Optimizing Powdery Emulsion Explosives with INForm

Explosives are used commercially in blasting applications, and cost is an important factor in establishing a new explosive into the market. Of course, issues like transportability, stability prior to detonation, detonation velocity, and water resistance can also be important factors.

Recent work by Wang, Duan and Song (*Proceedings of the Annual Conference on Explosives and Blasting Techniques* 2003 **29**(1) 423-429) reports a new powdery commercial explosive, Powdery Emulsion Explosive, which has the benefits of both emulsion explosives and powder explosives. They report 20 experimental formulations, in which the amounts of 5 ingredients were varied. 4 process conditions were also investigated, giving a total of 9 possible input variables. The measured output was the 'capability/cost' ratio, where the 'capability' in this case is the detonation velocity of the explosive.

As a typical rule, it is necessary to have about 3 times as many experiments as input variables, to develop a reliable model. In this case, we have about 2 times as many. However, a preliminary study with **FormRules** (described in a separate note) showed, that the amounts of water and emulsion, and the spray pressure, did not play a significant role in determining the measured ratio. Consequently, they were left out of this study. This left 6 inputs. However, since it is a requirement that the amounts of the 5 ingredients sum to 100%, these needed to be defined as variables in the problem, even though they were left out of the models.

Here, our aims are (1) to see how well **INForm** can model this problem, using **INForm** default values and (2) to predict a formulation with the highest capability/cost ratio.

Neural Network Models

Of the 20 data records, 2 were withheld at random, to validate the model. Neural network models can be 'black boxes' and so model validation is an essential step – even when, as in this case, the amount of data is limited. **INForm's** in-built rules for determining the model architecture suggested a single hidden layer with 2 nodes. More nodes are likely to lead to over-training, since more parameters would be included in the model. Other parameters were also left at the **INForm** default values, since the aim is to see how well **INForm** can model the data with minimal user intervention.

The one exception to this is that all network connections to Water and Emulsion were 'broken' so that these inputs did not feature in the model.

The model was assessed using ANOVA statistics, which showed an R^2 value of 0.88. This indicates a very good model that should be useful for 'what if' predictions and for optimization. The actual vs predicted values, for the training set, are shown in Figure 1.

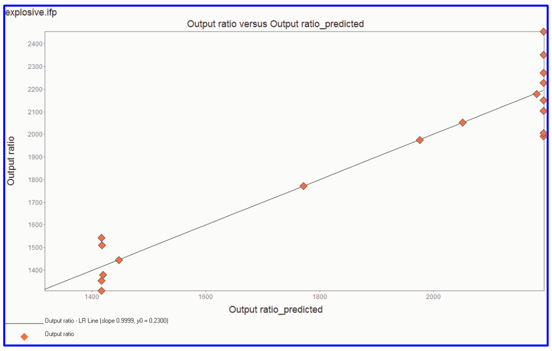

Figure 1. Actual vs predicted values for capability/cost ratio

Because the **FormRules** studies had suggested that Temperature and Whisk Rate were fairly unimportant, we also generated models in which these were excluded, i.e. a 4-input model. This gave a model which was as good (judged by ANOVA criteria) as the 6-input model above. However, it appeared that this model was more predictive, as judged by assessing the results for the Test Data set of 2 withheld records.

Results

Wang *et al* carried out their optimization by inspection, by making predictions for many possible formulations and seeing which was the best. With **INForm**, though, we can use its genetic algorithm optimization capability to home in on the best answer automatically.

For the optimization, there was a constraint on the ingredients because the amounts of all 5 ingredients needed to sum to 100%. Since the model did not involve the amount of water or amount of emulsion, the predictions for these must be treated with caution.

Our optimization searched for the formulation that gave the maximum capability/cost ratio. This formulation, as found by the optimization, is outlined in Table 1.

Nitrate	87.0
Water	5.7
Emulsion	2.3
Compound Oil	4.6
Additives	0.4
Addition speed	110

Table 1. Predicted optimum formulation for powdery emulsion explosive from 4-input model. Values are given as percentages.

The nitrate amount lies at the minimum value in the experimental data set (where it ranged between 87% to 93%, suggesting that it would be worth trying some experimental formulations in which the amount of nitrate was decreased.

The amount of water lies towards the high end of the experimental range – this can perhaps be expected, since water will be the cheapest ingredient so increasing it will lower the cost, increasing the capability/cost ratio.

The addition speed is at the high end of the range of variables used in the training experiments, suggesting that an increase in this parameter might be helpful.

We checked this with a 9-input model to see what the predicted optimum was – the results are shown in Table 2.

Nitrate	87.9
Water	5.7
Emulsion	2.5
Compound Oil	3.75
Additives	0.15
Addition speed	110
Temperature	120
Whisking rate	12.5
Spray rate	0.2

Table 2. Predicted optimum formulation for powdery emulsion explosive from 6-input model. Values for ingredients are given as percentages.

The temperature is at a minimum for the experimental rate studied – again, decreasing this could be useful.
The formulations predicted from **INForm** can be compared with the one from Wang *et al*, which had the values given in Table 3.

Nitrate	91.0
Water	3.0
Emulsion	1.7
Compound Oil	4.0
Additives	0.2
Addition speed	110
Temperature	130
Whisking rate	10
Spray pressure	0.2

Table 3. Predicted optimum formulation from Wang *et al*. Ingredient values are given as percentages.

The additional variables did not make much difference to the ability of the model to fit the data – Figure 2, for example, shows that the role of water is insignificant compared to that of nitrate

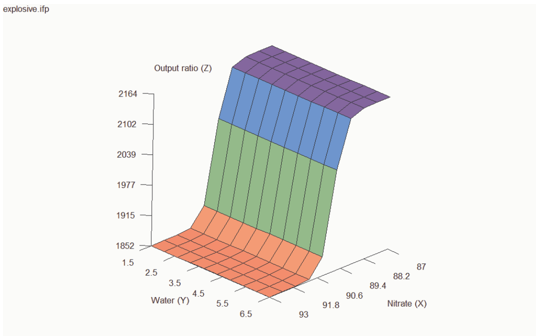

Figure 2. Effect of nitrate and of water on capability/cost ratio

Conclusions

The **INForm** default parameters gave satisfactory models for the capability/cost ratio, regardless of whether a 4-input, 6-input or 9-input model was used. The genetic algorithms also were useful in obtaining an optimum formulation.

Examination of the models and graphs showed that the key parameters were addition speed, and amounts of nitrate, compound oil, and additives, in line with the **FormRules** results presented separately

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