Optimizing Paint Rheology Using INForm

Rheology is important in controlling how paints behave when they are applied to substrates. Properties like sagging and levelling are critically dependent on the amounts of the solid components (pigment, extender, matting agent, rheology modifier) that is added to the formulation. There are interactions between the different ingredients (as confirmed by a parallel study we carried out using **FormRules**) and this can make it difficult to produce a formulation with optimum properties.

Leskovšek, Tušar, and Tušar (*Rheology* **95** 140-145 (1995)) have modelled the rheological and mechanical properties of a high-solids polyester-based paint, using both linear polynomial models and neural networks. Their work involved 5 input variables, specified as weight percentages, and they carried out 23 unique experiments (with two repeats of one of the formulations). They studied 11 output properties, but reported data only for one of these, the yield point τ_0. This is the property we have examined here; it is particularly relevant to sagging.

Neural Network Models

In the published paper, 6 nodes were used in the hidden layer; the backpropagation algorithm was not specified. Two models were developed – one for the 7 mechanical properties, and one for the 4 rheological properties. Here, we had the data only for one output, so our output layer had just one node. However, even when more properties have been measured, it can be advantageous to develop a separate model for each, since this allows optimizations to be carried out examining the 'trade-offs' between the different properties.

In our studies, two data records were withheld for validating the neural network. The remaining 21 unique formulations (using an averaged value for the point where they were repeats) were used for training. **INForm's** default parameters recommended a 2-node hidden layer, to avoid the risk of over-training. We used the **INForm** default (RPROP) backpropagation algorithm.

Our model for yield point gave ANOVA statistics for the training set with R^2 of 0.97 supported by an f-ratio of 12.1. This indicates a very good model. The results for the test data (the 2 data records that were withheld from the training set) gave an R^2 value of 0.72, so the model should be sufficiently predictive to be useful.

Results

A parallel study using **FormRules** showed that the matting agent and rheological additive played an important role in controlling the yield point. Figure 1 shows this relationship for the **INForm** model. This has broadly the same shape as that discovered by **FormRules**, and (as was clear in the **FormRules** study) shows that the rheology modifier has the greatest effect when the amount of matting agens is at a maximum.

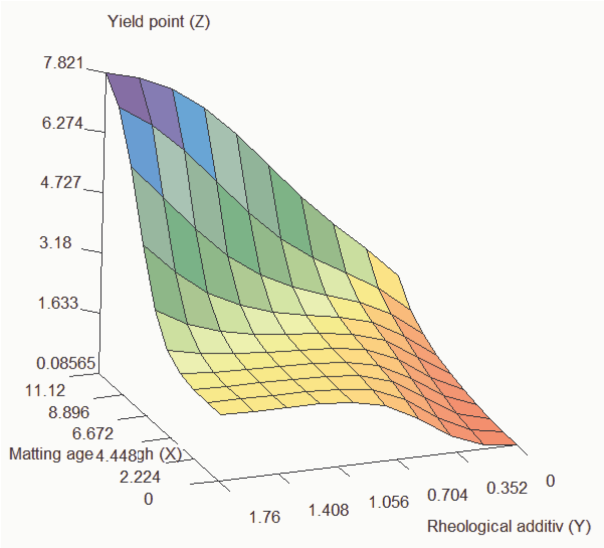

Figure 1. Yield point as a function of amount of matting agent and amount of rheology modifier

With this model, we have carried two types of study. In the first, the amount of rheology modifier was changed. To ensure that the ingredients still sum to 100% (since they are

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weight percentages) we have decreased the amount of extender present to compensate for this increase.

Table 1 shows what happens when the amount of rheological additive in one of the existing formulations ('old') is increased by 0.2%. As can be seen, the yield point increases significantly.

	'Old'	'New'
Pigment wt %	22.53	22.53
Binder wt %	44.12	44.12
Extender wt %	24.18	23.98
Matt.agent wt %	7.61	7.61
Rheo. Add. wt %	1.56	1.76
Yield point	3.726	4.743

Table 1. 'What if' trial of 'new' formulation, increasing amount of rheological additive

In Table 2, we have decreased the amount of rheological additive, compensating by increasing the amount of extender.

	'Old'	'New2'
Pigment wt %	22.53	22.53
Binder wt %	44.12	44.12
Extender wt %	24.18	24.38
Matt.agent wt %	7.61	7.61
Rheo. Add. wt %	1.76	1.36
Yield point	3.726	3.040

Table 2. 'What if' trial of another new formulation, decreasing rheological additive

These trials show that the yield point is very sensitive to the amount of rheology modifier added to the formulation. For these studies, the pigment weight percentage, matting agent percentage and binder percentage remained fixed. The fixed matting agent percentage is a bit higher than the mid-point between the minimum value of 0 and the maximum value of 11.12. As Figure 1 shows, if the matting agent percentage was larger, we might expect the sensitivity of the yield point to the amount of rheological additive to be even greater.

The second type of study that we undertook is an optimization, using **INForm's** genetic algorithm optimization capabilities. Here, we have information for only one property, so we cannot examine the trade-offs usually required in balancing yield point with other properties like hardness, elasticity and adhesion.

Within **INForm**, it is possible to constrain the optimization so that the ingredients sum to a fixed value – here, 100%. This constraint was implemented for our study.

Increasing the yield point will decrease the possibility of sagging – although of course it could impact negatively on other properties. In our optimization, we looked for a maximum in the yield point. This was found for the formulation outlined in Table 3.

	Optimum formulation
Pigment wt %	35.29
Binder wt %	39.33
Extender wt %	12.61
Matt.agent wt %	11.12
Rheo. Add. wt %	1.65

Table 3. Optimum formulation for high yield point

Conclusions

Using 21 data records for training, with 2 withheld for validation, good models were developed with a 2-node hidden layer. The models have been used successfully for 'what if' investigations, and to predict a new formulation