



CHALLENGE

To find the best way to speed innovation in research and development at a FORTUNE 500 multinational chemical company.

SOLUTION

Combining JMP® and SAS® software to create a cutting-edge virtual lab for researchers to explore chemical formulations using powerful predictive modeling.

RESULTS

Scientists are expanding experimentation while cutting the experimental cycle from weeks to minutes. The company saves substantial expense by adding JMP to existing SAS resources instead of building the virtual lab from scratch.

Accelerating innovation with a next-generation virtual lab

Creating products that appeal to consumer tastes and lead the market requires a fast-moving research and development department. That was clear to the leaders of a large multinational chemical company that makes household-name products. Staffed with the brightest scientists, the company has been a pioneer in its field for more than a century and wanted to remain at the forefront. But what was the best way to speed R&D?

The FORTUNE 500 company (whose name is withheld per confidentiality agreements) came up with an

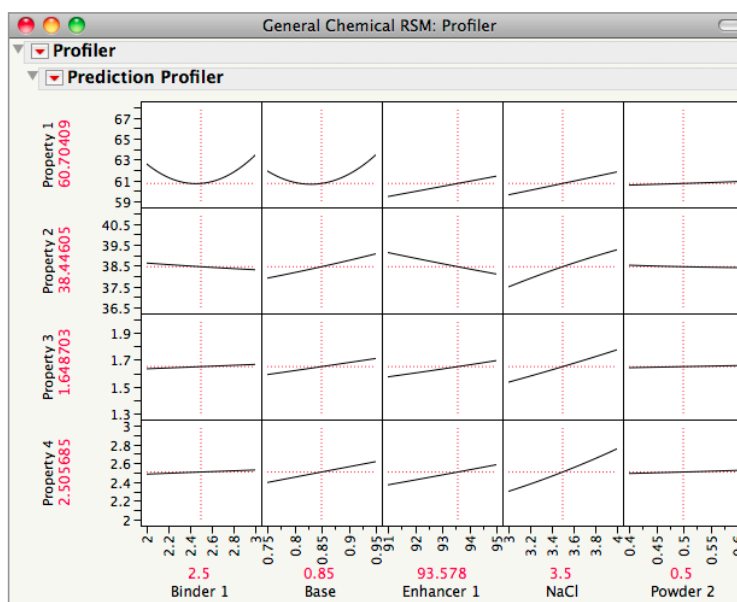
innovative idea: Let's build a virtual lab.

The lab would be a cutting-edge, powerful computer environment for researchers to explore chemical recipes using predictive modeling.

After studying several alternatives, leaders at the company decided that combining SAS and JMP software was the best way to get the virtual lab they needed. So they asked Predictum – a consultancy based in Austin, Texas, and Toronto, Canada – a JMP partner with expertise in SAS, to help them develop the virtual lab beginning in 2007.

“The whole purpose of analysis is to get insights. And if you're doing analysis on spreadsheets, you're getting just a fraction of those insights.”

Wayne Levin
President of Predictum



The Prediction Profiler in JMP enables virtual lab users to explore what-if scenarios quickly and easily. This example shows a predictive model. Users can change one factor (Binder 1, Base, Enhancer 1, NaCl, Powder 2) at a time and see the effect of that change on the predicted responses (Property 1, Property 2, Property 3, Property 4) and the interactions among the factors.

“Thousands of other companies are in the same situation: They have SAS in place, and if they added JMP, they would get substantial additional benefit.”

Wayne Levin

President of Predictum

And while companies typically expect new technology implementations to save money, that was not the primary objective of this project.

“Most of all, they wanted to boost research capabilities and substantially accelerate development,” says Wayne Levin, President of Predictum. “The virtual lab does that – in a big way – because researchers can quickly and easily examine the maximum possibilities before sending chemical formulations to the lab for physical development and testing.”

Accelerating R&D

This kind of efficiency was impossible when the company had only its physical labs. A scientist would develop a chemical compound that could make products better, safer or more profitable. She would send it to a physical lab to be tested 75 different ways and wait four weeks for the results.

The process has changed dramatically with the virtual lab, an application Predictum built using the JMP Scripting Language (JSL). Now scientists design comprehensive experiments using JMP’s Custom Design capabilities, evaluate the experiments with predictive models built on lab results collected over decades and assess the results visually – all in as little as 30 minutes. Scientists can now expand experimentation while cutting the experimental cycle from weeks to minutes.

“JMP’s graphical abilities and ease of use make it terrific for designing experiments and exploring data. SAS pulls data from just about any source and does the heavy analytical lifting. And JMP integrates with SAS. It’s a powerful combination,” Levin says.

The virtual lab in action

Before researchers could run the first experiment in the virtual lab, the predictive models had to be built. These models predict how new mixtures would perform in tests. Using SAS Enterprise Miner™, modeling experts created and “trained” models with the information collected over years of testing and experimentation in the physical lab.

With the models in place, work in the virtual lab follows a five-step process, explains Brian McFarlane, Predictum’s lead developer on this project.

First, the virtual lab pulls the latest data from the database into a customized user interface in JMP.

Next, researchers select from thousands of recipes and variants; they add or remove ingredients from a formulation; and then they design their virtual experiments using the Custom Designer in JMP. They may test the recipes for such properties as hardness or response to extreme heat.

“Formulations can be edited while the virtual lab provides important information about the current recipe and how it will be modeled,” McFarlane explains.

After that, the virtual lab generates SAS code, sending those experiments to SAS for modeling. SAS executes the experiments and performs the complicated modeling, returning a data table with the modeled properties to JMP.

Finally, researchers use JMP to explore and visualize the results with such features as the interactive Prediction Profiler and dynamic graphs like the Surface Plot. Researchers can then refine their recipes and physically test only the most promising formulations, thus accelerating innovation.

The screenshot shows a JMP window titled "2. Experimental Design" with a sub-tab "Design Editor". Below the tab is the "I-Optimal RSM Edit Panel". The panel contains a text box: "Enter AMT values for factors you wish to vary in your experimental design." Below this is a table with columns: "Ingredients", "AMT", "ACT", "Low Level", and "High Level". The table lists several ingredients with their current values and ranges. At the bottom of the panel is a "Build Design" button. Below the panel, there are two buttons: "Continue with current design to Submit for Analysis." and "Save and Submit for Analysis".

Ingredients	AMT	ACT	Low Level	High Level
binder	0.2	0		
Binder 1	60	0	60	90
Binder 2	5	0	2	8
Catalyst 1	45	0		
Enhancer 1	9	0		
KCl	10	0	8	12
NaCl	5	0		
Powder 2	6	0	4	8
Powder 3	46.4	0	44	48
Powder 4	48.6	0		

The virtual lab interface in JMP is a custom-made application built using JMP Scripting Language. The user identifies the factor levels so that the virtual lab can design an experiment, which SAS then runs.

JMP® and SAS®: A complementary pair

The virtual lab showcases how seamlessly SAS and JMP integrate and how well they complement each other because each brings unique capabilities to the project.

“The virtual lab extends the analytical power and benefits of SAS to scientists who typically wouldn’t use SAS. In fact, they probably don’t even know they’re using SAS,” says Erin Vang of Predictum, who focused on the JMP and SAS integration aspects of the project.

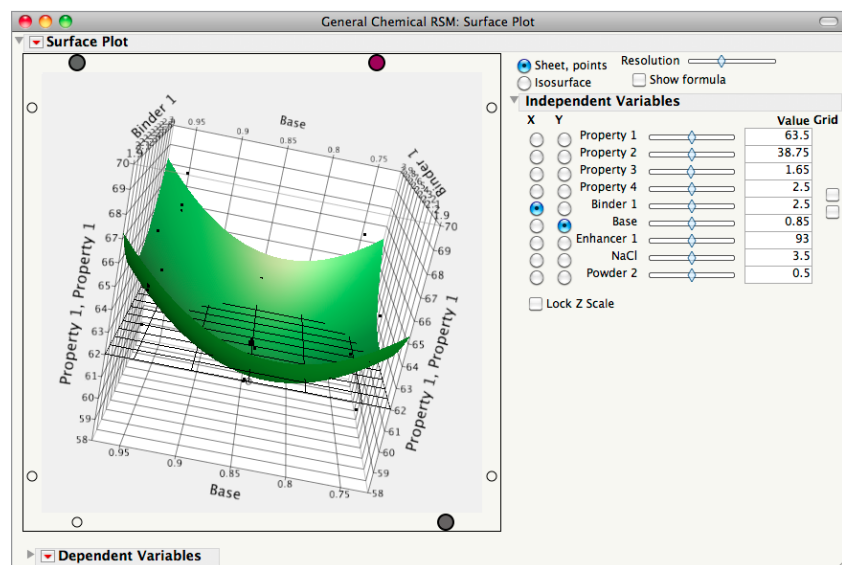
The JMP Surface Plot graphs points and surfaces in three dimensions. It enables users to examine the effect of two factors simultaneously. Users can rotate the plot and see relationships between the variables from all perspectives.

The scientists may not know much about SAS, but they are already sold on the value of the research method known as design of experiments, or DOE.

“They know DOE is the way to go for efficiently figuring out how to optimize a system by adjusting inputs to result in the best possible outputs,” Levin says.

Researchers are also enjoying the ability to explore trade-offs across different properties of materials using interactive, easy-to-use visualizations in JMP.

For example, the Prediction Profiler enables them to instantly see the effects of changing a single factor and to discover interactions among factors.



The JMP Surface Plot graphs points and surfaces in three dimensions. It enables users to examine the effect of two factors simultaneously. Users can rotate the plot and see relationships between the variables from all perspectives.

Creatively developing an interface with JMP® Scripting Language

Essential to the development of the virtual lab is the JMP Scripting Language (JSL). By using JSL, Wayne Levin and his Predictum team creatively built a custom interface for researchers to use in JMP.

For example, researchers needed to do some calculations on active ingredient levels in order to choose levels in their experiments.

“Rather than ask them to pull out their calculators or switch to another application, we quickly created and integrated an easy point-and-click facility right in the interface, which we had already largely developed,” says Brian McFarlane, Predictum’s lead developer of the virtual lab.

The Predictum team developed the virtual lab incrementally and sought feedback at each step so that the company got exactly the application it needed. JSL was a natural fit for this type of approach because it is flexible, requiring less rewriting of code as the company requested changes, Levin explains.

“The flexibility of JSL let us get a better sense of what the company was looking for and how the users wanted the application organized. Ultimately, it meant that we delivered value earlier in the implementation process.”

The next phase of development is to streamline the graphical user interface.

“We’ll add new features to take even more advantage of the unique capabilities that using JMP and SAS together offers,” says Levin.

“The visualization capabilities let scientists focus on their areas of expertise – making better formulations. They don’t need to be worrying about statistics,” Levin explains.

But they certainly needed more than spreadsheets, which Levin says are too limited in their analytics and visualization abilities to be of real help.

“The whole purpose of analysis is to get insights. And if you’re doing analysis on spreadsheets, you’re getting just a fraction of those insights,” Levin says.

Saving real money

Partnering with the Predictum team has resulted in substantial cost savings. The company got the virtual lab

for about a third of the expense of hiring a development team to build it from scratch. And the company was able to further leverage the SAS resources it already had.

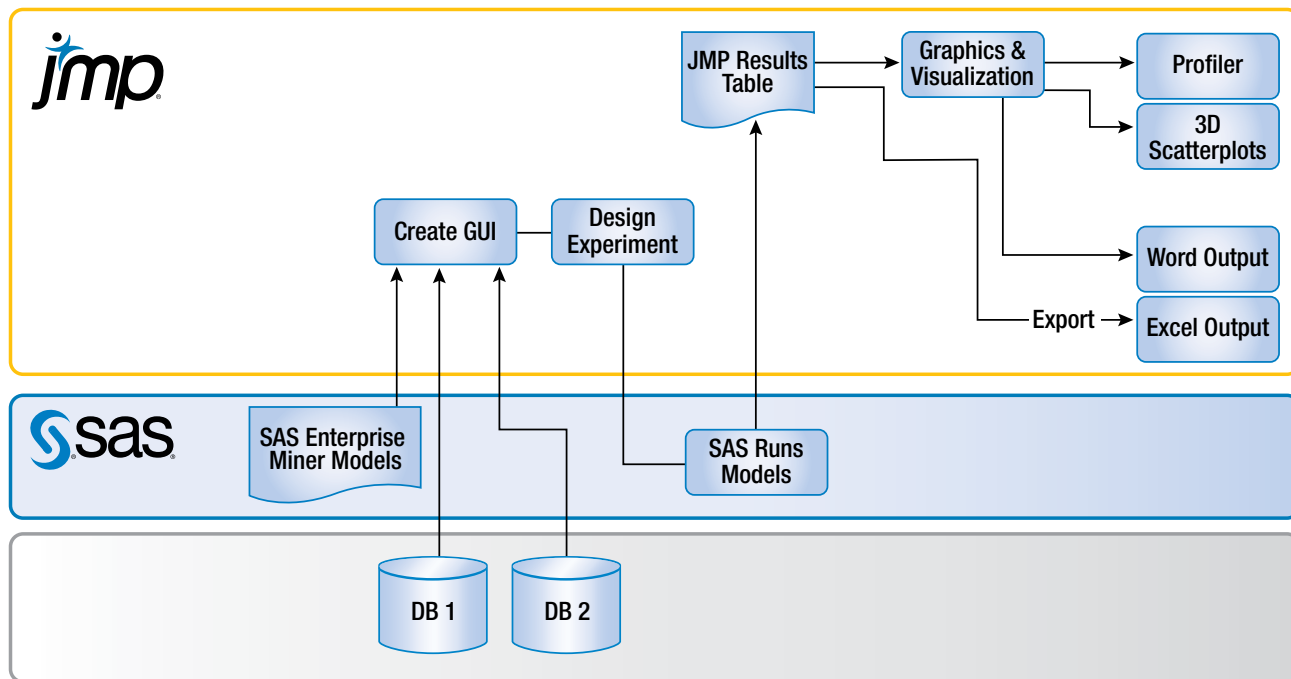
Competitors’ systems would have required more maintenance and customization. The JMP and SAS combination, on the other hand, is expandable and scalable as data increases, and it allows for continual improvements to the models without needing to edit the JSL that makes up the virtual lab.

The virtual lab is now in the company’s research centers in both the US and Europe, where each center employs its own model variants but uses exactly the same code. Researchers are increasing the pace of R&D and

getting the full benefit of decades’ worth of company data. Plus, the company is saving money in its physical labs, which no longer repeat tests unnecessarily.

For the Predictum team, the experience of working on this project has been both intellectually and professionally rewarding.

“Because of this uniquely capable software, we get to be creative and play a major role in this company’s future prosperity, and that’s exciting and very satisfying,” Levin says.



The virtual lab has a graphical user interface (GUI) that accesses databases and models created with SAS Enterprise Miner. Because it draws data from these sources, the GUI is complete with the most current information available. The virtual lab then assists scientists in designing experiments using JMP’s Custom DOE platform. It then combines the DOE with the SAS models and uploads the DOE to SAS for evaluation. The results are then returned to JMP for analysis and recorded for use in writing reports.