Finding Rules for Liquid Soap Viscosity with FormRules

Background

Controlling the viscosity of liquid soap is important in creating a product that meets consumer needs. In this particular example, a mixture of three different salts is used as a thickening agent, to give a liquid soap the correct viscosity. The thickening agent makes up 10% by weight of the final formulation.

The data used in this study were taken from *Response Surface Methodology: Process and Product Optimization using Designed Experiments*, by R H Myers and D C Montgomery. In their data, the formulators who supplied the original results performed an augmented simplex mixture design. No details on the exact nature of the salt have been provided in their study, and the only property that was measured was the viscosity, in centipoise.

In the present application note, we used **FormRules**, which is based on neurofuzzy logic, to mine their data to discover models and rules describing the cause-and-effect relationships in the data. **FormRules** does not require designed data, but since that was what was available, it is what is used here.

For the designed experiment, the centroid point had to be repeated 3 times. For our modelling study using **FormRules**, we averaged these three values, to give one unique centroid point. This left 10 unique data points for the modelling.

Model for Viscosity

In **FormRules**, models are fitted to the data. Over-fitting is avoided through use of a Model Selection Criterion, which is used to ensure that if models are made more complex, there is a sufficient return of information to justify the complexity. The default Modelling Selection Criterion is Structural Risk Minimization, which develops the simplest models. Structural Risk Minimization involves specifying a parameter, C_1. **FormRules** contains defaults for setting this according to the number of experiments that are available, and in the present case this value was 0.82.

Using the 10 data points available, a good model could be developed. ANOVA statistics give an R^2 value of 0.83.

Decreasing the C_1 parameter, or changing to a model selection criterion like Minimum Descriptor Length (which allows more complexity) gave R^2 values in excess of 0.99. This indicates that under those circumstances, the model has over-trained (i.e. it has fitted to the noise in the data, not just to the underlying important relationships).

The results discussed in this application note were therefore based on the simple model developed with the default parameters in FormRules (Structural Risk Minimization, with in this case C_1 = 0.82.)

Results for Viscosity

Interestingly, the only variable that was found to affect the viscosity was the concentration of the third salt, X3. This is illustrated graphically in Figure 1, which is a screenshot taken from **FormRules**.

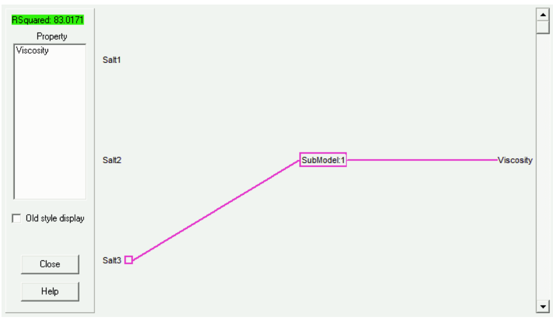

Figure 1. Graphical representation of model for viscosity of liquid soap

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The neurofuzzy approach used in **FormRules** automatically generates rules, with confidence levels, which express the relationships within the data.

In the present case, the model is very simple, and can be expressed in terms of the rules

IF Salt3 is LOW THEN Viscosity is LOW (0.77)
IF Salt3 is MID THEN Viscosity is LOW (0.96)
IF Salt3 is HIGH THEN Viscosity is HIGH (0.99)

The rule shown in red makes the greatest negative contribution to the model, while the rule in blue makes the largest positive contribution. Values in parentheses are 'confidence levels'. The value of 0.77 for the first rule indicates that the value is 'low-ish' i.e. lies towards the low end of the range.

The functional form of the relationship is also given, as illustrated in the screenshot shown in Figure 2. It is worth noting that this helps to clarify what is meant by the confidence limits given in the rules. For example, when X3 is low (at the left hand side of the plot), the viscosity is low, but not as low as it might be. On a 'low to high' axis, the value when X3 is at its lowest would lie at a point 23% from the low end, and 77% from the high end.

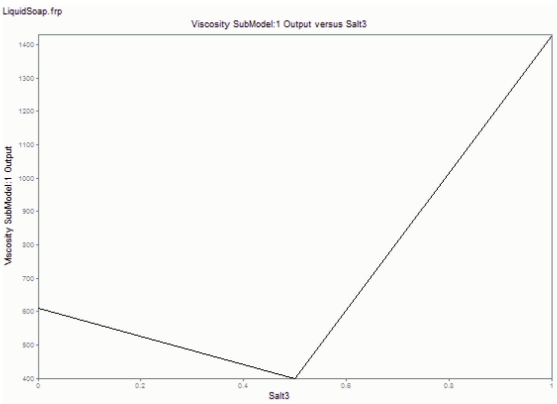

Figure 2. Relationship between amount of salt X3 and the viscosity of the liquid soap

Here, it is clear that at relatively low concentrations, salt X3 has relatively little effect on the viscosity. Indeed, increasing it up to about 50% of its possible range actually leads to a small decrease in viscosity. However, above this point, further increases show a sharp rise in viscosity.

Conclusions

In this simple example, **FormRules** has quickly discovered the most important relationships within the data. No assumptions on the part of the user were required, and the models were developed within seconds on a modern PC.

The results show that only one salt, X3, makes a significant impact on the viscosity of the liquid soap. The relationship between the amount of this soap and the viscosity is clearly very non-linear.

For further information on FormRules, and applying neurofuzzy logic to your problems, contact us at the address below.

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