

Optimizing Automotive Clearcoats with INForm

Automotive clearcoats are complex mixtures of mutually interacting components, formulated for specific customer demands. With new environmental pressures, the move is to decrease VOCs, leading to increased solids content in the coating. However, adding new monomers to increase the solids content tends to decrease the polymer T_g, and hence the hardness of the finished film.

Balancing these conflicting requirements is a design challenge even for experienced formulators.

The traditional approach involves statistical formulation models, with considerable experimentation and trial batching to determine how a change in formulation will change the solids content and hardness. This can become very complex when the task has nonlinear relationships and many variables.

Now, a powerful alternative, **INForm**, has been developed by Intelligensys.

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 (like the desired solids content and hardness) 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.

Modelling Clearcoats

Kruithof and van den Haak of Akzo Coatings B.V. have reported a study, using statistics, of a clearcoat containing novel monomers. Here, we have used their data, reported in *Journal of Coatings Technology* **62** 47-52 (1990) - but we have treated their data using a neural network. The present note therefore provides useful comparisons with the statistical treatment.

For each monomer, there were 20 experiments, varying the film thickness, the percent of novel monomer, and the percent of melamine formaldehyde crosslinker. Because of the limitations of the statistical package, only three variables were used - neural nets can of course cope with many more variables.

Kruithof and van den Haak found that, of the 4 monomers they considered, TMCMA led to the highest hardness, so we focused specifically on that case. **INForm** suggested a default architecture with a single hidden layer containing 3 nodes. Separate models were developed for Solids Content and for Knoop Hardness.

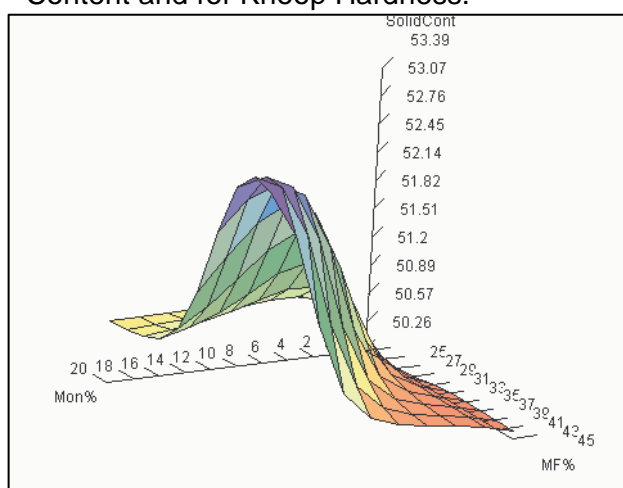


Figure 1. Solids Content as a function of MF% and Monomer %

The model for Solids Content is shown in Figure 1, and illustrates that there is a

maximum when the monomer % is high and the MF% is at the upper end. This curve is more complicated than was the relatively flat surface suggested by a simple statistical treatment. For this figure, the film thickness was constant, at 35 μm .

The effect on the Knoop Hardness is also non-linear, as Figure 2 illustrates. The Knoop hardness is at its maximum when monomer % is at the high end of the measured range, as is the MF%.

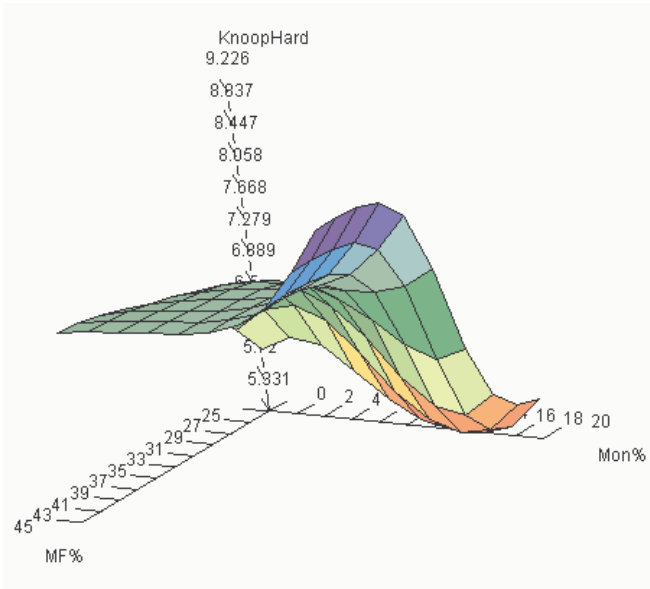


Figure 2. Hardness as a function of monomer% and MF%

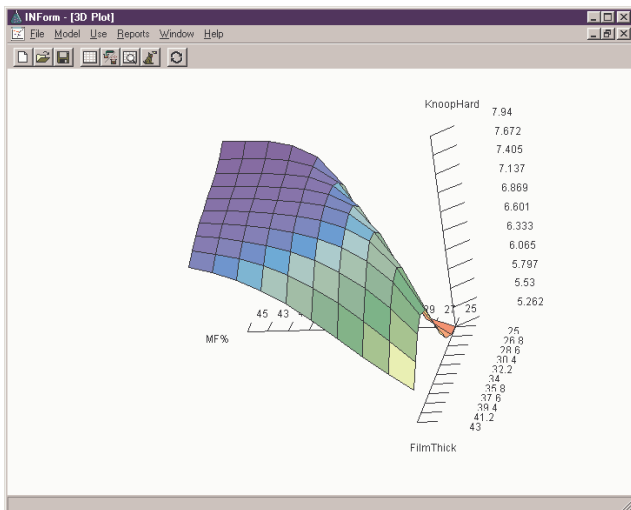
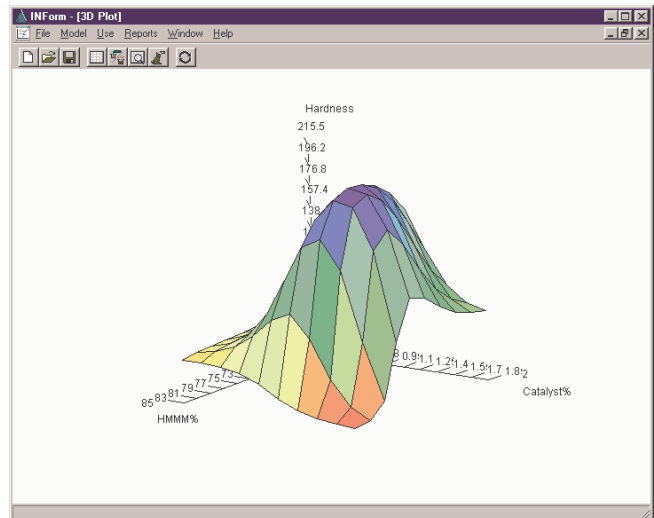


Figure 3. Maximum hardness is not necessarily attained at maximum film thickness.

High MF% therefore leads to high hardness, whatever monomer% is chosen. When monomer% is also high, then hardness is at a maximum.

Perhaps most surprisingly, the hardness is not linear with the film thickness, as plots involving film thickness show. In some cases - depending on the particular values of monomer% and MF% - hardness actually decreases with film thickness. Figure 3 shows that this is the case for high MF%, where hardness is highest for the thinner films.

Tusar and colleagues have published yet another study of clearcoat modelling, in *Surface Coatings International*, p427 (1995). Here, they present data for the change in hardness as they vary HMMM % (hexamethoxymethyl melamine), cure temperature, and catalyst concentration. They used a 3-level full factorial design with 27 experiments.



Using their data, we found (Figure 4, above) that at a temperature of 120, the maximum hardness is attained at intermediate catalyst values.

In all of these cases, since only three input variables were used, the 3D graphs showed the trends clearly. For more complex problems, **INForm's** Genetic Algorithm capability would find the best formulation quickly.

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