

Finding Rules for Paint Rheology with FormRules

Background

For high solids paints, flow control is vital because it determines important properties like sagging and levelling. The rheology of the uncured paint is determined by interactions of all the solid particles (pigment, extender, matting agent, rheology modifiers) with the binders and solvents in the system. Understanding these relationships is required if control of the properties is to be achieved.

Formulation Data

Leskovšek, Tušar, and Tušar, publishing in *Rheology* (95 140-145 (1995)) have modelled the rheological and mechanical properties of paint, using both linear polynomial models and neural networks. Their work involved 5 input variables detailed in the text-box; although they studied 11 output properties, they reported data only for 1 of these, the yield point τ_0 . This is the property we have examined here. 23 unique experiments were performed, with 2 additional repeats of one of the points.

Variables affecting Paint Rheology

- Weight % of pigment
- Weight % of binder
- Weight % of extender
- Weight % of matting agent
- Weight % of rheological additive

The data published by Leskovšek *et al* were used in **FormRules**, a package that uses neurofuzzy methods to 'mine' the data for significant interactions, presenting the results of the modelling as IF...THEN rules. 23 unique data records (with an average used for the one involving repeats) were available for the modelling.

Models for Paint Rheology

Using the default parameters (which were model selection criterion Structural Risk Minimization, $C1=0.846$ (as calculated by the **FormRules** AutoScale feature) the ANOVA statistics gave an R^2 value of

0.76. This indicates a reasonably good model, and, as the figure below shows, the yield point was affected primarily by the pigment weight, matting agent weight, and amount of rheological additive. **FormRules** discovered an interaction between the amount of matting agent and the amount of rheological additive.

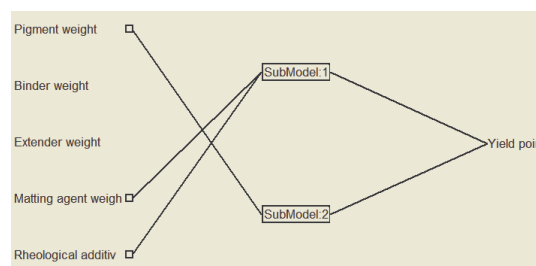


Figure 1. Important interactions discovered in model 1

Ideally, R^2 should be greater than 0.8. To achieve this, we tried a different model selection criterion – Minimum Descriptor Length. This gave a model involving all of the parameters, with an excellent fit to the training data (R^2 in excess of 0.995). However, there is a serious risk of overtraining. Since the 3 repeats show that there is an experimental scatter of between 0.159 and 0.188 for the yield point, we decided to use the rules from the simpler model.

The interaction between the rheological additive and the pigment weight, discovered by this simple model, is shown graphically in Figure 2.

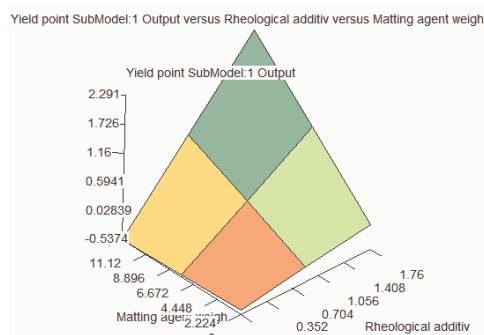


Figure 2. Yield point as a function of matting agent and rheological additive.

The more complicated model also discovered the interaction between rheological additive and matting agent. However, extender amount was involved in the same submodel, as illustrated in Figure 3.

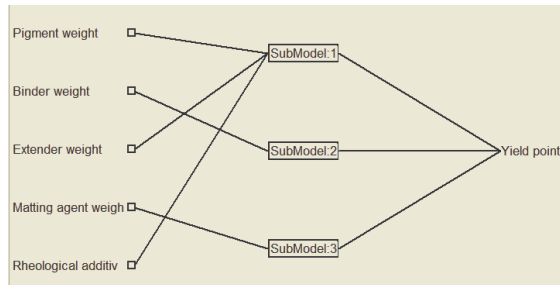
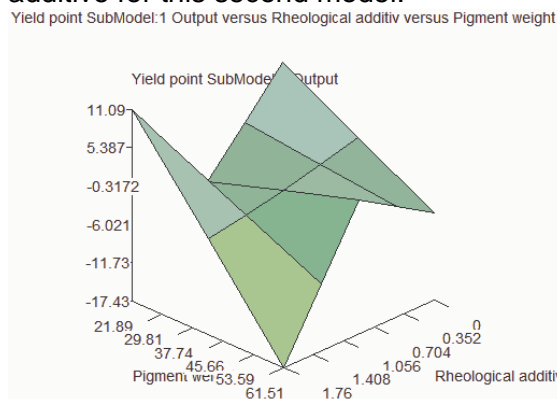


Figure 3. Model developed using MDL model selection criterion

Figure 4 shows the interaction between the matting agent weight and rheological additive for this second model.



Note that (in addition to involving different inputs) this is quite a bit more complicated than the plot from the SRM model (Model 1) shown in Figure 2. The model statistics, as discussed earlier, suggest that the model may be over-fitted – that it has fitted to noise in the system. This highlights the importance of knowing how accurately the data have been measured, in order to assess whether this complex relationship is a real effect, or an artefact of noise in the measurements.

Rules for Paint Rheology

For the simpler model (Model 1, using SRM model selection criterion) the rules from the

first submodel (combining matting agent and rheological additive) are:

IF Rheological additive is LOW AND Matting agent weight is LOW THEN Yield point is LOW (1.00)
 IF Rheological additive is LOW AND Matting agent weigh is HIGH THEN Yield point is LOW (1.00)
 IF Rheological additive is HIGH AND Matting agent weight is LOW THEN Yield point is LOW (1.00)
 IF Rheological additive is HIGH AND Matting agent weight is HIGH THEN Yield point is HIGH (1.00)

Values in parentheses are ‘confidence levels’. These rules show what Figure 2 has illustrated graphically – for low amounts of the rheological additive, the matting agent has little effect. For high values of the rheological additive, then the amount of matting agent becomes important – yield point is low when the amount of matting agent is low, but high when matting agent amount is high.

Pigment weight also affects the yield point, according to the rules

IF Pigment weight is LOW THEN Yield point is HIGH (0.69)
 IF Pigment weight is HIGH THEN Yield point is LOW (1.00)

Adding a significant amount of pigment therefore decreases the yield point.

Conclusions

FormRules has discovered the most important variables affecting the yield point. This is the amount of rheological additive, and to a lesser extent the matting agent weight and pigment weight. Although extender weight and binder weight may play a role, these materials are less significant in determining the yield point. This is consistent with results published by Leskovšek *et al.*

This study emphasizes the importance of understanding the quality of the data prior to a modelling study. In particular, experimental error in the measurements might mean that the more complicated models, developed by the non-default model selection criteria in **FormRules**, could lead to over-training.

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