Nonlinear modelling of material properties
of mineral wools of different compositions

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Outline of the presentation

- ❒ What Paroc wanted to achieve in this work
- ❒ Nonlinear modelling and feed-forward neural networks
- ❒ Modelling of material properties in general
- ❒ A few material properties of mineral wools
- ❒ A quick look at several other examples/concepts

What Paroc wanted to achieve in this work

- Given certain constraints on raw materials or the composition (x) of the material:

  $a_1 < x_1 < b_1$ or $a_1 = x_1$
  $a_2 < x_2 < b_2$
  $a_3 < x_3 < b_3$, etc.

  how do we produce a material which has the right properties (y):

  $c_1 < y_1 < d_1$ or $c_1 = y_1$
  $c_2 < y_2 < d_2$
  $c_3 < y_3 < d_3$, etc. ?

Material properties

- Materials have physical properties, chemical properties, mechanical properties, thermal properties, optical properties, electrical/magnetic properties, biological properties, etc.

- Biopersistence, viscosity, refractive index are also material properties.

- *in vitro* dissolution rates of mineral wool fibres are also material properties which are related to biopersistence.

- Simple conventional tools are inadequate for modelling material properties, as we shall see later in this presentation.

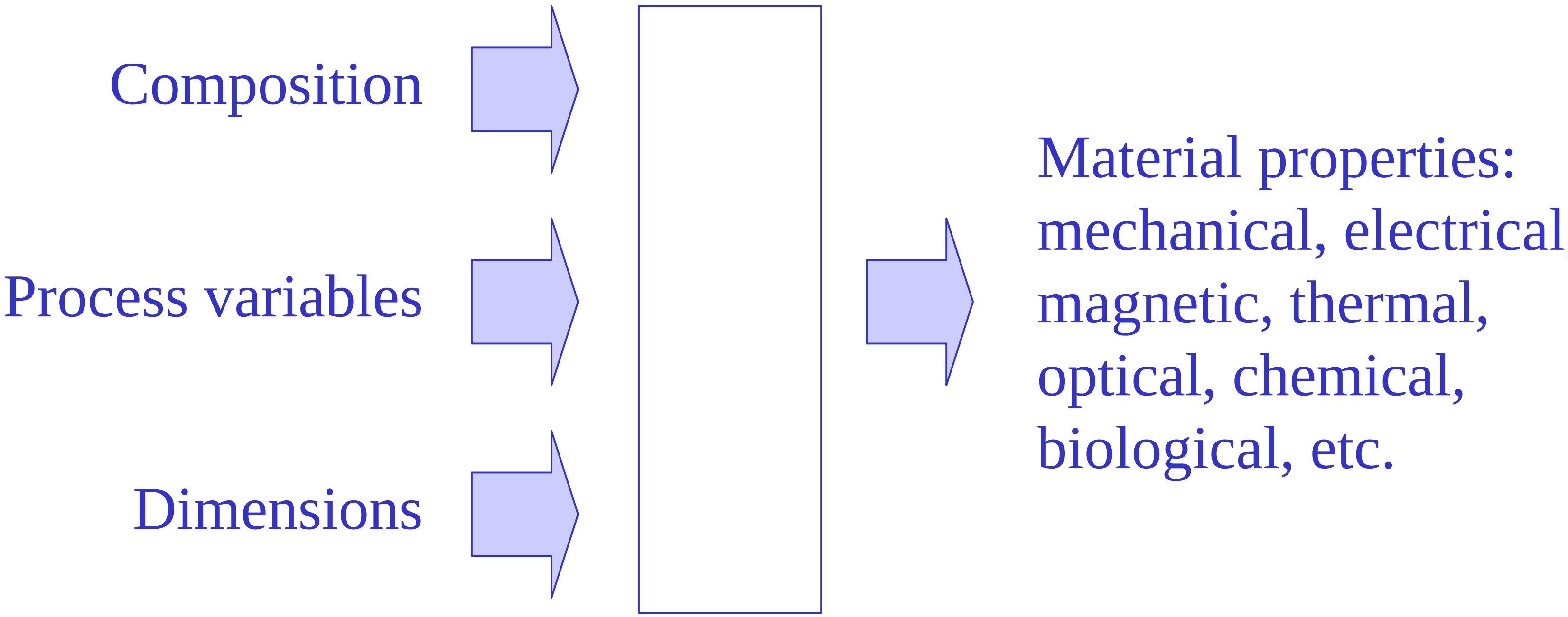
Modelling of material properties

- Material properties depend on the *composition* of the material, *process variables* by which the material was formed (if those variables are independent), and sometimes *dimension variables* like fibre diameter, particle sizes or thicknesses.

- This applies to various kinds of material properties of almost all kinds of materials.

- It applies also to biopersistence of mineral wool fibres. Process variables are not important in this case.

General framework for modelling material properties



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Development of better materials

- Development of better materials normally involves development of materials with more demanding combinations of a few material properties.

- To influence material properties, we need to know the quantitative effects of each variable on the material properties of interest.

- This is done by mathematical modelling. And mathematical modelling can be done in a number of different ways.

Forms of mathematical modelling

- Mathematical modelling can be classified into
  - physical (phenomenological) modelling
  - empirical modelling
  - semi-empirical modelling
  - stochastic modelling
- Models can be static or dynamic.
- Every mathematical model has “output variables” as well as some input information in some form.

Various mathematical modelling approaches

Mathematical modelling

others

physical modelling

Empirical, semi-empirical modelling

stochastic modelling

linear empirical modelling

nonlinear modelling

linear regression
without nonlinear terms

linear regression
with nonlinear terms

polynomial regression

nonlinear regression

Approaches with free-form nonlinearities including splines, basis functions, kernel regression, feed-forward neural networks

In addition, all these approaches may be static or dynamic.

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Nonlinear modelling

- Nonlinear modelling is empirical or semi-empirical modelling which takes into account at least some nonlinearities.

- Nonlinear modelling can be carried out in several ways including

  - linear regression with nonlinear terms
  - polynomial regression
  - nonlinear regression
  - splines, multivariate splines (MARS)
  - other series of basis functions, kernel regression
  - feed-forward neural networks

Approaches suitable for biopersistence and viscosity

- Physical modelling is hardly possible.
- That leaves empirical modelling.
- The effects of composition variables are known not to be linear.
- .. which leaves nonlinear empirical modelling,
- .. as in most cases of modelling of various kinds of material properties of various kinds of materials.

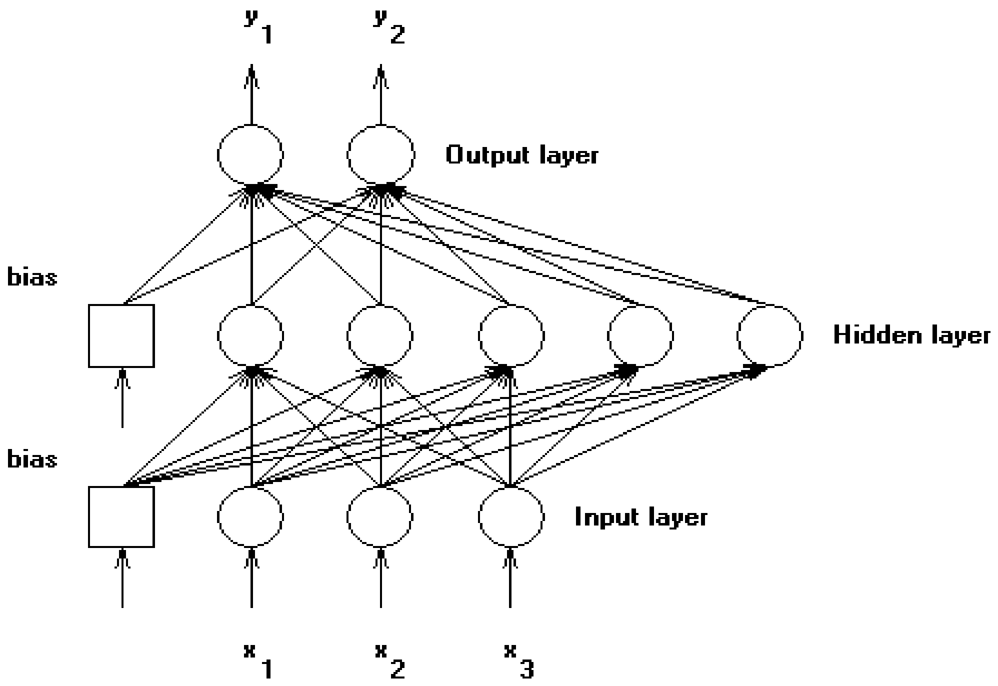
Feed-forward neural networks

- Feed-forward neural networks are capable of approximating any continuous, bounded, first order differentiable function to any desired degree of accuracy with a finite number of nodes on a single hidden layer with sigmoidal activation functions.

- This is referred to as the ***universal approximation capability***. This result became clear as late as in 1989, although Kolmogorov had come quite close in his results on superposition of functions in 1957.

- With this approach, we do not need to know in advance the kind of nonlinearities present.

A typical feed-forward neural network



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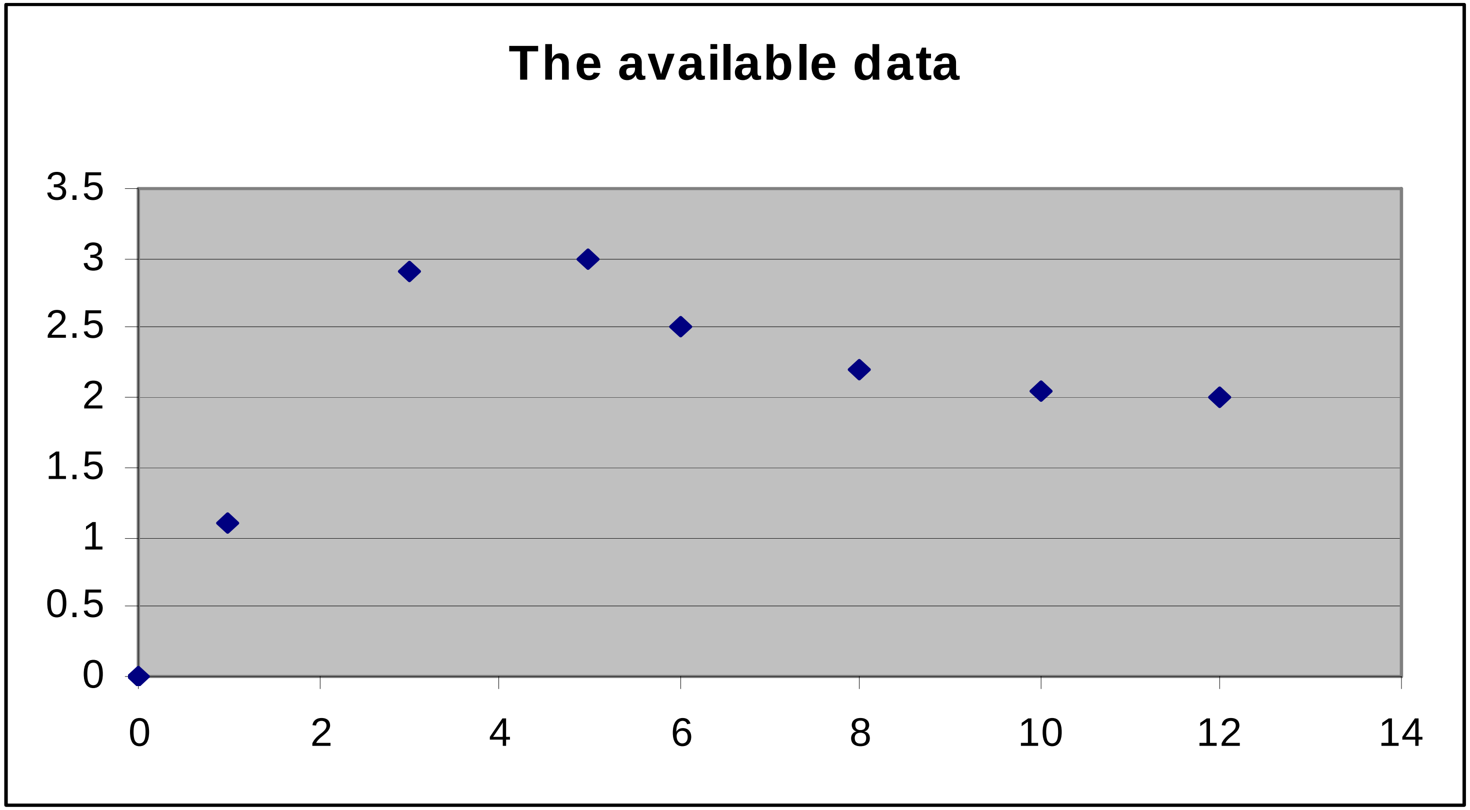
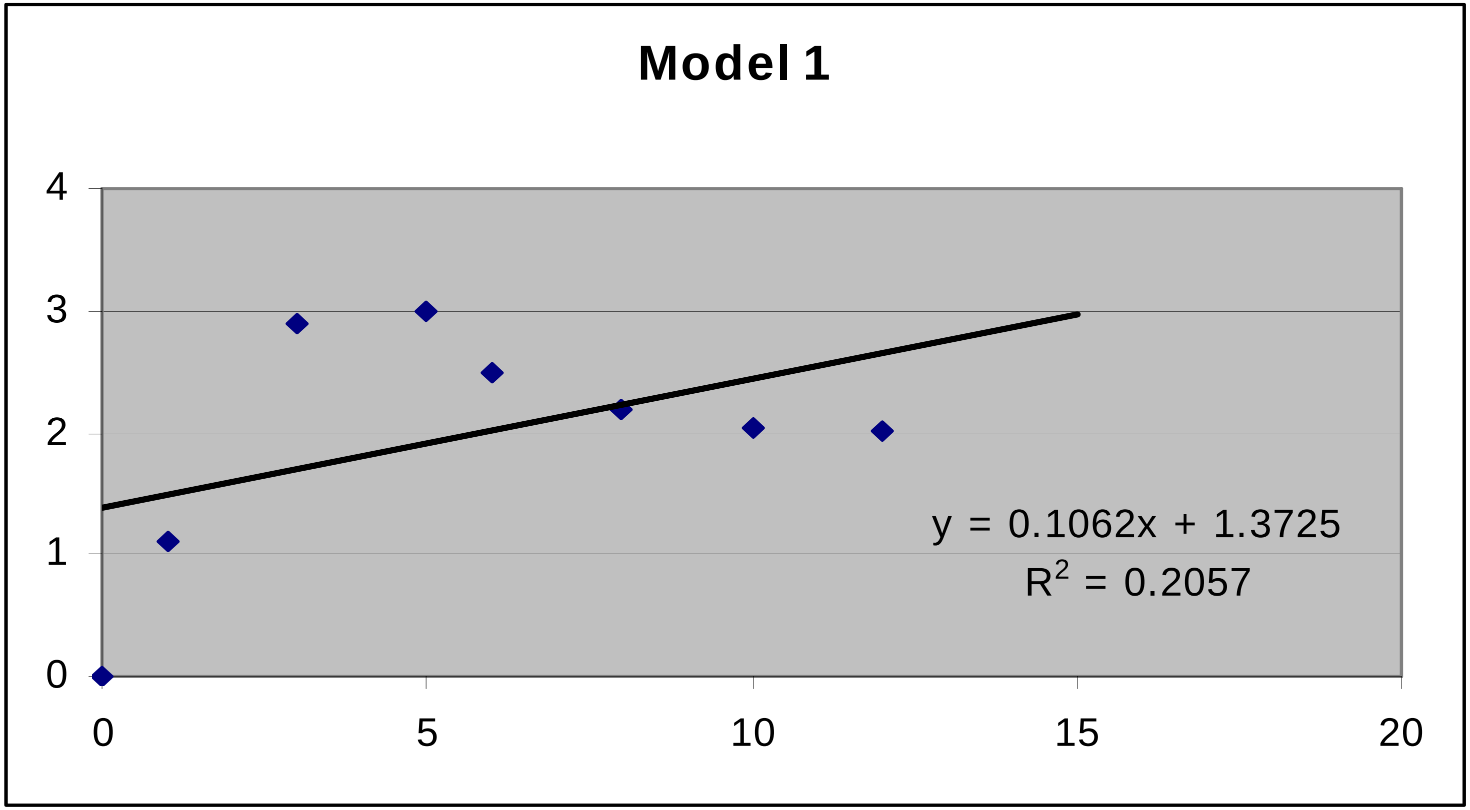
A simple, one input example



Linear regression model



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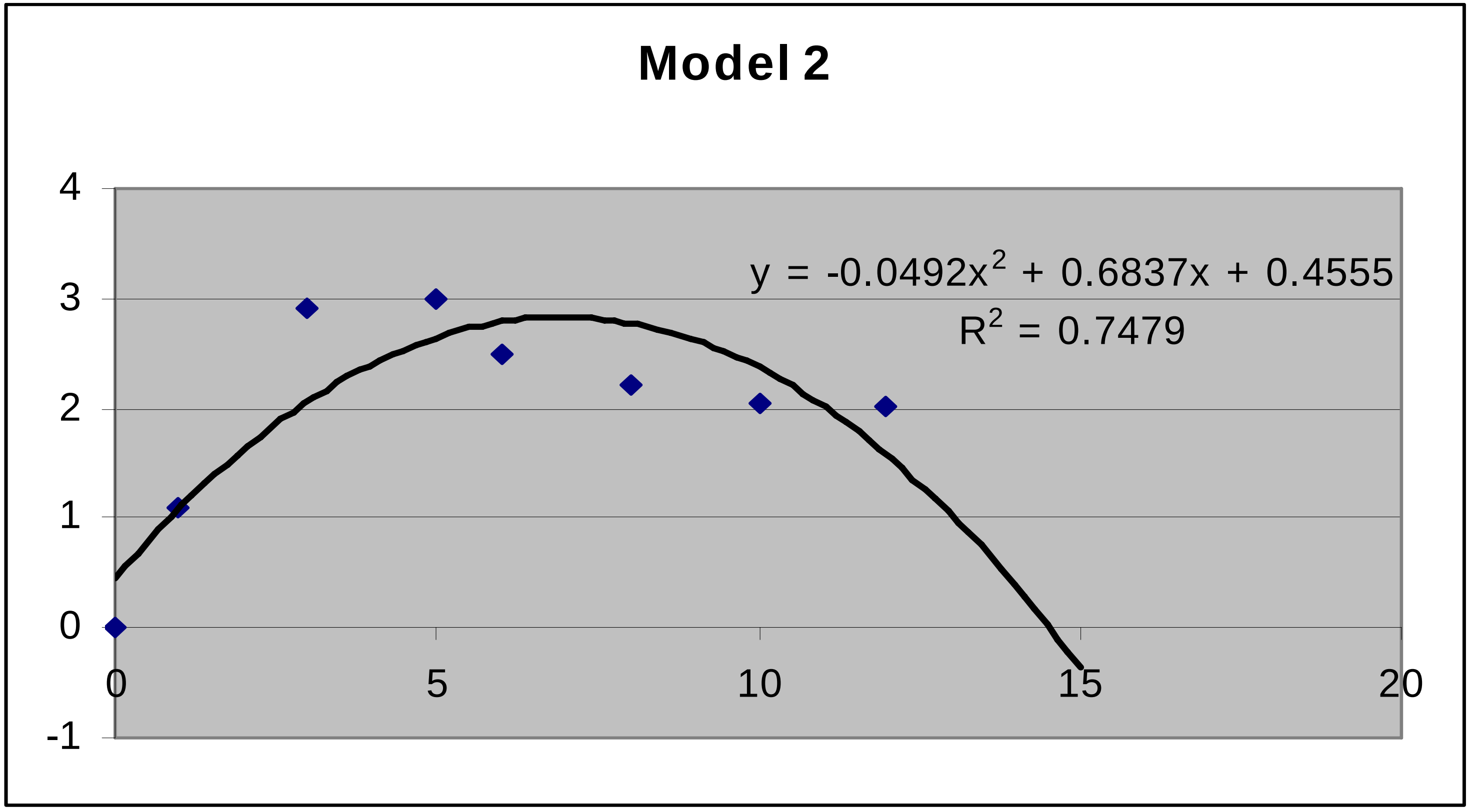
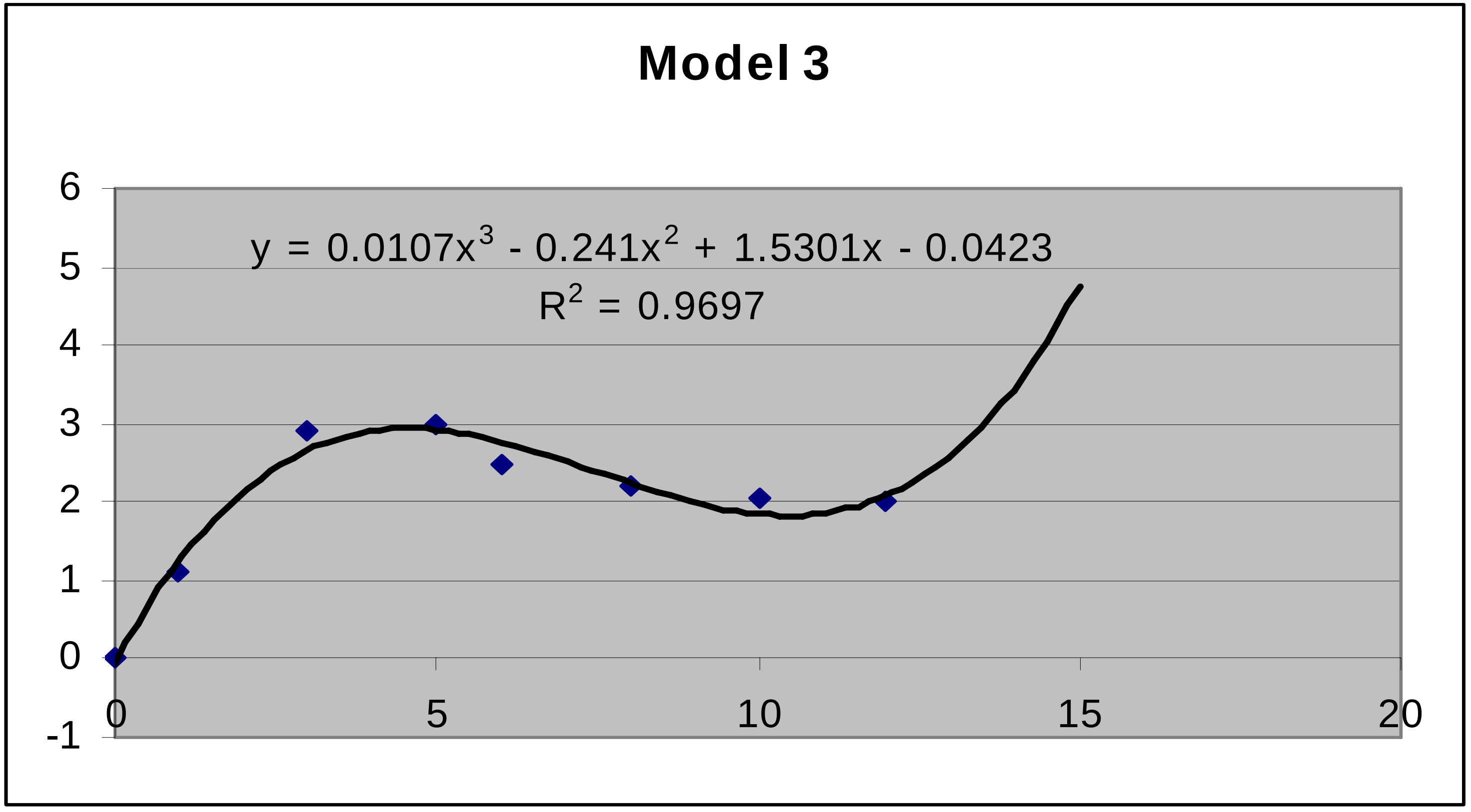
A nonlinear empirical model (quadratic)



Another nonlinear empirical model (polynomial)



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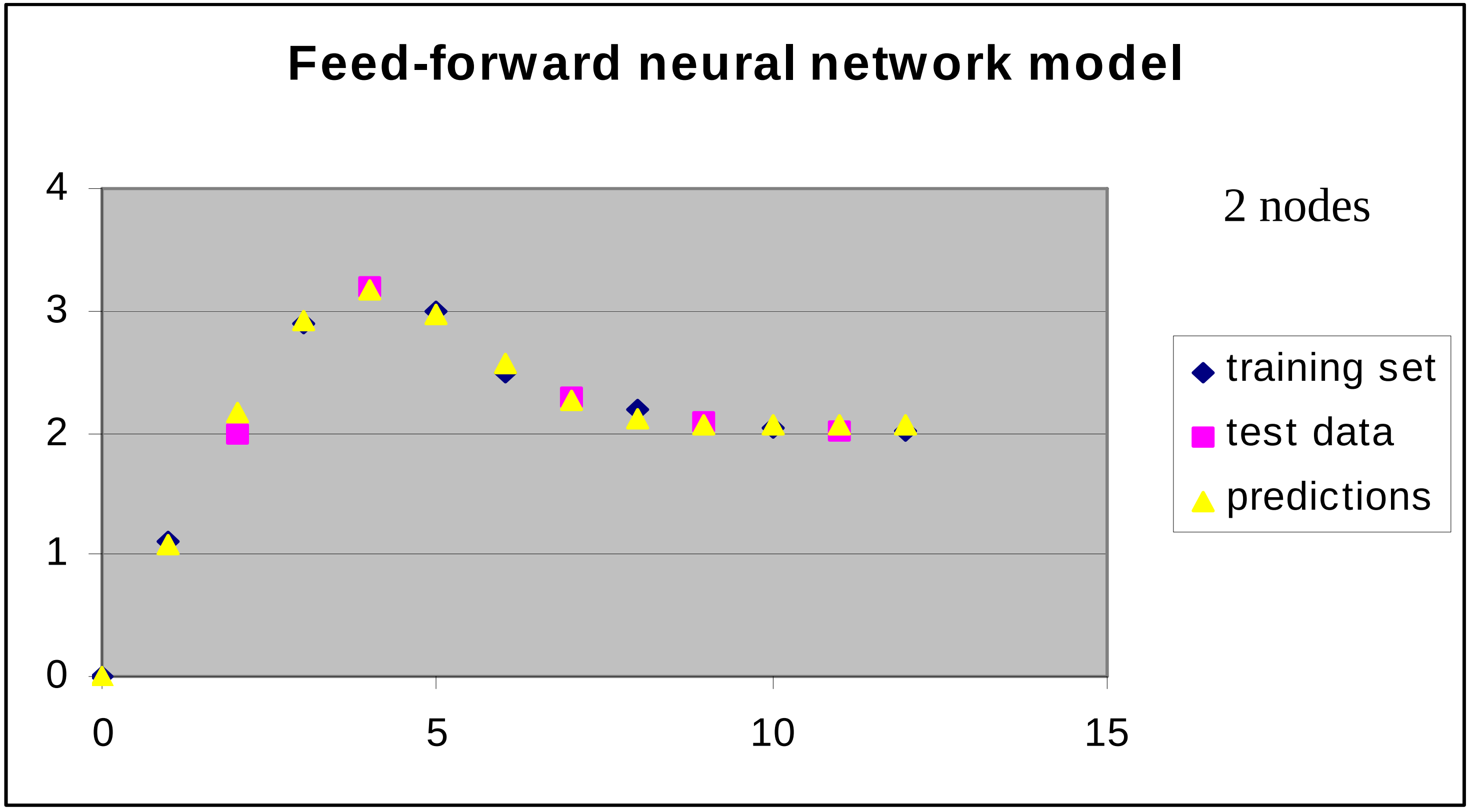
Predictions from a simple feed-forward neural network



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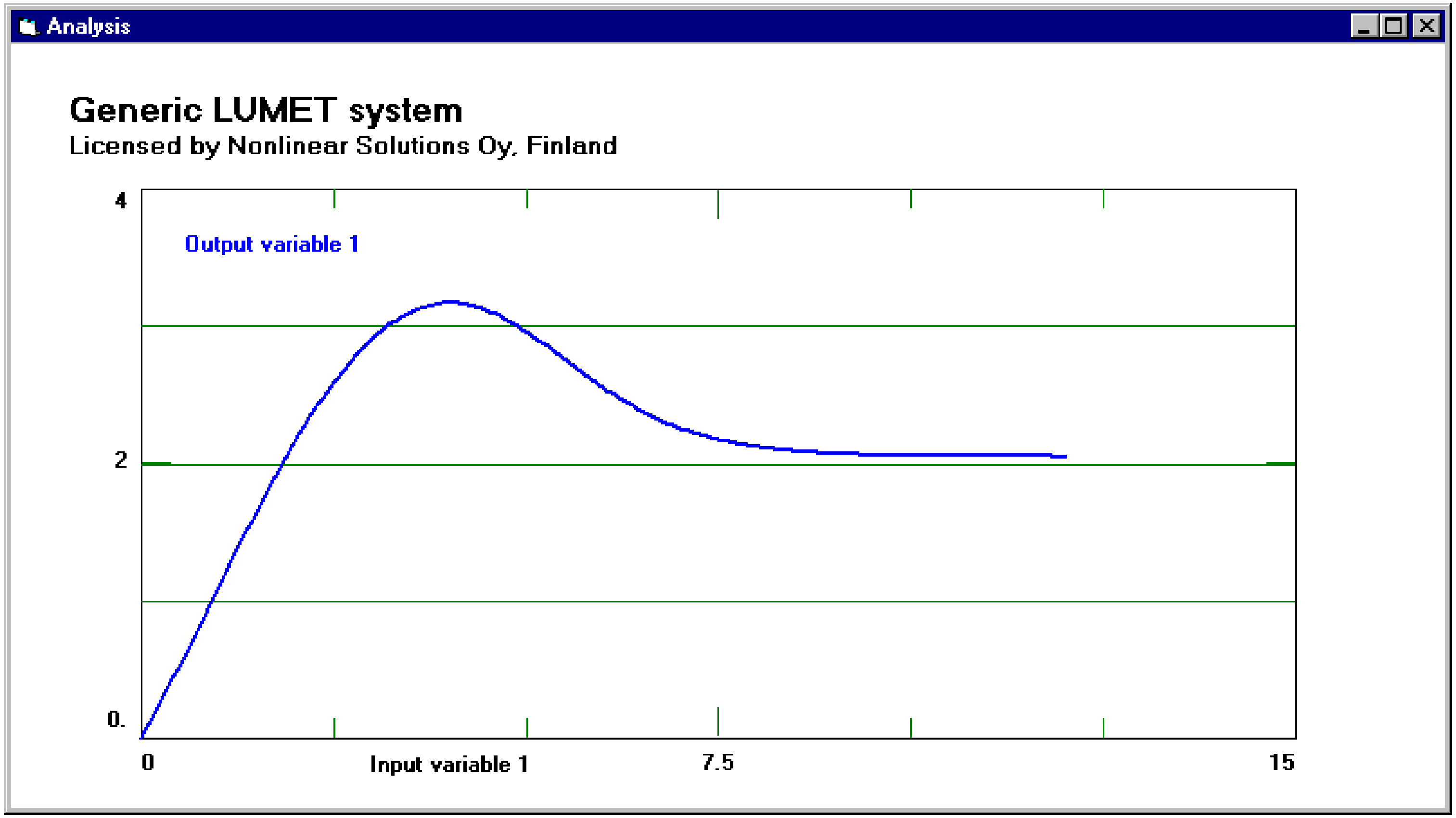
A feed-forward neural network model



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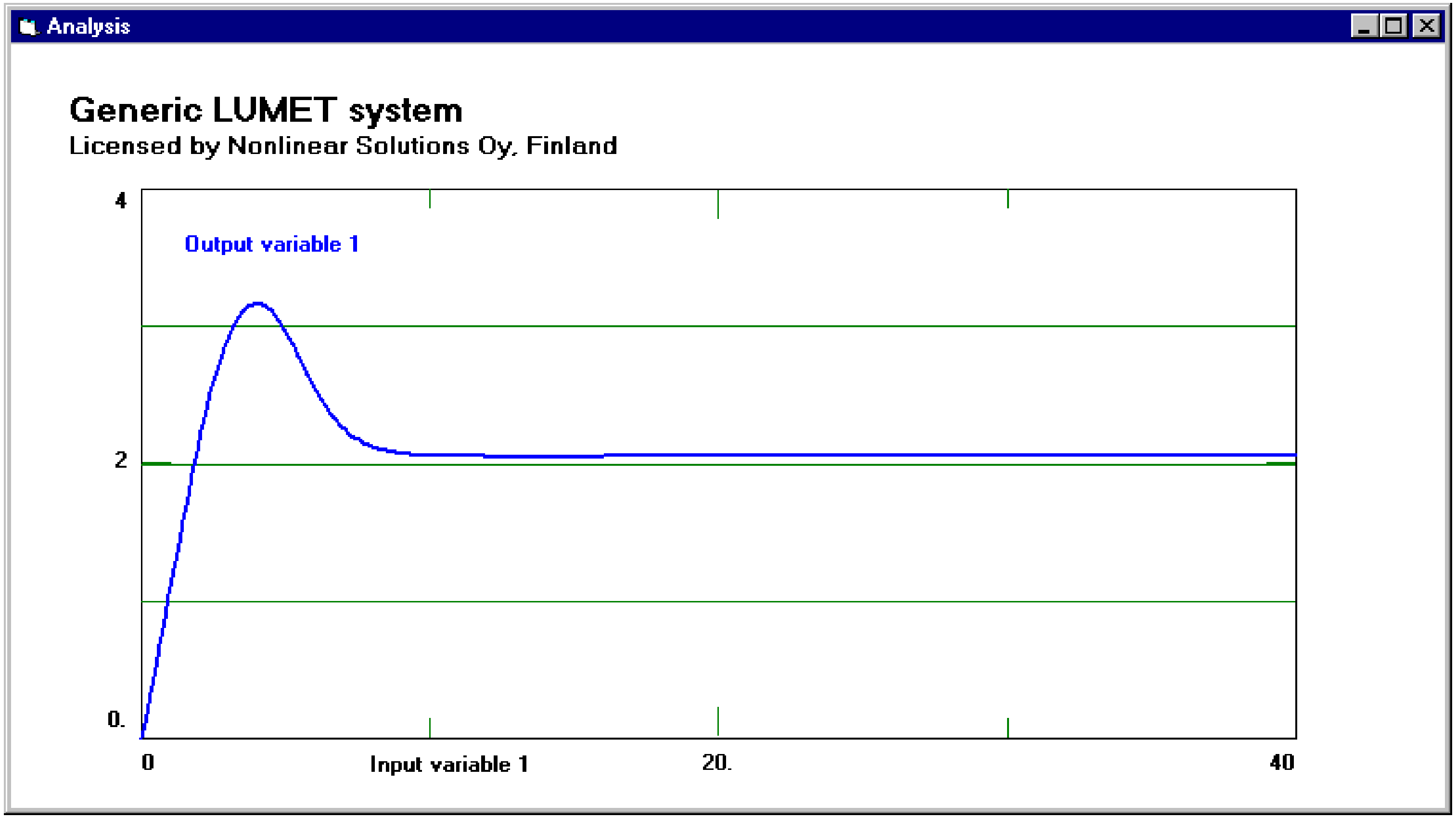
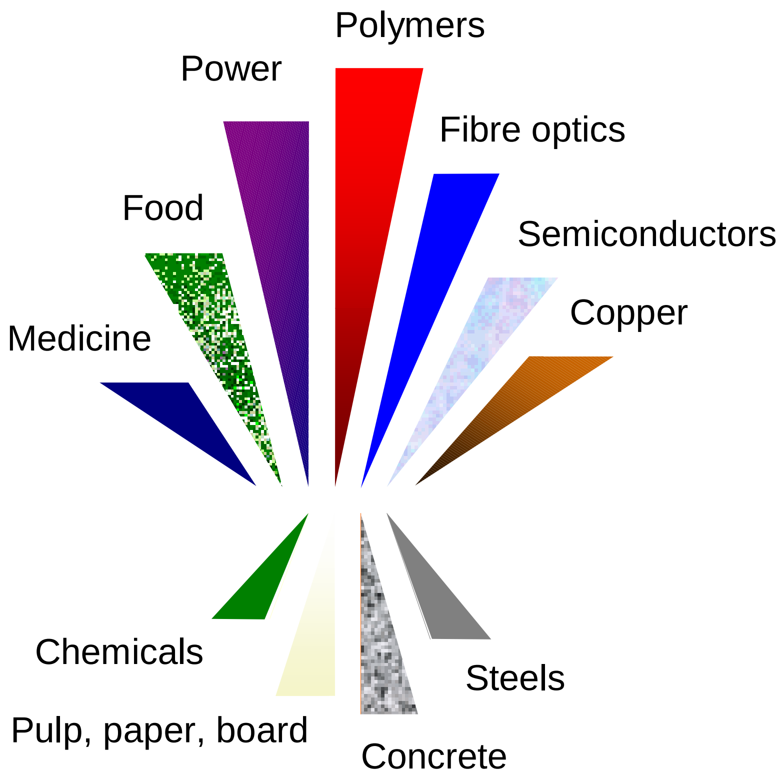
A good model can extrapolate to some extent



Lessons from the example

- Nonlinearities can be introduced in empirical models in many ways.
- Polynomials are not a very effective way. Nature is not linear. It is not very quadratic either. “Free-form” nonlinearities worked well in this case.
- Nonlinear regression would have worked about as well if we knew for sure the form of the nonlinearities.
- These observations become more pronounced in higher dimensions (more input variables).

Various industrial sectors utilise nonlinear modelling



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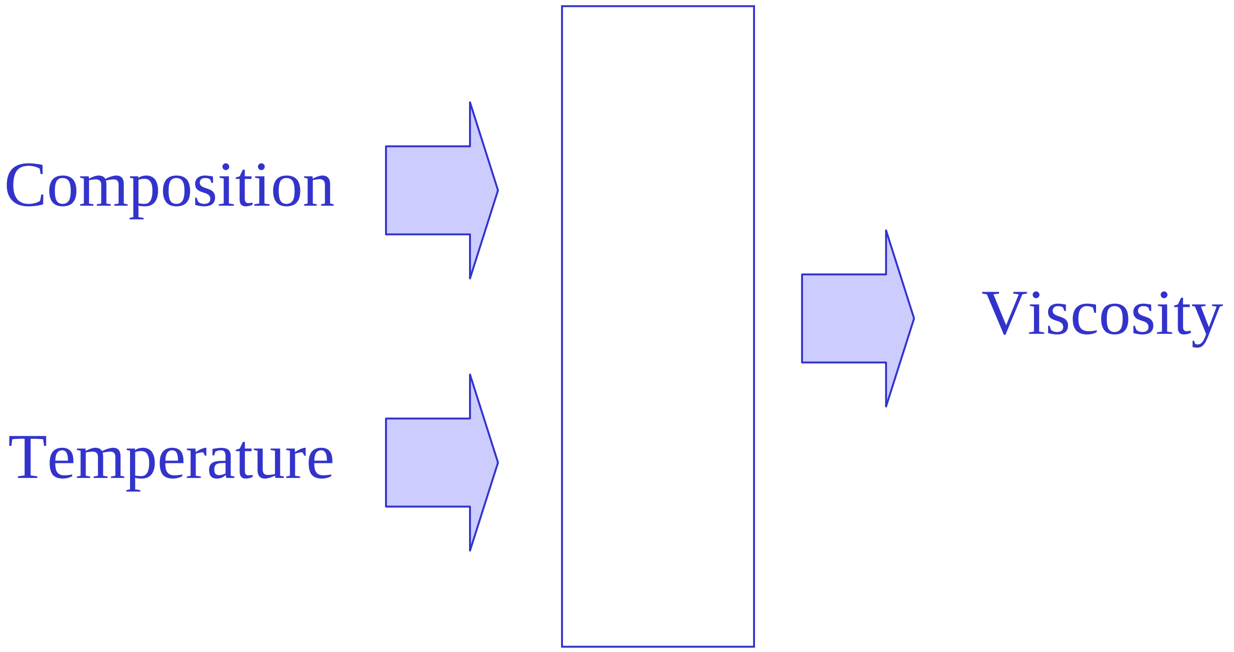
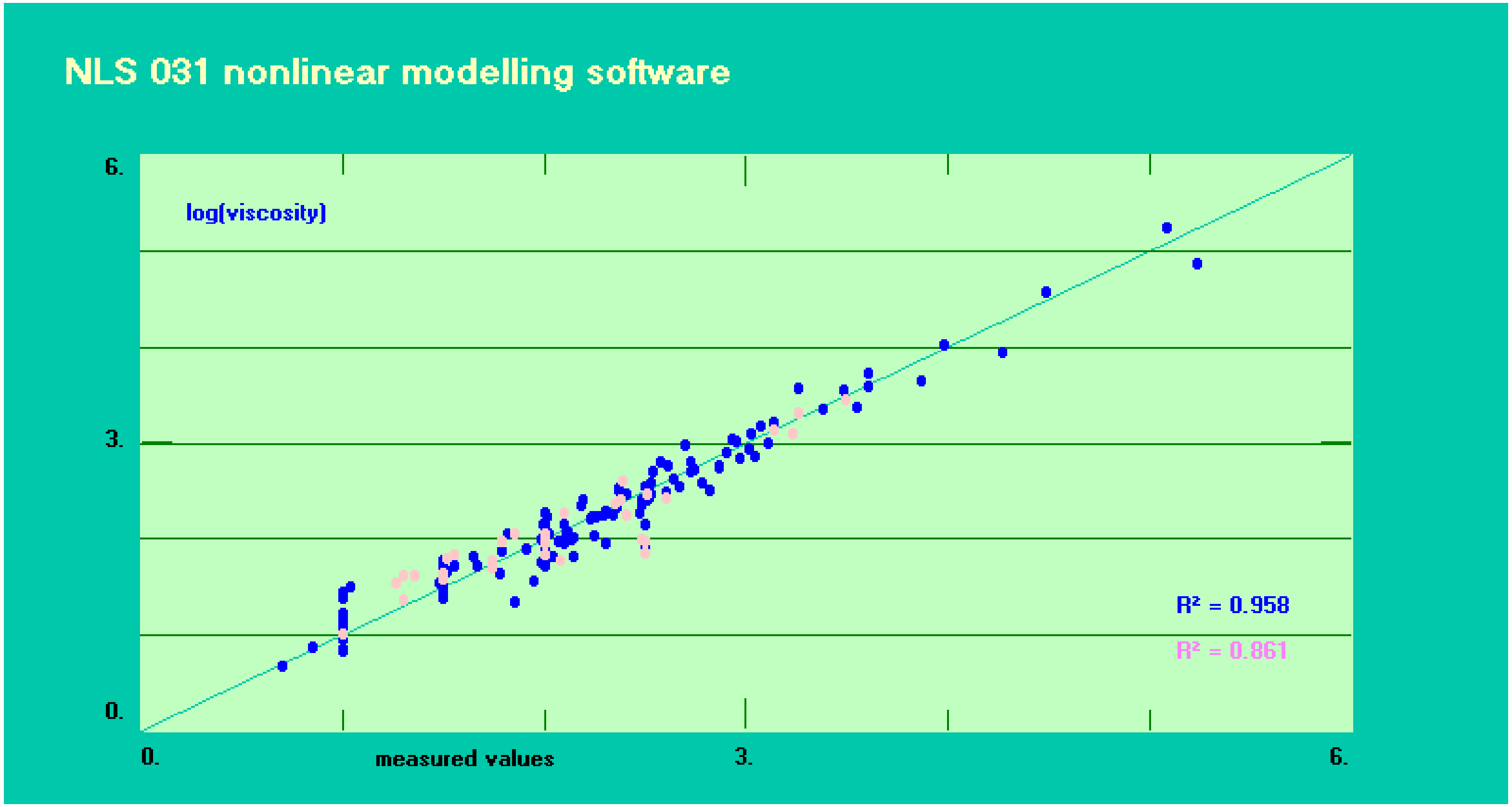
Viscosity (Paroc’s data)



Results from one of the nonlinear models of viscosity



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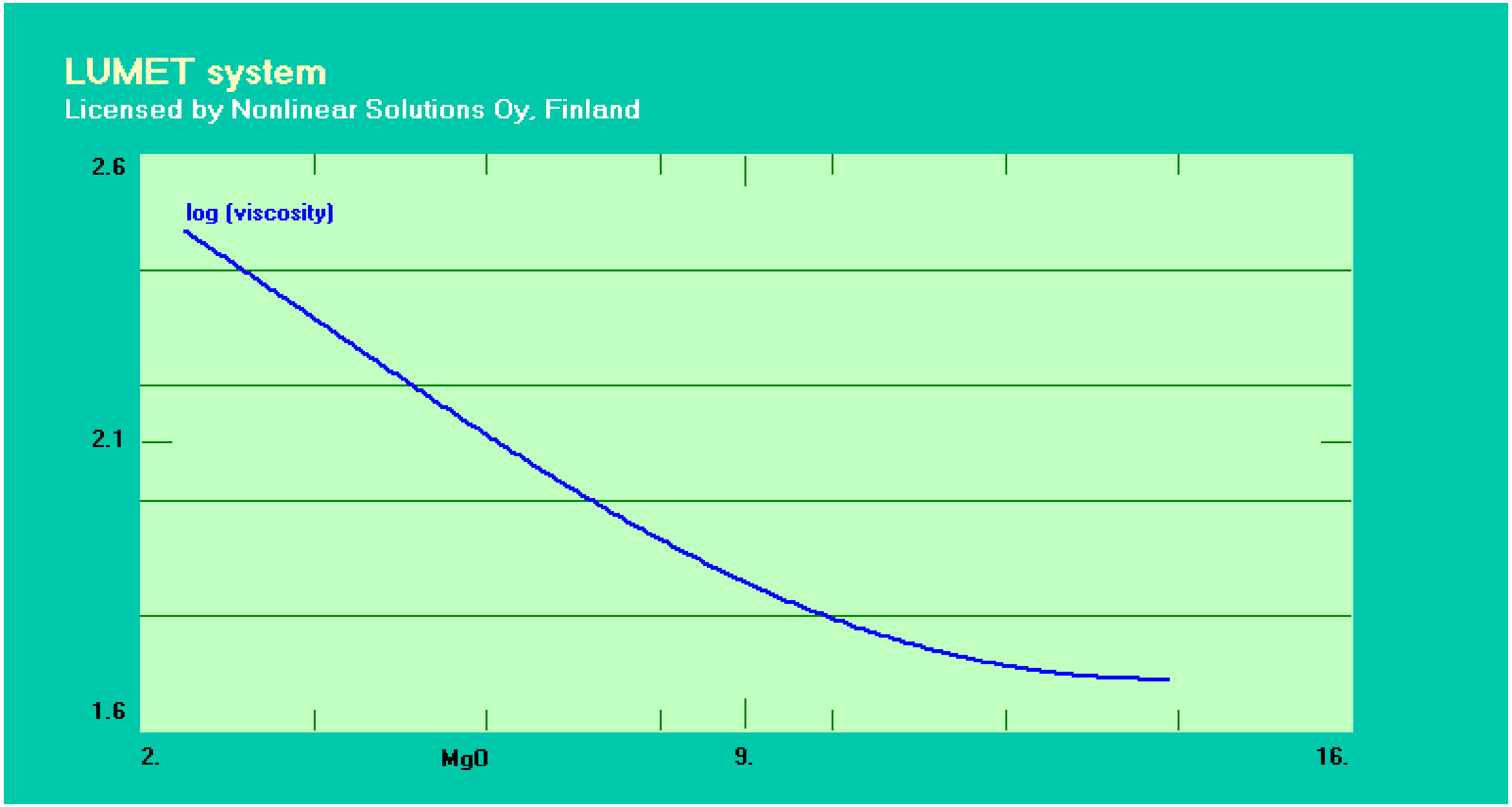
Effect of MgO on log(viscosity) as shown by the model



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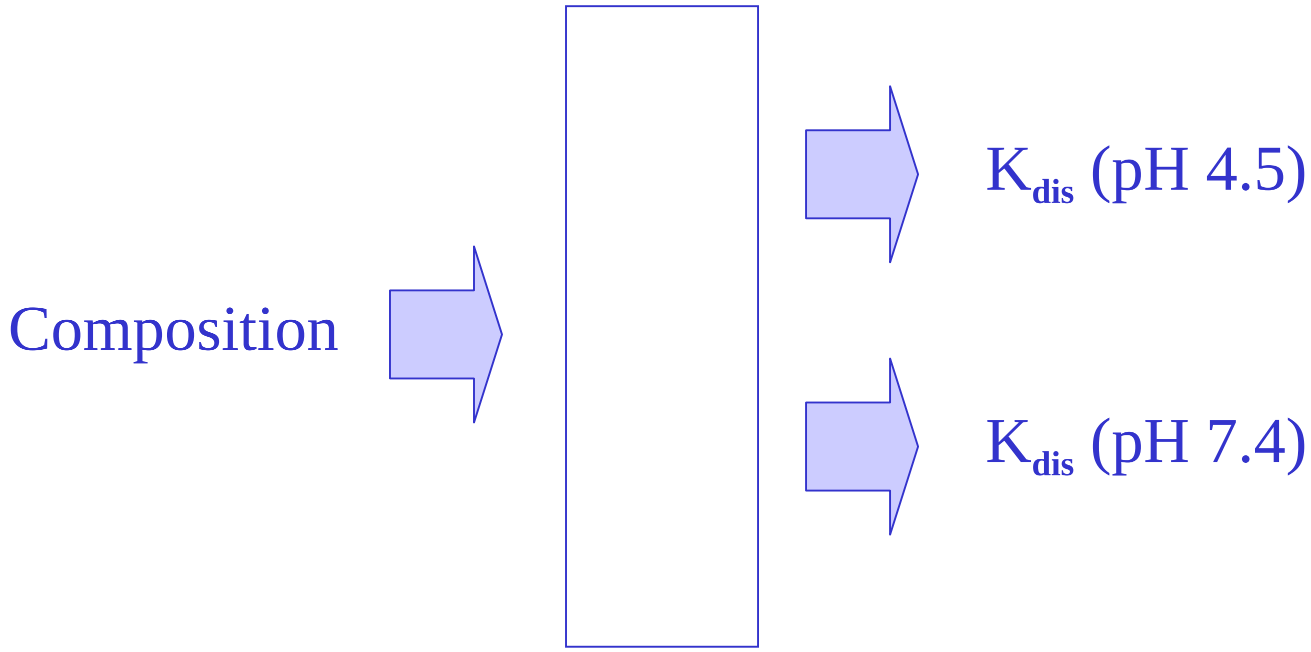
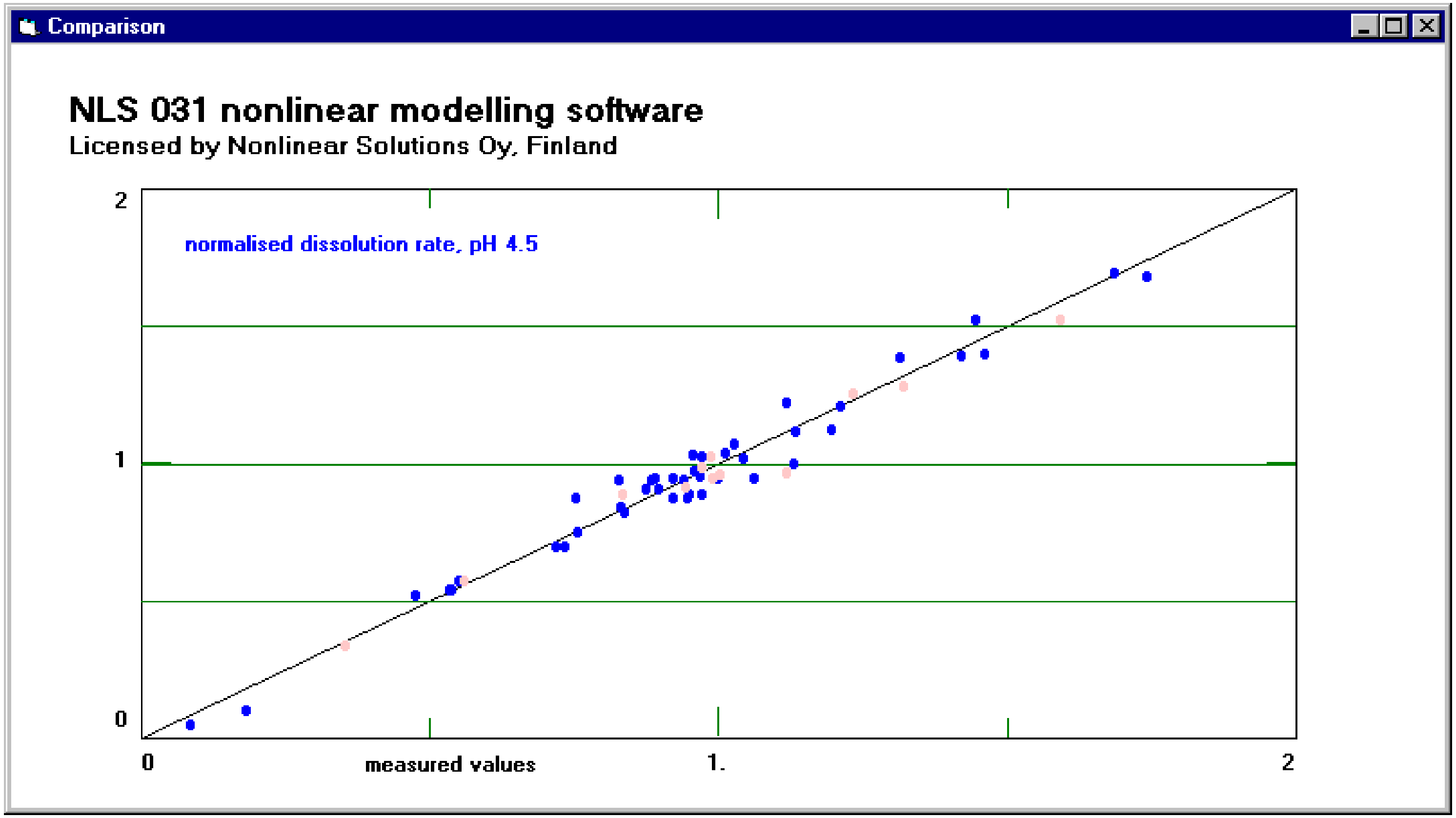
Dissolution rates at pH 4.5 and 7.4 (Paroc's data)

This has been attempted earlier with simpler methods.

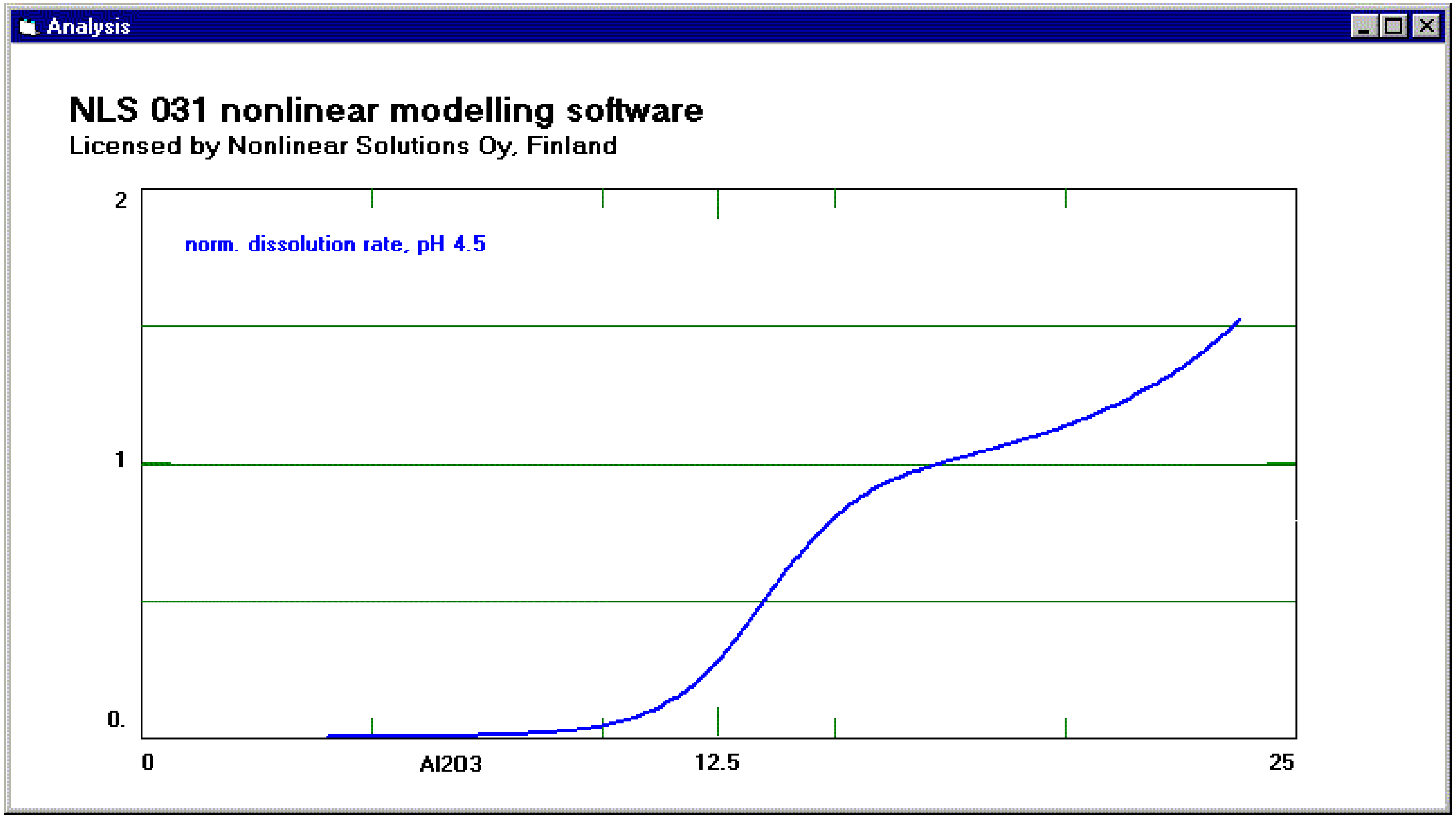
Those results have not been very useful.



Results from one of the models for pH 4.5



Effect of alumina content as shown by the model



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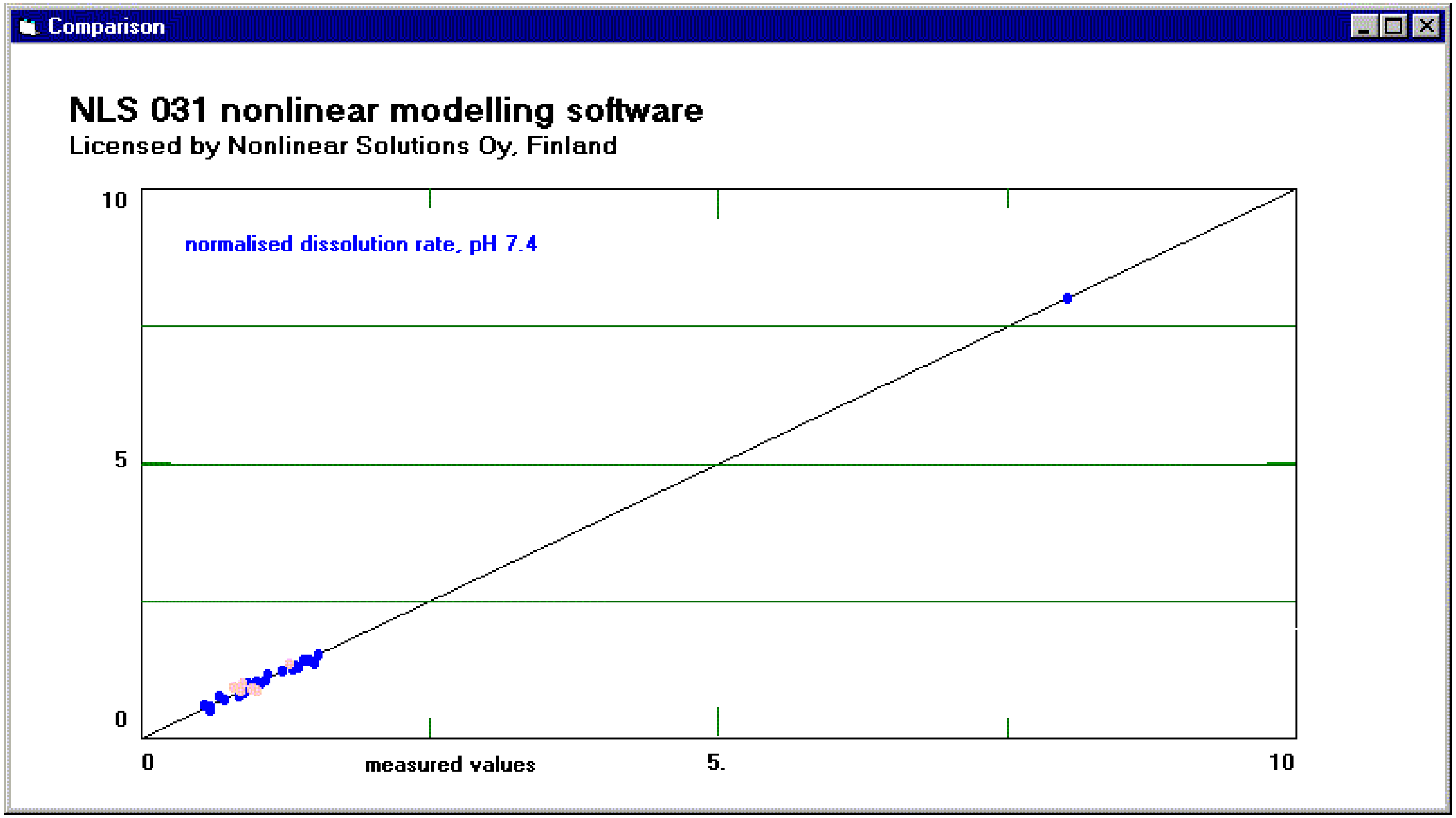
Results from one of the models for pH 7.4



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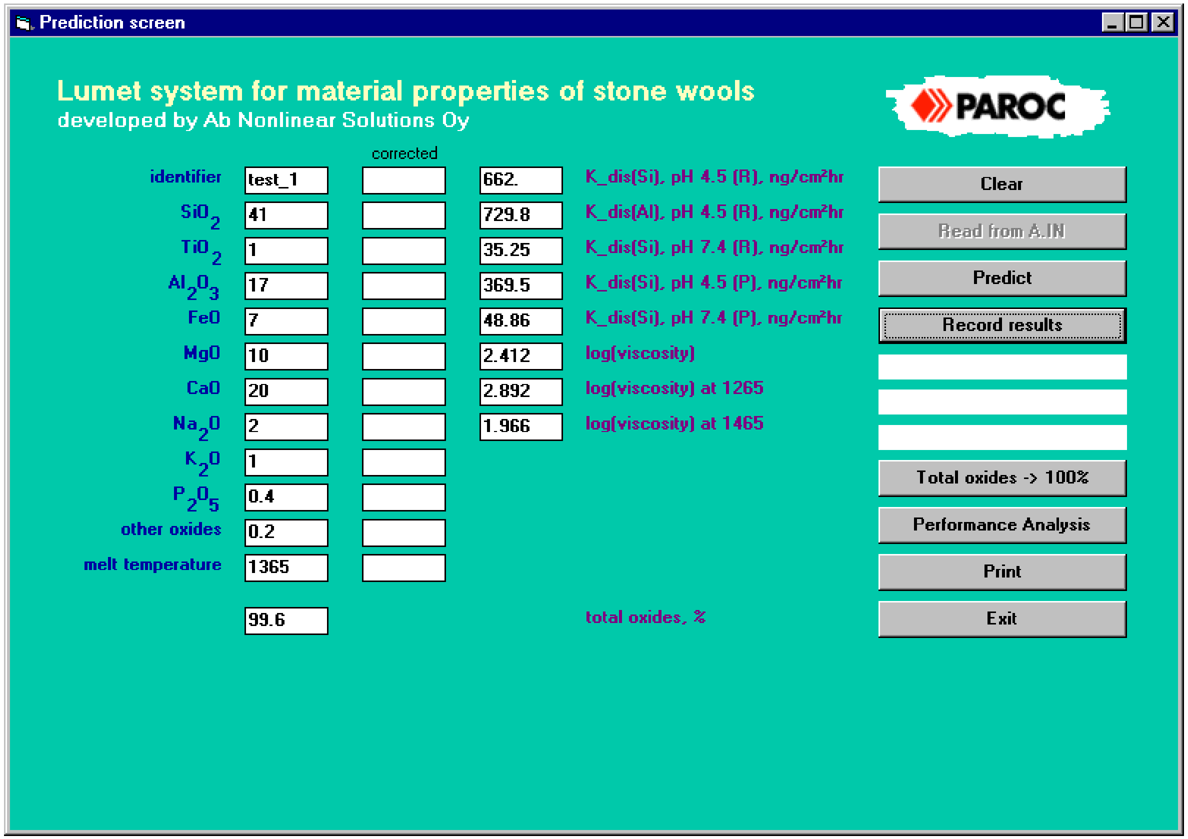
Nonlinear models implemented in the *LUMET* system



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literature on neural networks in process engineering

If you want to read more: