Optimizing Architectural Coatings with INForm

Rheology modifiers are added to architectural coatings to ensure that they have the required flow properties, to facilitate improved application behaviour, as well as enhancing storage properties. The aim is to have a coating that is easy to apply, and that does not readily sag or drip. Especially with recent legislation that requires lower VOC emissions, formulators need to meet he challenge of using cost effective replacements for traditional thickeners. An added complication is that rheology modifiers affect properties that directly impact upon the customer's perception of the quality of the coating.

Traditionally, statistical methods have been employed to generate models, with response surfaces used to try to determine optimum formulations. However, this often means that the problem is over-simplified in order to render it tractable. The current data, taken from a statistical study, provide a case in point, since only three ingredients and two properties have been included.

A powerful alternative, **INForm**, has now been developed by Intelligensys. **INForm** integrates neural network modelling with efficient optimization routines based on Genetic Algorithms. **INForm** lets the user bypass many "what if" questions typically required to find an acceptable formulation, and instead tells the user directly how to achieve certain properties (like viscosity, flow, and hiding power) with minimum effort.

To use **INForm**, you carry out some initial experiments, and feed these into the neural network directly from your spreadsheet package. Once your model is developed, you can then specify the values of the properties you want, and the relative importance of any conflicting properties. The optimization process will tell you what conditions are required to obtain them. Cost can even be included as a factor if you wish, and the optimum solution is obtained in seconds, saving you valuable time.

Rheology Modifiers for Coatings

Although **INForm** does not require 'designed' data, the study we found in the literature did use a statistical experimental design, in which the amounts of three different rheology modifiers were varied. The sum of the amounts of the rheology modifiers had to add to 100%, and a simplex lattice was used in the experimental design. Experiments at vertex points (those which involved only one modifier) were carried out twice, to give an idea of the experimental variation in the results. This meant that there were 13 experiments, 10 of which were unique combinations of rheology modifiers.

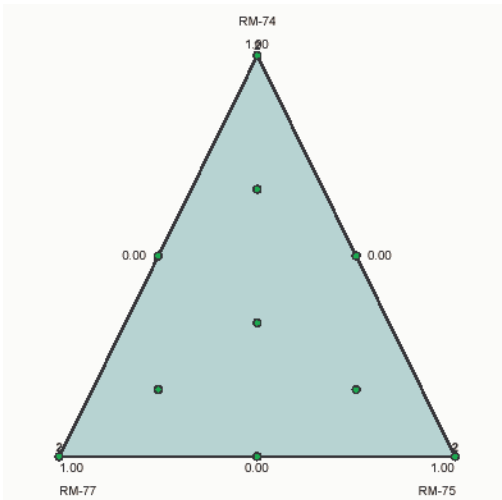

Figure 1. The 10 unique points used in the experimental design.

Two properties were measured. These were the ICI Viscosity, and the Leneta flow (which gives an indication of the anti-sag properties of the coating).

The 13 experiments were typed directly into **INForm**. One of the experiments was withheld for experimental validation, and the models were trained on the other 13 values, using the default parameters set up within **INForm**.

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Results

As expected from well-designed data, good models were developed for both properties, with ANOVA statistics giving R^2 values of 99% and 96% for the ICI Viscosity and Leneta Flow respectively. This is encouraging because it indicates that other variables, not included in the study, are not having a significant effect on the results – therefore, accurate cause – and - effect relationships have been captured.

The Leneta flow depends non-linearly on the amount of the modifiers, as Figure 2 indicates.

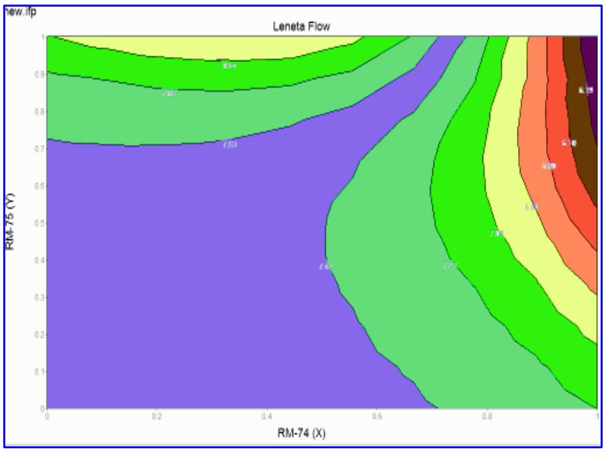

Figure 2. Contour plot for Leneta Flow as a function if RM-75 and RM-74 amounts.

Figure 3 shows the effect of changing RM-74 and RM-77 on the ICI viscosity. Clearly, RM-74 has relatively little effect – although we must bear in mind, of course, that the amount of RM-75, not shown in the plot, might have an effect. The analogous plot for RM-77 and RM-75, not shown here, indicates that RM-75 also has a small effect on viscosity.

Optimizing the Formulation

In the present example, we are looking for a formulation that has viscosity in the range of 0.5 to 0.7 poise, and Leneta flow in the range of 7.5 to 8 ASTM units.

Both properties were treated as equally important here. However, it is worth noting that for **INForm**, it is easy to weight different properties differently, emphasizing the most important ones – something that is not easily achieved with response surface methods.

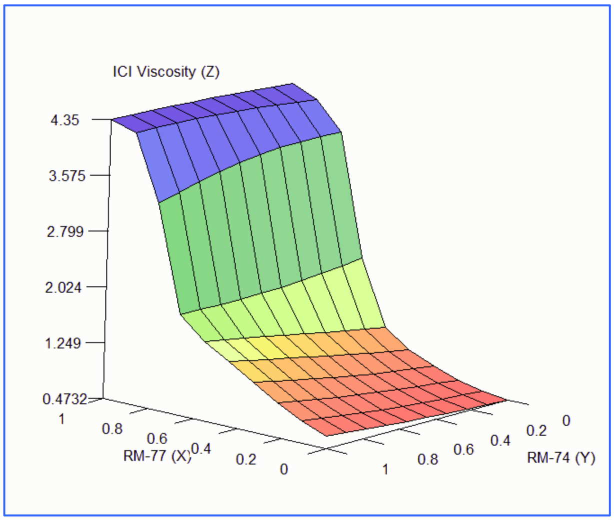

Figure 4. Effect of RM-77 and RM-74 on ICI Viscosity.

The optimum formulation was predicted to be

- 0.14 parts RM-74
- 0.26 parts RM-77
- 0.60 parts RM-75

and has an expected ICI viscosity of 0.57 poise, and Leneta flow value of 7.68 ASTM units. These properties are well within the ranges specified in the optimization, showing clearly that both properties can be achieved by a judicious blend of rheology modifiers.

Conclusions

- Despite the relatively few data points, good models could be developed. These compare well with statistical models.

- The genetic algorithm optimization found an optimum as good as that obtained by response surface methods.

- The neural computing modelling and genetic algorithm optimization could have coped with a significantly larger and more challenging problem!

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