Optimizing Hot Melt Adhesives with INForm

Because of its low surface energy, bonding to polypropylene poses a major challenge. Polypropylene has potential as a major engineering material, but only if it can be 'welded' successfully both to itself and to other materials. Consequently, hot melt adhesives have been developed to meet this challenge, but they need to be designed carefully so that reasonable bond strengths are obtained. In a typical formulation, oligo(propene) can be mixed with SEBS (Hydrogenated polystyrene - block polybutadiene - block polystyrene) and a range of tackifiers. But determining the optimum formulation can be difficult.

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

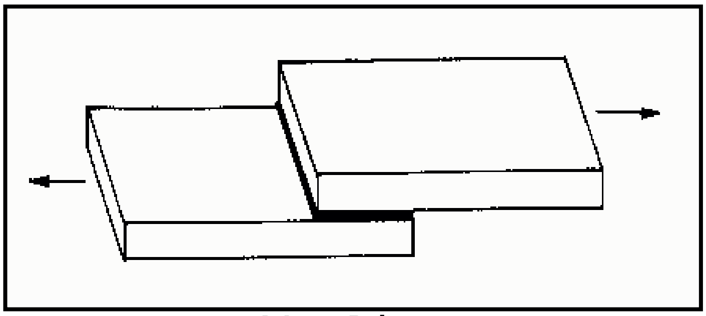
Now, a powerful alternative, ***INForm***, has been developed by Intelligensys.

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 release profile) 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 release profile you want, and the optimization process will tell you what ingredients and process conditions are required to obtain it.

Modelling Hot Melt Adhesives
Here, we have used data reported by Setz and coworkers (*Journal of Chemometrics*, **11** 403-418 (1997)) to see what neural network models can tell us about this problem. Setz *et al* used a statistical approach, and found that one model would not fit the data satisfactorily, since the mode of failure was sometimes adhesive, and sometimes cohesive (when failure took place within the adhesive itself).

The properties they measured included τ_B (the lap shear strength), $\Delta\tau_B$ and the viscosity η.



A Lap Joint

Their early 'scoping' studies indicated that the formulation should contain

- **IPP10k - an isotatictic oligo(propene) with M_n = 10,000**
- **TPE - hydrogenated polystyrene - block polybutadiene - block polystyrene thermoplastic elastomer, M_n = 83000**
- **TPEm - like TPE, but with grafted maleic acid anhydride**
- **T1 - a hydrocarbon resin tackifier, Mn = 690**
- **T2 - a straight mineral oil**

The total amount of the material had to add to 100%.

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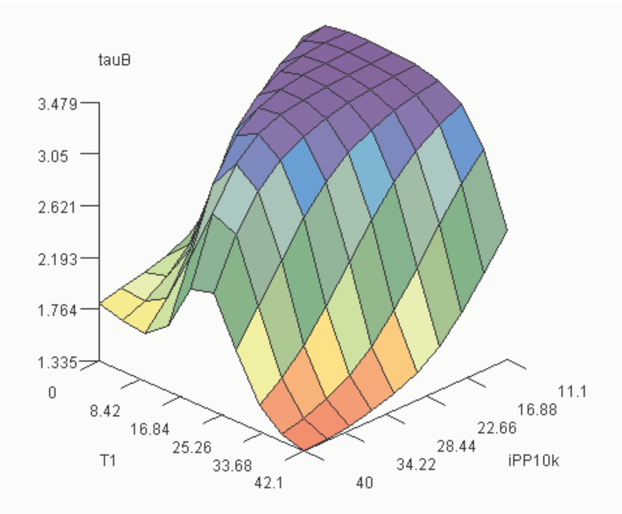
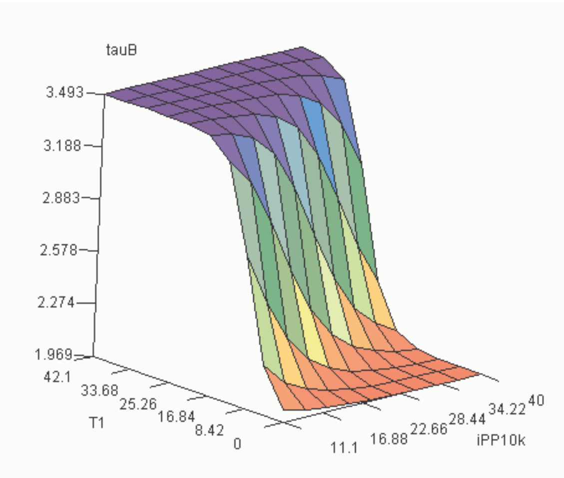
The 29 experiments were fed into ***INForm's*** main spreadsheet, and cause-and-effect models developed for each of the separate properties, using a 2-node hidden layer network. ***INForm's*** ANOVA model statistics showed that good models were obtained for the lap shear strength and for the viscosity, but the model for $\Delta\tau_B$ was relatively poor. It is worth noting that this was achieved with a single model, rather than the two separate models required by the published statistical treatment. The response surface is highly non-linear, as the figure below shows.



Of course, the shape of this plot depends on the values of the 'unspecified' variables. In the plot shown here, T1 and iPP10K have been varied. Both TPE and TPEm are at their minimum values, and T2 is zero. Within the constraint that the ingredients must sum to 100%, lap strength would be very low.

However, increasing the amount of TPE to the maximum 75% shows very different behaviour.



This is consistent with the findings of Setz *et al*, who determined that if the total concentration of the elastomers (TPE and TPEm) was too low, the joint would fail cohesively, with a low lap strength. This makes intuitive sense, since with little TPE, the low molecular weight material cannot support much strain.

Using ***INForm***, we looked for a formulation that would satisfy the two criteria:

Lap strength > 3.5 MPa
Viscosity < 3 Pa s

The constraint that the ingredients must sum to 100% was applied. Lap strength was assigned an importance of 10 on the 1 to 10 scale, and Viscosity was given an importance of 8.

The genetic algorithm optimization quickly found a suitable formulation, suggesting that we should use

28.5% T1
4% T2
28.5% iPP10K
7.2% TPEm
31.8% TPE

Conclusions

In searching a multidimensional space, ***INForm's*** ability to handle constraints and to deal with multiple objectives makes it very suitable for looking for new hot melt adhesive formulations within a known design space.

The integrated 3D graphics provide a useful check on the effect of the 'unspecified' ingredients, but a range of plots were needed to do this.

Most importantly, the neural network model could reproduce the complex experimental information satisfactorily, without needing to invoke a two-model strategy.

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