

Finding Rules for Rheology Modifiers with FormRules

Background

Increasingly strict environmental legislation is driving a move towards waterborne coatings, even for demanding applications like architectural coatings. The ease of application of the coatings and the properties (for example, resistance to sag during cure) are crucial properties that must be maintained. Rheology modifiers are often added to help to produce the desired properties. New types of modifiers are frequently needed to replace traditional thickeners, but their behaviour may (initially at least) be poorly understood.

Formulation Data

Here, data were taken from a designed experiment in which amounts of three rheology modifiers were varied, with the total adding to 100%. A simplex lattice design was used, giving 10 unique points. The experiments at the vertex points were each carried out twice, to give an idea of the experimental scatter. This meant that there were a total of 13 experimental points, shown in Table 1.

Inputs were the amounts of 3 rheology modifiers referred to by the code names

- RM-74 (0 to 100%)
- RM-77 (0 to 100%)
- RM-75 (0 to 100%)

Unlike most statistical techniques, **FormRules** could have coped easily with a much larger number of inputs. As we see later, though, the experimental properties could be described well in terms of these three inputs.

Measured outputs included the ICI Viscosity and the Leneta Flow, which measures the tendency of the film to sag during cure.

We have imported the published data directly into **FormRules**, and have used the neurofuzzy technique to examine the data. The models were assessed using the Minimum Descriptor Length criterion, which aims to minimize the model complexity while ensuring there is a good fit to the experimental data used to develop the model. ANOVA statistics were used to assess the quality of the models, and for both properties gave values in excess of 0.98. This indicates an excellent fit to the experimental data.

Models for Architectural Coatings

The model for ICI Viscosity showed that this property is primarily dependent on RM-75 and RM-77. Figure 1 illustrates this clearly.

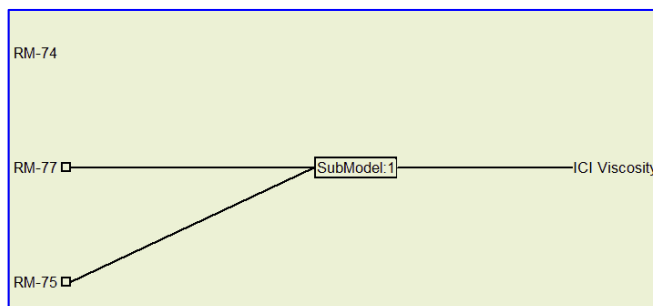


Figure 1. ICI Viscosity depends on RM-75 and RM-77

Leneta Flow depends on all three of the rheology modifiers, as shown in Figure 2. There is an interaction between RM-74 and RM-77, shown by the fact that both participate in the same submodel.

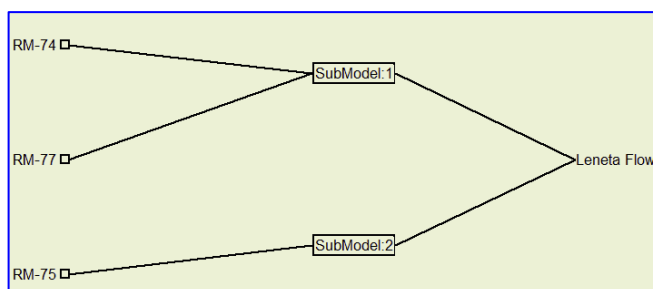


Figure 2. Leneta Flow depends on all modifiers

RM-74	RM-77	RM-75	ICI Viscosity	Leneta Flow
1	0	0	0.76	8
1	0	0	0.75	8
0.5	0.5	0	1.4	7
0.5	0	0.5	0.55	8
0	1	0	4.1	4
0	1	0	4.4	4
0	0.5	0.5	0.9	7
0	0	1	0.42	9
0	0	1	0.4	10
0.67	0.17	0.17	0.8	7
0.17	0.67	0.17	1.7	7
0.17	0.17	0.67	0.55	8
0.33	0.33	0.33	0.8	8

Table 1. Data used in modelling study

Rules for Architectural Coatings

The rules for ICI Viscosity are found by **FormRules** to be:

- IF RM-77 is LOW AND RM-75 is LOW THEN ICI Viscosity is LOW (0.92)
- IF RM-77 is LOW AND RM-75 is HIGH THEN ICI Viscosity is LOW (1.00)
- IF RM-77 is MID AND RM-75 is LOW THEN ICI Viscosity is LOW (0.76)
- IF RM-77 is MID AND RM-75 is HIGH THEN ICI Viscosity is LOW (1.00)
- IF RM-77 is HIGH AND RM-75 is LOW THEN ICI Viscosity is HIGH (0.96)
- IF RM-77 is HIGH AND RM-75 is HIGH THEN ICI Viscosity is LOW (1.00)

The numbers in parentheses represent 'confidence' in the rules. It is clear that if the amount of RM-77 is low then the viscosity is low, regardless of the amount of RM-75. If the amount of RM-77 is high, on the other hand, then RM-75 has a big factor in determining the viscosity – if there is a small amount of RM-75, viscosity is high, but when there is a large amount, viscosity is low.

The full relationships are captured graphically as shown in Figure 3.

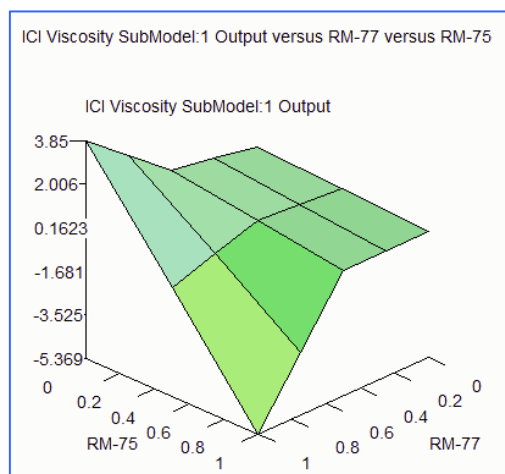


Figure 3. Graphical representation of ICI Viscosity model

The rules for Leneta flow are, from one submodel:

- IF RM-75 is LOW THEN Leneta Flow is HIGH
- IF RM-75 is HIGH THEN Leneta Flow is LOW,

both with 100% confidence. The second submodel gives a complicated set of rules:

- IF RM-77 is LOW AND RM-74 is LOW THEN Leneta Flow is HIGH (1.00)

- IF RM-77 is LOW AND RM-74 is MID THEN Leneta Flow is HIGH (1.00)
- IF RM-77 is LOW AND RM-74 is HIGH THEN Leneta Flow is LOW (1.00)
- IF RM-77 is MID AND RM-74 is LOW THEN Leneta Flow is HIGH (1.00)
- IF RM-77 is MID AND RM-74 is MID THEN Leneta Flow is LOW (1.00)
- IF RM-77 is MID AND RM-74 is HIGH THEN Leneta Flow is LOW (1.00)
- IF RM-77 is HIGH AND RM-74 is LOW THEN Leneta Flow is LOW (1.00)
- IF RM-77 is HIGH AND RM-74 is MID THEN Leneta Flow is LOW (1.00)
- IF RM-77 is HIGH AND RM-74 is HIGH THEN Leneta Flow is LOW (1.00)

FormRules automatically assigns the categories LOW, MID and HIGH as required in order to fit the data. The fact that 3 classes were required for each of RM-74 and RM-77 means that 9 rules are produced.

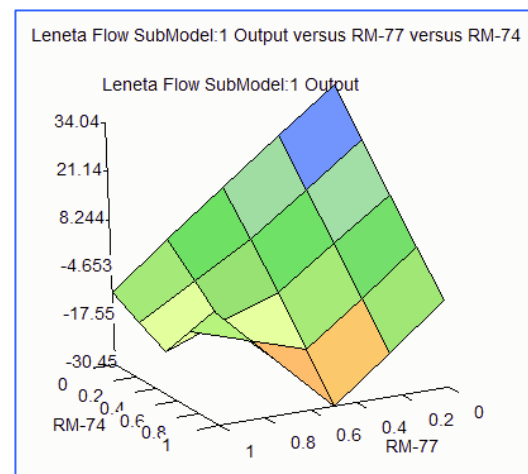


Figure 4. Leneta Flow as a function of RM-74 and RM-77

In the figure above, the point at RM-74 = 1 and RM-77 = 1 must be treated with caution, since this was not an experimental point in the design.

Conclusions

Despite the fact that there are relatively few data points, **FormRules** has been able to extract useful information largely because the data are of high quality.

The rules have found interactions between the variables that are broadly in line with the conclusions from a detailed statistical study (Stat-Ease Inc.) with no assumptions required from the user.

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