Optimizing Viscosity of Liquid Soaps with INForm

Liquid soaps usually containing thickening agents that give them the correct viscosity to meet consumer needs. In the present study, a thickening agent made up of three different salts was added to a liquid soap formulation, so that it made up 10% of the total weight.

The data used in this study have been taken from the book *Response Surface Methodology: Process and Product Optimization using Designed Experiments*, by R H Myers and D C Montgomery. The amounts of the three different salts were varied, subject to the constraint that they made up 10% by weight of the final formulation. Other ingredients in the liquid soap, and the process variables, were kept fixed in this study.

Just one property – viscosity – was measured. Values are given in centipoise.

Although neural networks do not require designed experiments, because this data set was available we have chosen to investigate it using the **INForm** formulation modeling and optimization program. 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 product properties you want, and the optimization process will tell you what ingredients and process conditions are required to obtain them, within the limits of the overall data you have scoped out.

In the case of the data taken from the book by Myers and Montgomery, the data set followed a simplex mixture design. (The term 'mixture design' indicates that the three ingredients had to add up to a fixed amount, in this case 10% of the weight of the liquid soap.)

The centroid point was replicated three times in their study, and in the present application note these three replicates were averaged to give one point. This meant that there were 10 unique points in total available for the modeling study.

Model for Viscosity

A data mining study using **FormRules** showed that a good model could be developed from this data set, and as expected the neural network within **INForm** was able to generate a good model using the default parameters.

However, there is one point to note here. Usually with neural networks, some of the data points are removed from the training set, and used to 'test' the predictivity of the network. When the data has been experimentally designed, there is always some risk associated with removing some of the data. Testing the network is important, though, so one data point (10% of the total) was withheld from the training set so that it could be used in training.

INForm selects the neural network architecture taking account of how many ingredients there are, and how many experiments have been performed, and in the present case this led to a network with 2 nodes in the hidden layer. The default parameters within **INForm** gave a model with R^2 value of 0.88 indicating a good fit to the data. (Different values, of course, might be obtained if alternative data records had been withheld from the training set, and used in testing the network.)

The predicted vs. actual values are shown in Figure 1. This shows that the model is predicting the data well, and in addition shows clearly that one formulation, involving pure X3, is significantly more viscous than any of the others.

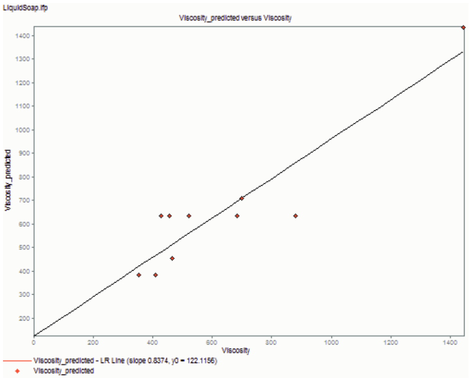

Figure 1. Actual vs predicted viscosities

Results for Viscosity

The viscosity responds non-linearly to the concentrations of the various salts, and is most sensitive to changes in the amount of salt X3.

This can be seen by using **INForm's** Visual Explorer, which lets the user examine interactively how the response surface is affected when the value of one of the hidden variables is changed. Figures 2 and 3 show how the response surface (with X3 and X2 as the main variables) changes when the amount of salt X1 is changed. Figure 2 shows the surface when X1 is 0, and Figure 3 when it is at its maximum value.

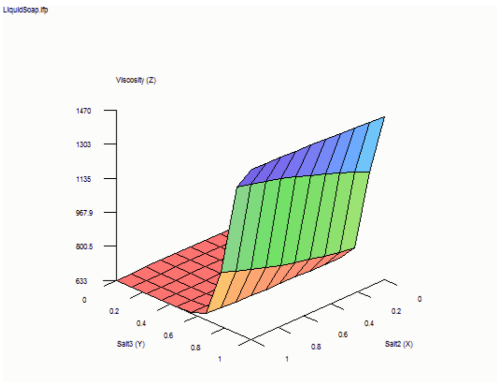

Figure 1. Response surface when X1 is 0

There are clearly some substantial changes. However, one noteworthy feature is that the value of the viscosity remain virtually unchanged with the amount of X2 is varied.

Optimizing Viscosity

One of **INForm's** strengths lies in its ability to combine modeling with optimization, to obtain specific desirable properties. In the present study, there is only one property, so **INForm's** ability to examine trade-offs cannot be demonstrated here. However, it is possible to develop a formulation to meet specific requirements.

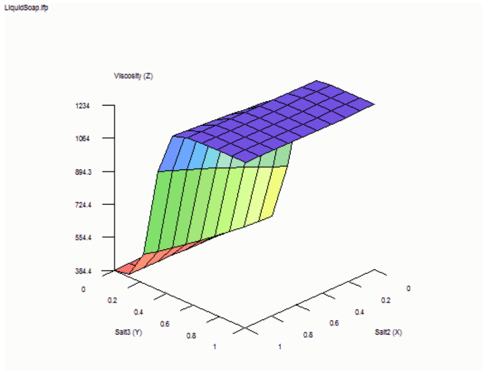

Figure 2. Response surface when X1 is at its maximum

Myers and Montgomery ask the reader to find a formulation with viscosity 900 centipoise. We used the same requirement in **INForm**, and set up a constraint that the amount of the three salts had to sum to a constant value (10% by weight of the final formulation).

Five different populations were used, to develop five optimum solutions. These are shown in the table below.

	X1	X2	X3	Viscosity
1	0.016	0.009	0.075	900.
2	0.006	0.014	0.080	902.
3	0.023	0.006	0.072	902.
4	0.003	0.016	0.081	898.
5	0.024	0.005	0.071	901.

These results show that a significant amount of X3 is required. However, too much X3 will give too high a viscosity, and the other salts must be present in small amounts to give the correct behaviour.

Conclusions

Neural networks have been able to generate a good model quickly and easily, using the default parameters within **INForm**. The model could be used to produce an optimum formulation.

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