

Controlling Catalyst Quality with FormRules

Background

Delivery of a quality product to the market is the aim of every catalyst manufacturer, but this is complicated by the fact that there is little knowledge of how the properties of the product are affected by process conditions.

ICI's 52-8 catalyst for the low temperature water-gas shift reaction is a case in point. It is a co-precipitated mixture of copper oxide, zinc oxide and alumina, which is subsequently calcined and reduced prior to use. In order to produce a catalyst which can be handled easily, it is precompact, crushed and formed into cylindrical pellets before reduction. This process is shown schematically in Figure 1.

Characterization of the catalyst pellets is generally used to assess their quality. Tensile strength is an important property, since in a packed catalyst bed, the pellets can fail in a tensile mode. Other parameters that are important include surface area, permeability, effective diffusivity, porosity, and tortuosity.

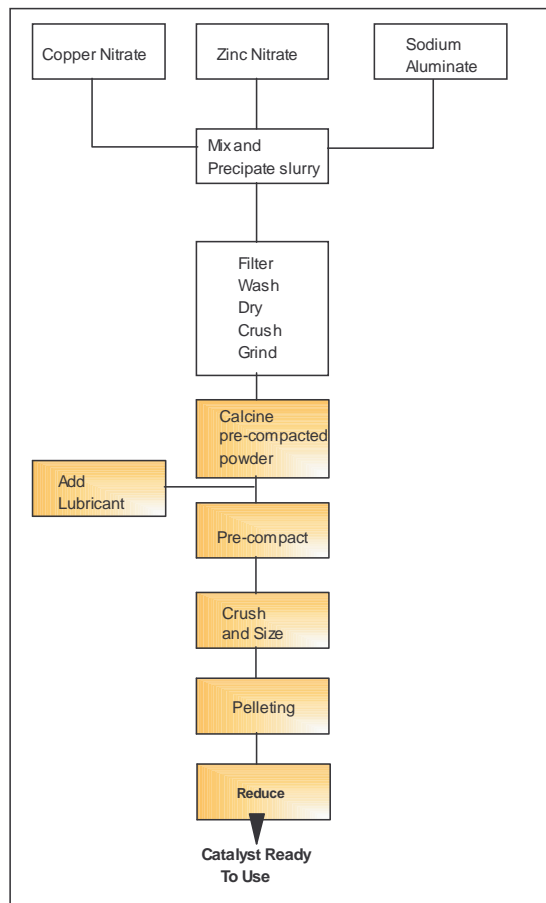
Catalyst Formulation Data

FormRules is based on neurofuzzy logic, and has been applied to catalyst formulation by Ken Waugh of UMIST, Elizabeth Colbourn of Intelligensys and Ray Rowe of AstraZeneca. This study used data from a doctoral thesis published at University College London (Waldram, *Manuf. Chemist*, Feb. 1991).

Properties that were measured were those mentioned above - tensile strength, porosity, surface area, tortuosity, effective diffusivity and permeability.

The variables in Waldram's study - which were used as the inputs to the neurofuzzy network - were

- ◆ Calcination temperature
- ◆ Amount of lubricant added prior to precompaction
- ◆ Pre-compaction load
- ◆ Particle size range of pre-compacted catalyst
- ◆ Effect of reduction - whether the pellet was 'green' or reduced
- ◆ Pelleting density



Schematic of Process Used to make 52-8 Catalyst

Catalyst Formulation Rules

Neurofuzzy logic was used to train and validate the neural network and to generate the fuzzy rules. The rules were all expressed in the form *IF (condition 1) AND (condition 2) AND (condition 3), THEN (conclusion 1 with confidence factor)*. The number of conditions in each rule is determined automatically by the neurofuzzy system.

The rules discovered for tensile strength are shown in Table 1, overleaf, while rules for effective diffusivity are given in Table 2.

| POWDER SIZE | TENSILE STRENGTH |
|-------------|------------------|
| Low | Low (0.66) |
| High | High (0.52) |

| PELLETING DENSITY | REDUCTION | TENSILE STRENGTH |
|-------------------|-----------|------------------|
| Low | Green | Low (0.85) |
| Mid | Green | High (0.63) |
| High | Green | High (0.69) |
| Low | Reduced | Low (0.89) |
| Mid | Reduced | Low (0.70) |
| High | Reduced | Low (0.72) |

Table 1. Summary of Rules for Tensile Strength

As expected, neurofuzzy logic has discovered that when pelleting density is low, the tensile strength is low. Reduction lowers the tensile strength, in agreement with Waldram's findings. Powder size is also a significant variable, especially for the green catalyst pellets. When the powder size is low, then tensile strength is low.

| PELLETING DENSITY | EFFECTIVE DIFFUSIVITY |
|-------------------|-----------------------|
| Low | High (0.59) |
| Medium | Low (0.76) |
| High | Low (0.83) |

| POWDER SIZE | REDUCTION | EFFECTIVE DIFFUSIVITY |
|-------------|-----------|-----------------------|
| Low | Green | Low(0.64) |
| Medium | Green | Low (1.00) |
| High | Green | Low (0.90) |
| Low | Reduced | Low(0.82) |
| Medium | Reduced | Low(0.78) |
| High | Reduced | Low(82) |

Table 2. Summary of Rules for Effective Diffusivity

Low pelleting densities lead to a high effective diffusivity. However, this is also the condition which (from Table 1) leads to low tensile strength, and consequently to a high probability of catalyst pellet disintegration.

Table 3 shows the rules for Surface Area, which is one of the traditional measures of catalyst behaviour. Neurofuzzy logic has discovered rules that involve the calcination temperature and the reduction of the catalyst; however, powder size and pelleting density are relatively unimportant in determining the surface area.

| CALCINATION | REDUCTION | SURFACE AREA |
|-------------|-----------|--------------|
| Low | Green | Low(0.58) |
| Medium | Green | High (0.69) |
| High | Green | Low (0.89) |
| Low | Reduced | High (0.82) |
| Medium | Reduced | High (0.68) |
| High | Reduced | Low (1.00) |

Table 3. Rules for Surface Area

In the neurofuzzy study, porosity was affected by powder size and pelleting density, with high porosity found except when the particle size was relatively large and the pelleting density was high. The calcination temperature and reduction play a smaller role for porosity.

We found tortuosity depended on reduction, and on the pelleting density - for the green catalyst, high pelleting densities led to high tortuosity. Tortuosity decreased when the catalyst was reduced.

For the reduced catalyst, low permeability related to high calcination temperatures. For the green catalyst, calcination temperature showed no significant effect.

Conclusions

This problem is of special interest since a straightforward examination with statistics did not show any strong correlations between the input variables and the output properties. Much more information has been discovered using neurofuzzy logic than was apparent from the statistical treatment.

The rules generated are those which would be expected by experienced formulators, showing that the technique can be used confidently by relatively inexperienced formulators, and for new problems where experience is lacking.

These rules can be incorporated into an expert system environment to create a genuinely self-learning formulation package.

*For further information on **FormRules** and on applying neurofuzzy logic to your problems, contact us at the address below.*

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