

Optimizing Shampoo Foam Height with INForm

The amount of foam produced by a shampoo is often one of the criteria that consumers use to assess how good it is, largely because it is readily visible to them. Consequently optimizing the foam height can be an important part of developing a product to be marketed.

In a study discussed in the book *Response Surface Methodology: Process and Product Optimization using Designed Experiments*, R H Myers and D C Montgomery give data from a designed experiment in which three different ingredients were varied, and the foam height (in mm) was measured.

The three ingredients that were varied were

- Lauryl sulphate: between the limits 20% and 30% (X1)
- Cocamide: between the limits 7% and 10% (X2)
- Lauramide: between the limits 13% and 20% (X3)

Just the one property – foam height – was measured.

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.

The **INForm** software package integrates neural networks with efficient optimization routines based on Genetic Algorithms. The neural network-based formulation model lets the user bypass many "what if" questions typically required to find an acceptable formulation, and instead, tells the user directly how to achieve certain properties with minimum effort.

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 Montgomery's data, it followed a D-optimal design involving a number of replicates. In the study undertaken in this application note, the replicate values were averaged so that only unique points were used. 9 unique points were available for modeling, once the averaging procedure had been undertaken.

Modelling Shampoo Foam Height

A corresponding study undertaken with **FormRules** showed that good models could be found from this data, although it required adjustment of some of the parameters.

The same is true here. Because there were so few points, none were held back for validation of the network, and assessment of the goodness of fit was based solely on the ANOVA statistics.

We found that a neural network with 2 nodes in the hidden layer, and asymmetric transfer functions on both the hidden and output layers, gave a good model when the standard batch backpropagation algorithm was used.

This gave a model whose ANOVA statistics showed an R^2 value of 0.91. The fit of actual vs. predicted values is shown in Figure 1. The agreement is well within the experimental error as indicated by the results from the replicate studies.

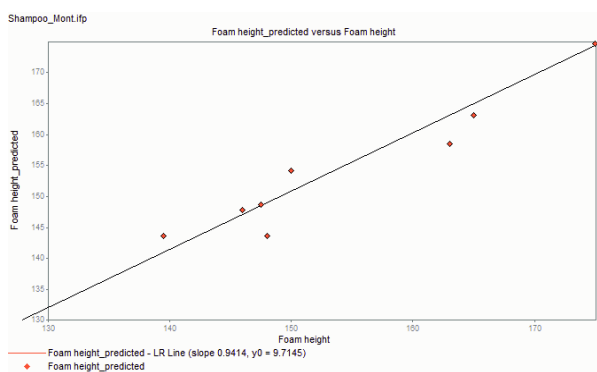


Figure 1. Actual vs. predicted values for shampoo foam height

The related **FormRules** study (given in a separate application note) showed that cocamide and lauramide concentrations were the most important variables.

The **INForm** Visual Explorer allows the user to investigate interactively the effect of changing ‘hidden’ variables, which affect the response surface indirectly. Response surfaces in this case are complicated to interpret, because there is a summation constraint that the sum of the three ingredients must be 50% of the shampoo formulation. Therefore, not all possible points on the response surface are accessible in practice.

Two different ‘snapshots’ from the Explorer are shown in Figures 2 and 3. In Figure 2, the amount of lauryl sulfate is at a maximum, while in Figure 3, it is at a minimum.

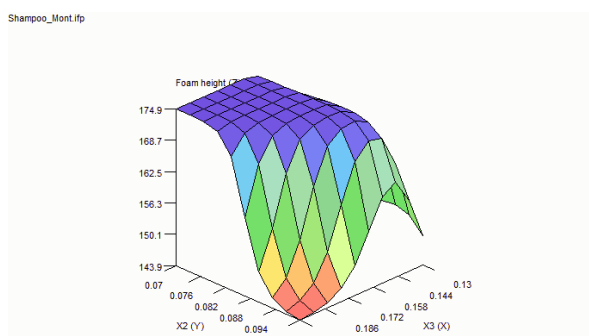


Figure 2. Response surface for 30% lauryl sulfate

INForm’s other strength lies in optimization. In the present case, there is only one property, so the full advantages of being able to explore the trade-offs in achieving one property rather than another cannot be

investigated. However, it is quick to find an optimum formulation i.e. one in which the foam height is at a maximum.

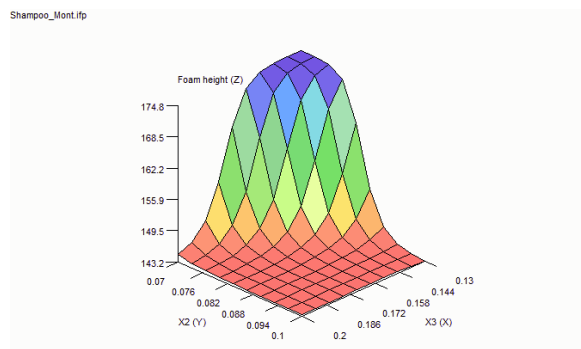


Figure 3. Response surface for 20% lauryl sulfate

INForm’s optimization allows for constraints to be set, so we postulated a requirement that the amounts of the three ingredients had to add to 50%. A population of 5 optimum solutions was generated, and all 5 were substantially the same, with.

- Lauryl sulfate 26%
- Cocamide 7%
- Lauramide 17%

The amount of cocamide is the minimum that was in any of the formulations in the ‘training’ set, and the optimization suggests that perhaps it should be decreased further.

Conclusions

Good models could be developed, although this required some changes to the default parameters within **INForm**. These were of similar quality to the models extracted from statistical methods. However, it was much quicker to find the models than it was via statistics.

Optimization using **INForm’s** genetic algorithms was also very fast. With a requirement that the foam height be as high as possible, a formulation within the range of the experimental results – but differing from any of the trial formulations – was discovered.

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