Optimizing Polyester Hot Melt Adhesives with INForm

Hot melt adhesives have some stringent design requirements. Typically, they are thermoplastic polymers which can be applied in the molten state, and which bond to the substrate to provide an adhesive joint. The melting point must not be too high, and they must have a degree of crystallinity. They must not be too viscous when they are applied, but must also not be too tacky once they are cooled. One class of hot melt adhesives that has been examined is comprised of copolyesters, in which various acids are reacted with an alcohol like 1,4-butanediol. Which acids to use, and what relative amounts of each are best, must be assessed.

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.

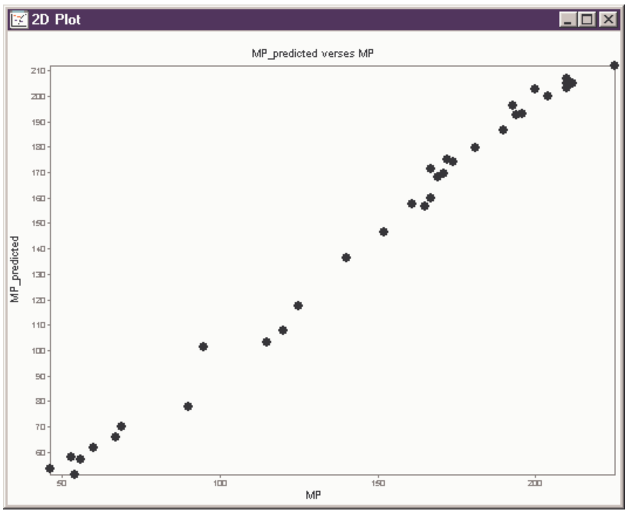
Modelling Hot Melt Adhesives

Scientists working in Dynamit Nobel (now part of Akzo Nobel) have worked extensively in designing hot melt adhesives, and much of their data is included in patent specifications.

We have used some of their data, from UK Patent Specification 1,515,727, to see how ***INForm*** can be used to understand hot melt adhesive design.

In this patent, they cite conventional polyesters in which1,4-butanediol has been mixed with terephthalic and one or two additional acids, selected from the range:

- Isophthalic acid
- Adipic acid
- Azelaic acid
- Sebacic acid
- Dim. Fatty acid, an aliphatic dibasic acid containing 36 carbon atoms



Actual and Predicted Melting Points from *INForm's* Neural Net Model

A reference formulation, containing simply terephthalic acid with the diol, was also

Intelligensys Ltd, Springboard Business Centre, Stokesley Business Park, Stokesley, N. Yorks TS9 4JZ, UK
Tel:(+44) 1642 715380 Fax:(+44) 1642 715301 E-mail: sales@intelligensys.co.uk

made. Measurements for all the adhesives included the melting point, the glass transition temperature, the damping decrement (to assess crystallinity) and the reduced viscosity.

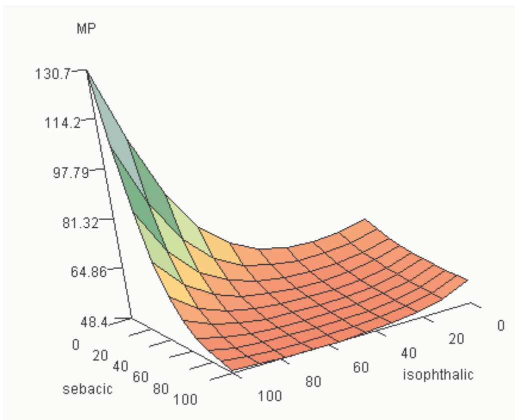
The data were typed into ***INForm's*** spreadsheet; we then defined which were ingredients and which were properties, and used the neural net to seek some cause-and-effect models. There were 37 different formulations, with the six input variables being the amount of each of the acids. We withheld 3 experiments to assess the validity of the model, training with the other 34 records. We developed a separate model for each of the properties, using a 3-node single hidden layer in each case. Excellent models were obtained for melting point and glass transition temperature, and a satisfactory model was obtained for the damping decrement. However, we obtained a poor model for reduced viscosity, suggesting that perhaps there are some other parameters which are important in determining the properties, but which have not been measured so are not taking part in the model.

We can use ***INForm's*** optimization capability to search for mixtures with specific properties. In this search, the ability to be able to constrain the ingredients is absolutely essential. Here, the sum of all the acids must equal 100, so we need to be able to define a constraint that forces this condition. In ***INForm***, when we implement a constraint, it means that non-compliant candidates are given a lower measure of 'fitness' in the genetic algorithm search.

The lower the value of the damping decrement, the higher the degree of crystallinity. Therefore, if we are looking for a material with low melting point and low damping decrement, we can set up a multi-objective optimization search. When we asked for a melting point less than 130^o, and a damping decrement less than 0.5, the optimization suggested that a mixture of adipic and azelaic acid (not a combination which had been tried in the original set) would have the best properties. Both of these acids were present in relatively large amounts in the optimum formulation, with only about 10% molar quantity of terephthalic acid in the formulation.

If we wish to search only part of the design space, it is possible to fix some of the variables (amounts of each acid) to be zero, therefore excluding them from the formulation. Within ***INForm***, this simply involves toggling 'on' the Fixed option for each variable. For example, if we search a formulation which will give Tm < and damping decrement < 0.5, but exclude azelaic acid from the formulation, then the optimization finds that the best formulation contains a lot of sebacic acid, with about 12% of adipic acid - and virtually no terephthalic acid.

Of course, in a real life situation, there will be other constraints - not least of which is the cost. ***INForm*** can optimize the cost as well, simply by allowing you to define a 'cost' output function which is a simple function of the input ingredients.



Conclusions

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

The optimizations take only seconds on a modern PC, allowing many ideas to be tested out in a short period of time.

Intelligensys Ltd, Springboard Business Centre, Stokesley Business Park, Stokesley, N. Yorks TS9 4JZ, UK
Tel:(+44) 1642 715380 Fax:(+44) 1642 715301 E-mail: sales@intelligensys.co.uk