

Optimizing Catalyst Pellets with INForm

Heterogeneous catalysts need to work in demanding environments, and often conflicting demands are made of catalyst pellets. To make them robust in use and do not disintegrate, a high tensile strength is demanded. However, so that the product yield is high, we also want a porous material with high effective diffusivity, so that gaseous reactants can access the maximum surface.

Controlling the variables in the catalyst pellet production process is essential to obtain consistent quality and the desired properties. But the interplay between the many process variables, and the range of measured properties, is very complex.

The traditional approach involves statistical formulation models, with considerable experimentation and trial batching to determine how a change in processing will change the catalyst pellet 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.

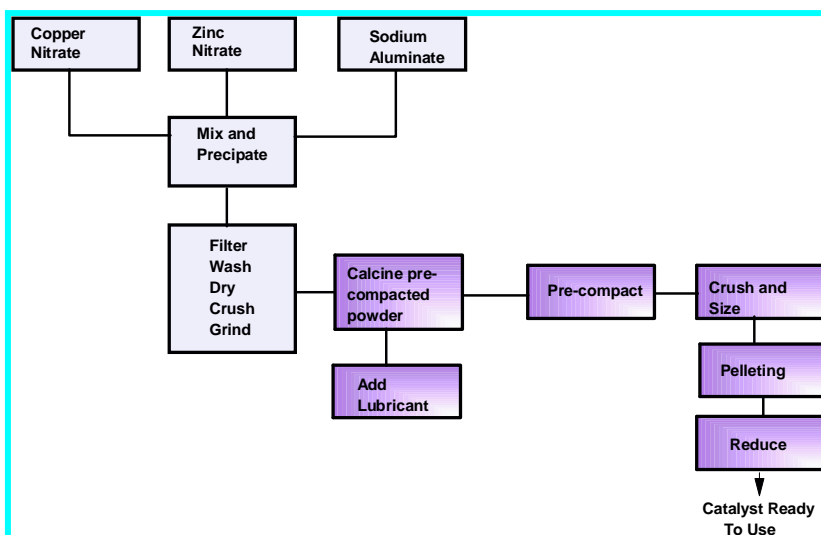
The **INForm** software package integrates neural networks with efficient optimization routines based on Genetic Algorithms. The neural network-based formulation model lets the user bypass many "what if" questions typically required to find an acceptable formulation, and instead, tells the user directly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

ICI's 52-8 low temperature shift catalyst - a co-precipitated alumina/copper oxide/zinc oxide system - is used worldwide in low temperature shift reactors. The catalyst is supplied as cylindrical pelleted particles, and is made following the process shown in the schematic below.



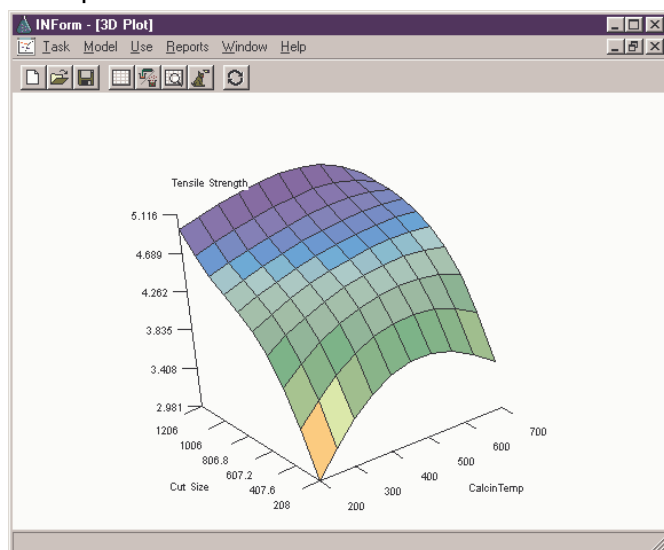
The areas shown in darker boxes involve the processing of the catalyst powder into pellet forms.

Simon Waldram and S Bhomik of University College London, UK, working with Godfrey Chinchin of ICI, have carried out a systematic study of the effects of varying six process parameters - lubricant %, precompaction load, calcination temperature, powder cut size, pelleting density, and effect of reduction - on six different pellet properties. The properties they considered were tensile strength and effective diffusivity (which they judged to be

the most important) together with porosity, tortuosity, permeability and surface area.

We used their data - 84 different experimental points - with **INForm**, to develop a cause-and-effect model that we could use to investigate the inter-relationships between pellet properties, and the process conditions used in their manufacture. **INForm** suggested that a 9-node single hidden layer network was our best option. The model statistics showed that satisfactory models were developed for most of the properties, although that for surface area was relatively poor compared to the others.

Looking at the effect of cut size and calcination temperature on the tensile strength, we see that cut size is especially important, although temperature also plays a part.



However, it is not feasible to come up with the optimum processing conditions simply by looking at the 3D graphs - there are simply too many variables to make it possible.

So, we turned to **INForm's** genetic algorithm optimization capability in our quest to see how pellets with high effective diffusivity and high tensile strength could be determined. **INForm** is ideal for complex optimizations like these, because it allows different properties to be given different weights (reflecting their importance) and

also allows us to specify the ranges in which each property should have its best values.

We weighted tensile strength and effective diffusivity at 10 and 9 (on a 1 to 10 scale), with other variables regarded to be of much less importance. Our results showed immediately that, within the range of process conditions, there was no one set of process variables which would produce a pellet with high tensile strength and high effective diffusivity. The only way that a pellet could be produced with high tensile strength was to sacrifice the effective diffusivity; in that case, the optimizer suggested that a cut size as high as possible, with a high pelleting density, would give the highest tensile strength.

If, on the other hand, effective diffusivity was of paramount importance, then cut size needed to be much lower; pelleting density also lay at the lower end of the range.

In a real-life situation, both parameters are important, and an optimization suggested that a high pelleting density, with an intermediate cut size, is best.

Conclusions

- ✕ **INForm** was able to discover the cause and effect models within the processing data with a satisfactory level of accuracy
- ✕ Optimization allowed the trade-offs between conflicting objectives to be understood and assessed
- ✕ Because of this, an experienced practitioner could use **INForm** to design a set of process conditions which will lead to reasonable values for effective diffusivity and for tensile strength
- ✕ **INForm's** modelling and optimization capability will show if a viable set of conditions can be found within the experimental space investigated

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