	1.13	7.73	1.30	-0.93	1.12	7.76	1.09	-0.93
8	60	40	5.00	170.00	15.00	0.35	19.52	5.23	-6.45	0.36	19.55	4.63	-6.45
9	60	40	5.00	205.00	10.00	0.81	9.20	2.17	0.00	0.82	9.23	2.56	0.00
10	90	40	6.50	170.00	10.00	1.07	5.77	1.07	-0.37	1.05	5.81	1.08	-0.37

Optimizing an Anodizing Process

Select Profiler from the Graph menu option.

The Prediction Profiler launch window will allow us to simultaneously optimize the four predicted responses for this experiment.

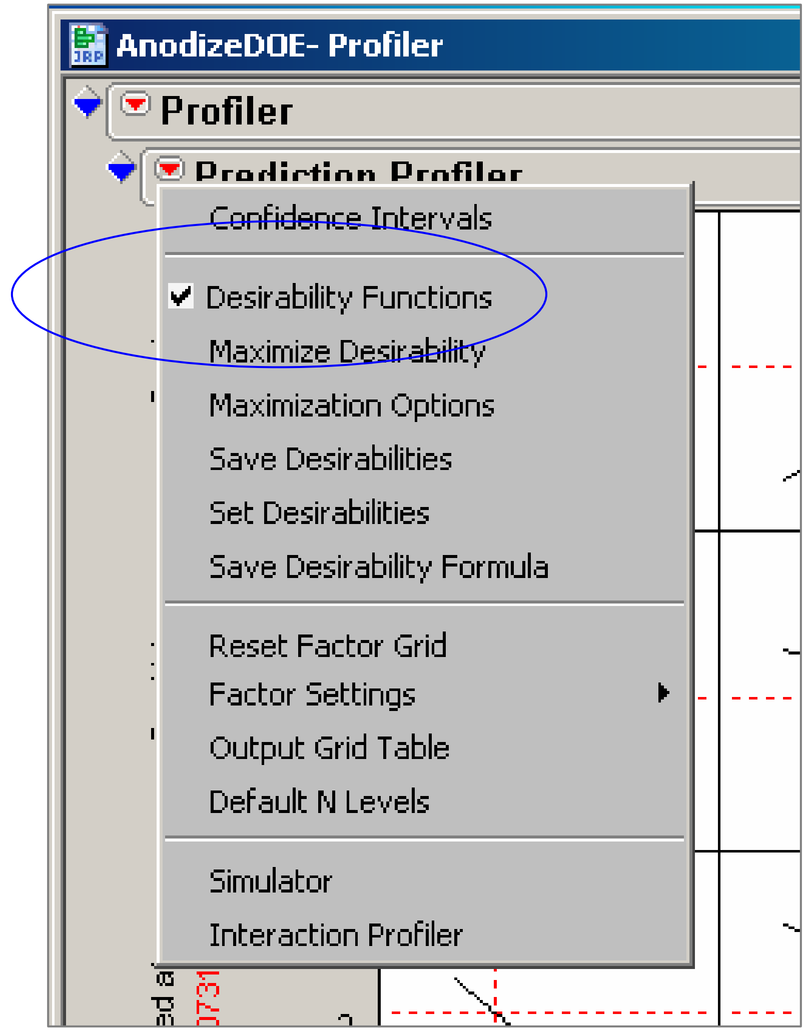




Optimizing an Anodizing Process

Once in the Profiler Report Window, one can select the menu items **Maximization Options** and **Maximize Desirability** function.

These set up the multiple optimization of the four responses, based upon the saved prediction formulas.



Optimizing an Anodizing Process

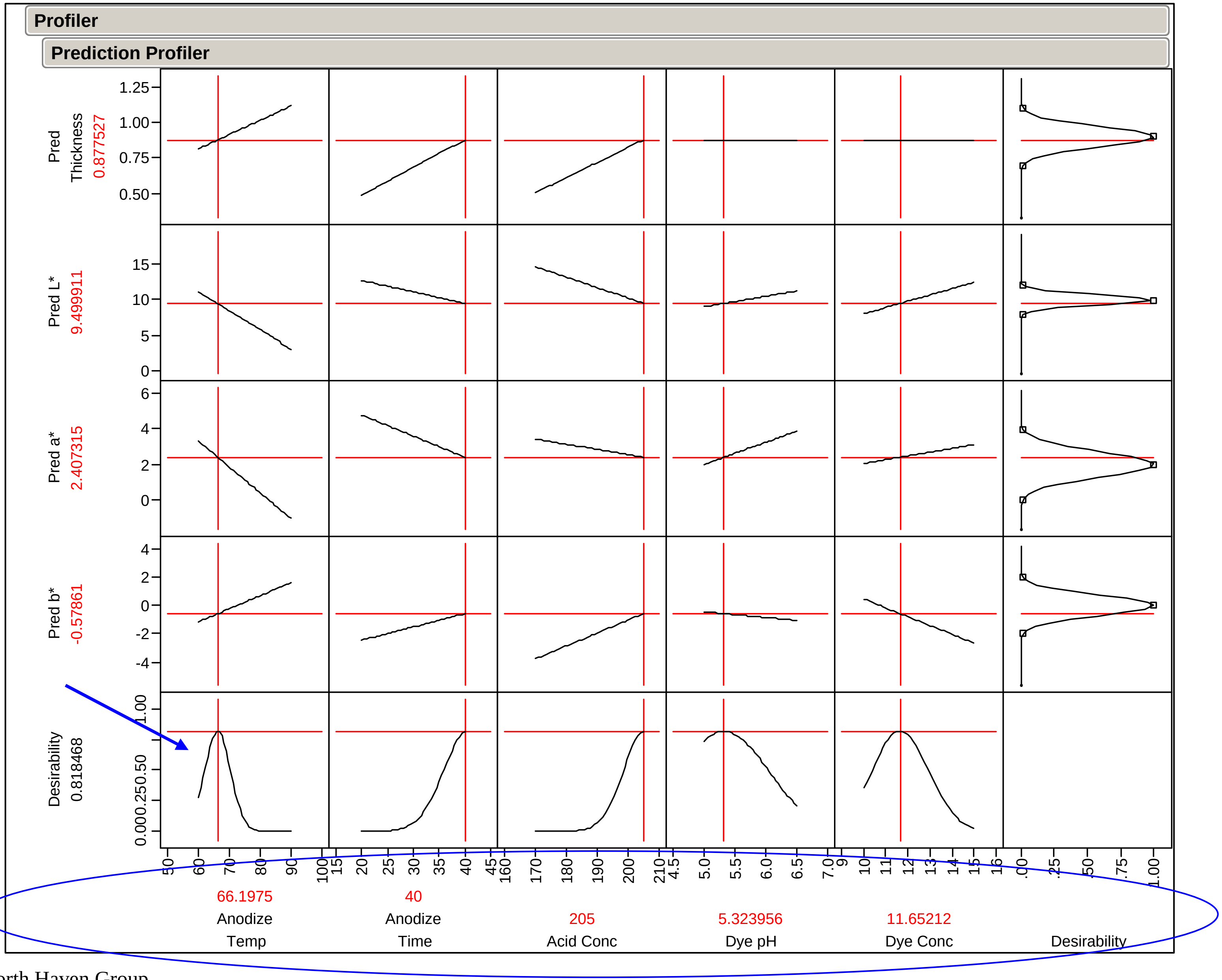
The next slide depicts the results of the multiple optimization using the Prediction Profiler.

A calculated desirability of 1.0 indicates that all response goals were simultaneously achieved.

The output indicates that the overall desirability was 0.82. However, all predicted response levels are well within the specification range.

The settings for the five factors that achieve the most desirable response values are depicted at the bottom of the output.

Note that all four responses are **very sensitive** to Anodize Temp, based upon the desirability trace in the last row of the output.


Profiler
Prediction Profiler
Pred Thickness
0.877527
Pred L*
9.499911
Pred a*
2.407315
Pred b*
-0.57861
Desirability
0.818468
66.1975
Anodize Temp
40
Anodize Time
205
Acid Conc
5.323956
Dye pH
11.65212
Dye Conc
Desirability

NHG
North Haven Group, LLC

Optimizing an Anodizing Process

Anodizing Experiment Issues

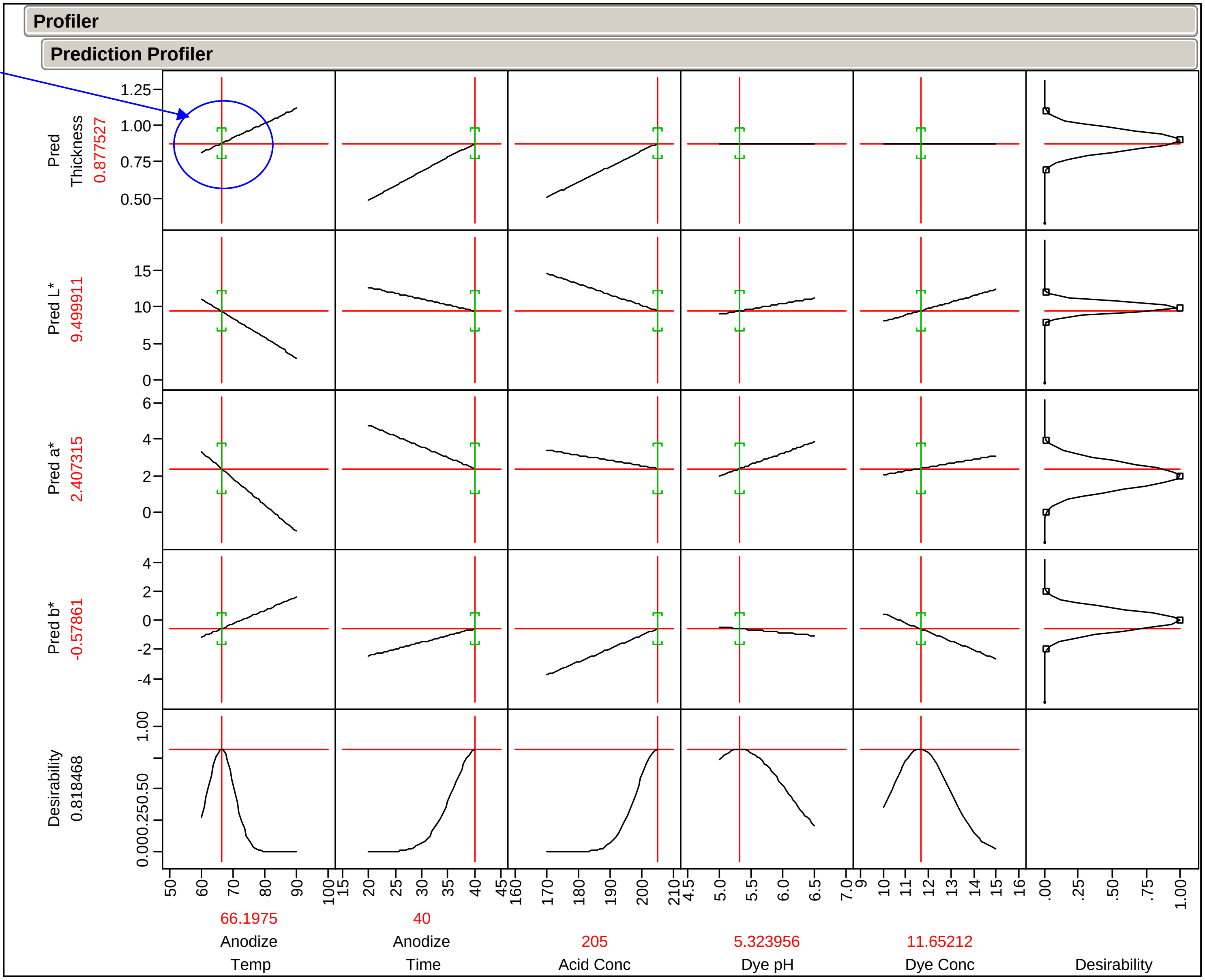
In production, not all of the five factors could be tightly controlled.

- In fact, from standard deviation estimates, the team concluded that only Anodize Time could be precisely controlled.
- In the **Column Info** window for each of the process factors, if the column property **Sigma** is specified, then JMP will provide propagation of error (POE) bars for the factor in the Profiler.

The next slide shows the optimized process settings in the profiler with the POE bars.

- The bars represent a $\pm 3\sigma$ window of variation in the response caused by the factor variation.

POE bars


Profiler
Prediction Profiler
Pred Thickness
0.877527
Pred L*
9.499911
Pred a*
2.407315
Pred b*
-0.57861
Desirability
0.818468
66.1975
Anodize Temp
40
Anodize Time
205
Acid Conc
5.323956
Dye pH
11.65212
Dye Conc
Desirability

Optimizing an Anodizing Process

The Profiler contains a Simulator function that can be used to illustrate the POE in the responses due to the factors.

To the right, are the settings for the factors used in the simulation.

Simulator

Factors

Anodize Temp	Random	Normal	Mean 66.197497	Std Dev 3
Anodize Time	Fixed		40	
Acid Conc	Random	Normal	Mean 205	Std Dev 1.625
Dye pH	Random	Normal	Mean 5.3239561	Std Dev 0.1
Dye Conc	Random	Normal	Mean 11.652119	Std Dev 0.323

Responses

Pred Thickness	No Noise
Pred L*	No Noise
Pred a*	No Noise
Pred b*	No Noise

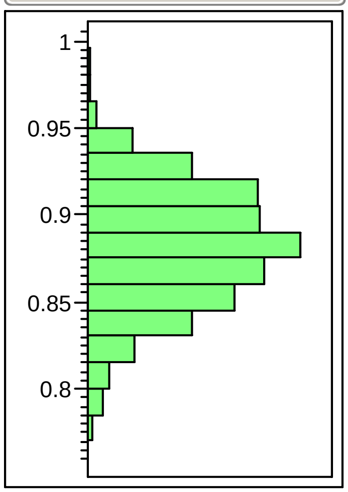
N Runs: 1000

Optimizing an Anodizing Process

These simulation results for the responses quantify anticipated variation due to lack of control of the process factors.

Distributions

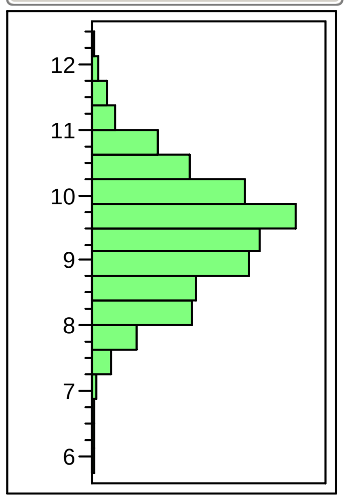
Pred Thickness



Moments

Mean	0.8808721
Std Dev	0.0351241
Std Err Mean	0.0011107
upper 95% Mean	0.8830517
lower 95% Mean	0.8786925
N	1000

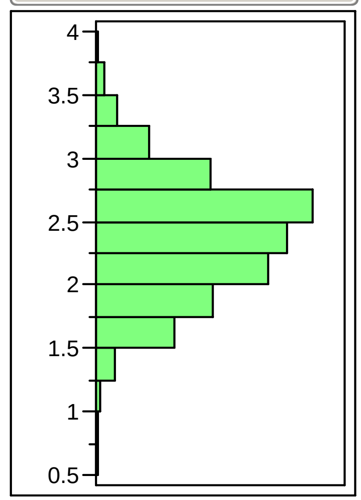
Pred L*



Moments

Mean	9.4268638
Std Dev	0.9351656
Std Err Mean	0.0295725
upper 95% Mean	9.4848952
lower 95% Mean	9.3688324
N	1000

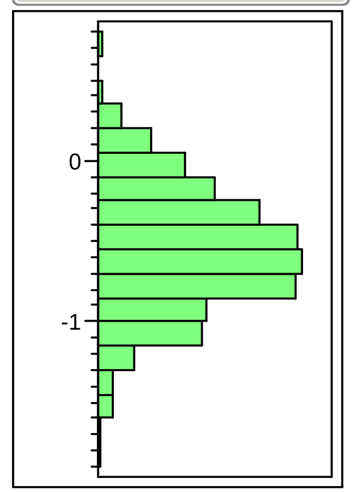
Pred a*



Moments

Mean	2.3708303
Std Dev	0.4712389
Std Err Mean	0.0149019
upper 95% Mean	2.4000728
lower 95% Mean	2.3415877
N	1000

Pred b*



Moments

Mean	-0.552679
Std Dev	0.3905999
Std Err Mean	0.0123519
upper 95% Mean	-0.528441
lower 95% Mean	-0.576918
N	1000

Optimizing an Anodizing Process

Further Issues

Since the experiment was a resolution III design, main effects were aliased with two-way interactions.

Furthermore, since all five factors were significant for one or more of the responses, it was not possible to resolve the aliases in most cases.

No production equipment time was available to perform additional experiments to resolve which interactions might be active.

The new process settings recommended by the Prediction Profiler optimization where far different from the current settings.

Optimizing an Anodizing Process

The experimental results suggested that the new conditions would substantially increase yields and produce higher quality coatings.

Equipment time was provided to perform **two confirming runs** at the new process conditions.

The two confirming runs achieved 100% yields with very high quality anodize coatings on all parts.

The current process had yields in the range of 40% with marginal quality coatings.

Although aliases were unresolved, engineers decided to perform no further experimentation, since the suggested factor settings worked extraordinarily well in practice. This is not ideal!

Using Importance Values

Often, multiple responses do not have the same level of importance to experimenters.

JMP allows the user to specify weights or importance values for each of the responses.

The default is to weight all responses equally.

Recall, that each weight should be between 0 and 1 and the sum of the weights across the factors should equal 1.

The response goals and importance values can be set in the JMP Profiler. They can also be set in the Column Info window as Column Properties (recommended).

Using Importance Values

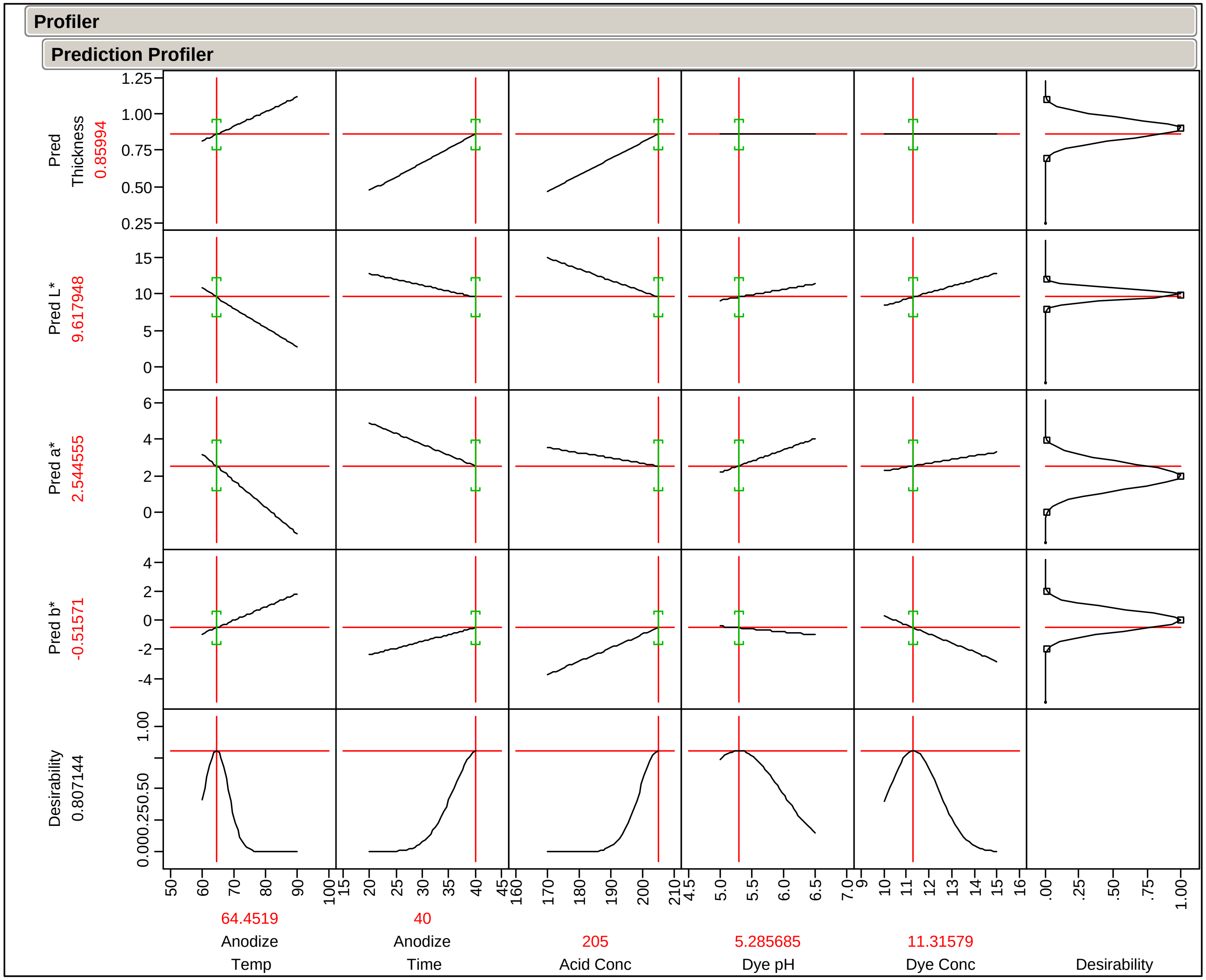
We revisit the Anodize experiment, but apply different importance values for each response.

Note that the previous optimization weighted the four responses equally.

The importance values for the four responses are:

- Anodize Thickness – 0.15
- L* – 0.35
- a* – 0.20
- b* – 0.30

The next slide depicts the optimization with the new importance values.


Profiler
Prediction Profiler
Pred Thickness
0.85994
Pred L*
9.617948
Pred a*
2.544555
Pred b*
-0.51571
Desirability
0.807144
64.4519
Anodize Temp
40
Anodize Time
205
Acid Conc
5.285685
Dye pH
11.31579
Dye Conc
Desirability

Constrained Mixture Example

The next example illustrates the use of the Profiler Desirability function to optimize a mixture subject to upper and lower bound constraints on each component.

In this example, the data were collected by observation of a process to produce a type of composite material.

There were nine mixture components and each had upper and lower bound constraints.

There were 3 responses.

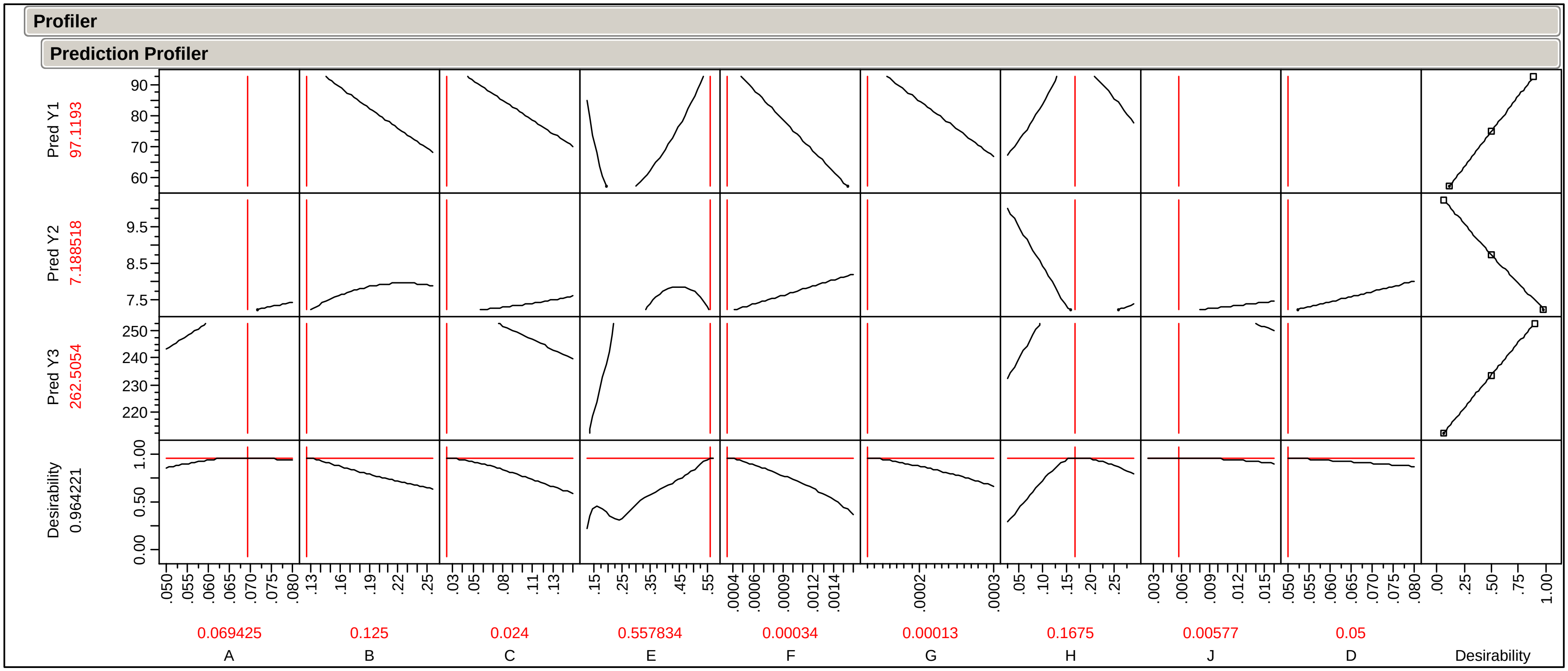
Y1 and Y3 were to maximized, while Y2 was to be minimized.

North Haven Group, LLC

Constrained Mixture Example

Each of the three responses had a different statistical model.

The Profiler analysis, below, shows a most desirable mixture.



NHG
North Haven Group, LLC

Constrained Mixture Example

Because the data were obtained by observation, as opposed to from a formally designed mixture experiment, there was considerable uncertainty as to how the predicted optimum mixture would actually perform.

Responses Y1 and Y3 are considered inversely related by scientists, so considerable skepticism existed as to validity of the suggested optimum composition.

Having no better solution to the problem, several trial batches were created.

The responses in all three cases actually exceeded the predicted optimum values from the Profiler.

Constrained Mixture Example

As a result, a multimillion dollar contract was saved and millions in new business were obtained for the improved, unique material.

NHG
North Haven Group, LLC

Summary

Desirability is a popular and proven technique to simultaneously determine optimum settings of input factors that achieve optimum performance levels for one or more responses.

The JMP® statistical software implements desirability optimization through the Fit Model platform and the Profiler.

JMP® allows the user to perform the desirability optimization with a different statistical model for each of the responses. The responses can be differentially weighted in terms of importance.

Two multiple response case studies were presented where the optimum input factor settings suggested by the Profiler where confirmed, with substantial financial benefits to the businesses.