Advanced nonlinear models help plastics processors in many ways

New technology, new possibilities

Nonlinear modeling has been around for over ten years. It has been successfully utilized by various industries for a variety of purposes from quality control, product development and process guidance to software sensors and fault detection.

This new technology benefits you in several ways. Besides higher level process control of injection moulding and extrusion whereby the final properties of the extruded or moulded products are controlled by adjusting the process variables based on nonlinear models, even your raw material production benefits from them, as a consequence of which, you can now demand more from your polymer suppliers. Many companies around the world produce and supply polypropylene and its heterophasic copolymers of various kinds. Ask them if and when they can provide you the material with specified narrow ranges of mechanical properties, and specified constraints on MFR and crystallinity, and then you can start to see the difference between the producers. Ask them the maximum tensile modulus they can provide you while keeping impact strength and other variables within narrowly specified limits, and the difference between them becomes more pronounced. Thanks to the new technology, this task is now much easier. Engineers can calculate the polymer structure variables and polymerisation conditions that will lead to the desired properties in a matter of seconds, while you are still on the phone, and if it is not possible, they can tell you the closest they can get.

Currently polypropylene (PP) is the fastest growing bulk polymer, with a consumption today of around 30 million tonnes globally and an estimated consumption of 40 million tonnes in 2005. PP is the most versatile polymer and has the advantages of having light weight and a broad range of properties. Impact PP materials are used for wide range of applications. High modulus and thin walled pipes, packaging items, packaging films and automotive parts are the important end products.

The reason for the development of PP heterophasic copolymers is the improvement in the low-temperature impact strength. This is achieved with a polymer structure where an elastomeric phase, usually ethylene-propylene copolymer rubber, is dispersed uniformly within the PP homopolymer matrix

The present trend in the market is to enhance the rigidity of the material while retaining the impact properties. This translates to thinner walled extruded and moulded products, resulting in raw material savings to the plastics processors. The stiffness of heterophasic PP copolymers varies from high modulus PP of 2000 MPa to soft PP of 200 MPa . Another trend among plastic converters is reduced cycle times in processing which is obtained by nucleation seen as fast crystallisation of the material.

The fast growth and the need to find economical ways to design new and improved properties required new approaches in development work. In line with Borealis' policy of using the best available technology, nonlinear modeling was introduced in this development activity. Combined knowledge of PP structure property relationship and experimental data by nonlinear modeling permits us to investigate the final properties by fewer experiments, and lesser development costs. It helps to gain the quantitative knowledge necessary for quick tailormaking of polypropylene to suit the requirements of plastics processors.

New techniques of nonlinear modeling

New techniques of nonlinear modeling which have come up within the last ten-twelve years, have made possible the development of highly sophisticated nonlinear empirical models, without knowing the type and severity of nonlinearities present in the relations. It is also possible to combine process knowledge with this kind of empirical models, which often leads to better models. These new techniques have opened up new possibilities. It is now possible to develop accurate and reliable nonlinear models of material properties like tensile modulus and impact strength from experimental or production data, when the data has sufficient information content.

There are hardly any processes or materials in this world which have absolutely linear characteristics. It is therefore wise to treat the nonlinearities rather than ignore them. To treat the nonlinearities, one can use new techniques of nonlinear modeling, like artificial neural networks. The proponents of linear techniques draw on their simplicity and the possibility of adding nonlinear terms in linear regression. Often this is not done, and is not efficient even if it is done. Nature does not follow the simplicities that we try to fit it in, using linear techniques.

Neural networks, on the other hand, have the so-called universal approximation capability which makes them suitable for most function approximation tasks we come across in process industries. The user does not need to know the type and severity of nonlinearities while developing the models.

Nonlinear modeling and neural networks

Nonlinear modeling can be roughly defined as empirical modeling which takes at least some non-linearities into account. Nonlinear modeling can be performed in many ways. The simpler ways include polynomial regression and linear regression with nonlinear terms. One can also use basis functions and splines, and in cases where the form of the nonlinearities is known, nonlinear regression can be used. Artificial neural networks are a set of efficient tools for nonlinear modeling, for reasons mentioned earlier, particularly the universal approximation capability of feed-forward neural networks.

There are many different types of neural networks, and some of them have practical uses in process industries. Neural networks have been in use in process industries for about ten years. The multilayer perceptron is a kind of a feed-forward neural network. Most neural network applications in industries are based on them. They have been used for nonlinear modeling of material properties of steels, copper, plastics, concrete, paper, pulp, etc.

Nonlinear modeling has its disadvantages too. Nonlinear models of good quality are not developed in a week or a month. It takes several months to develop highly reliable and robust nonlinear models, and needs special expertise which is rare. A lot of people claim to be able to develop neural network models and can offer you nice looking user interfaces which don’t show the details of the models. However, not many can offer models of a high quality. This makes nonlinear modeling quite expensive. Still, as evinced by the Borealis case, the benefits clearly outweigh the expenses.

Nonlinear models in plastics engineering

Nonlinear modeling can contribute a lot to plastics engineering. Nonlinear models can help improve the properties of products produced with almost all the plastics engineering processes including injection moulding, extrusion and blow moulding. Nonlinear modeling can also help in designing polymer blend compositions and composites to produce the desired properties. Several nonlinear models of this kind have been provided to metal industries, where the effects of each alloying element can be quite complicated.

Nonlinear models for injection moulding correlate the process variables with product properties including their dimensional accuracy, mechanical properties and other special properties. Nonlinear Solutions has developed models for reflectivity of certain injection moulded parts of automotive headlamps. Extrusion models have been developed correlating process variables like temperatures of different zones and screw speed with the properties of extruded pipes. Several of our nonlinear models for extruded loose buffer tubes of optical fibre cables are in industrial use. Figure 1 shows a typical form of a linked group of nonlinear models for extruded loose tubes for optical fiber cables.

Nonlinear models for Borealis Polymers

The models for Borealis Polymers are of another kind. Some of the models correlate the polymerization conditions with the structure of the polymer. Other models correlate the structure variables with mechanical properties.

The catalyst and the polymerization conditions used influence the structure of the polymer. The final properties are defined together by the polymer structure and the processing conditions. The microstructure of both the matrix and dispersed phase affect the properties of PP heterophasic copolymer material. A high stereoregularity homopolymer as a matrix is a key to the high stiffness products. Whereas when designing low temperature properties, the amount, the composition and the dispersion of the rubbery phase has to be optimised. A successful tailoring of the copolymer structure results in a good stiffness/impact balance for moulding applications, an improved impact/optical balance for film, or a high stiffness and improved creep resistance for pipe.

Figure 2 gives a glimpse of the accuracy of some of the models developed for mechanical properties. Correlations are very good for all the three properties. However, it is more interesting to see a comparison between linear regression models and nonlinear models.

Often linear and nonlinear models have similar accuracies. Nonlinear models should be at least as accurate as linear models, but sometimes the improvement may be small in magnitude. Even in such cases, nonlinear models are usually better in many respects.

There is a remarkably large difference between the accuracies of linear and nonlinear models for the Charpy impact test. Figure 3 shows a comparison of linear and nonlinear models. The maximum error goes down by almost an order of magnitude, from 39.2 to 5. The rms error also goes down by an order of magnitude, from 14.27 to 1.53. It does not take much to see why this new technology is worthwhile inspite of its cost.

***processMax+* system**

Advanced and complicated models like the ones often implemented in *processMax+* systems are cumbersome to use in their raw form. Unlike simple regression models, the equations look clumsy and the free parameters don't tell you very much unless you are very familiar with these kinds of nonlinear models. processMax+ systems make it easy for the user to utilise the models without needing to understand the technology in detail. At the same time, this is no black box. If the user wants to see what the models are doing, a few clicks of the mouse will also show what is going on inside.

A few neural network models of mechanical properties of heterophasic PP copolymers of Borealis were implemented in the second version of processMax+ systems, and Figures 4 and 5 are based on some of those models. These systems also have facilities to calculate the structure variables for desired mechanical properties in presence of constraints.

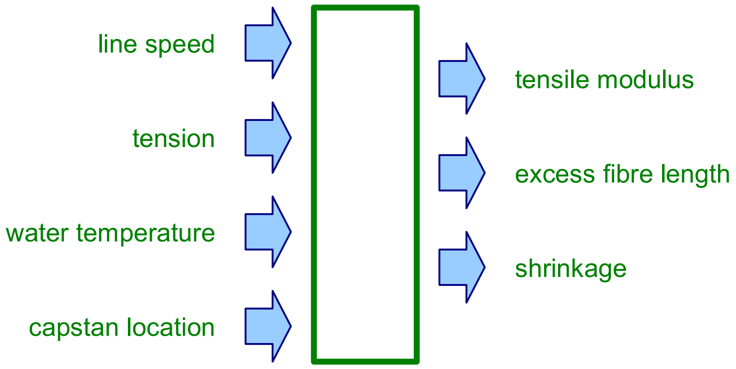

Figure 1. Nonlinear models of this kind are used for extrusion of loose buffer tubes for optic fibre cables

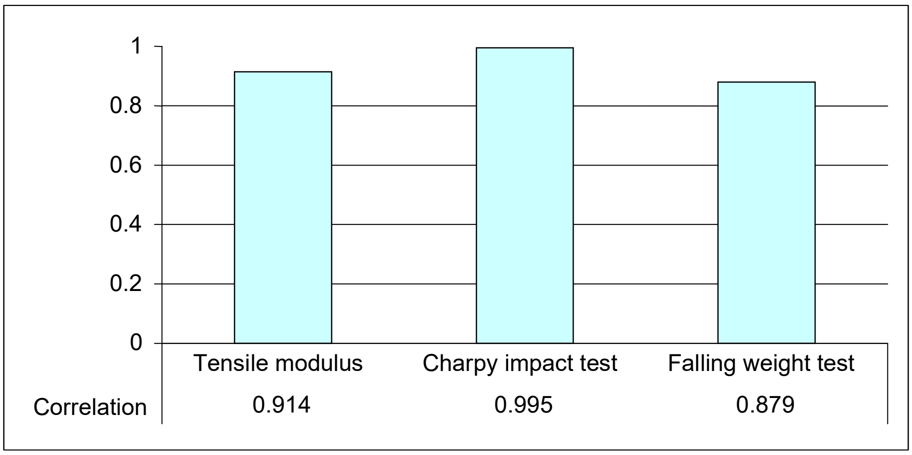

Figure 2. The correlations for all the three material properties were quite high.

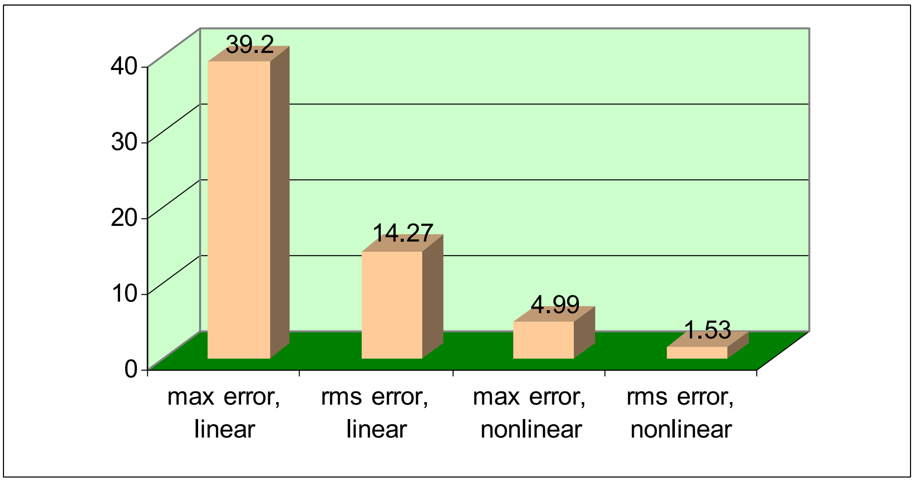

Figure 3. A comparison of errors from linear and nonlinear models for Charpy impact test at room temperature

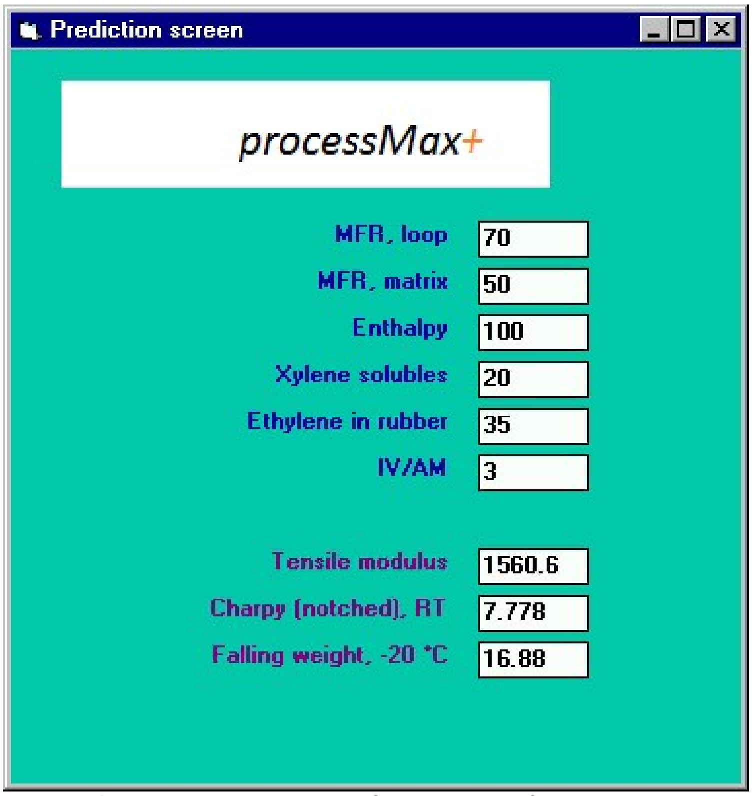

Figure 4. A typical prediction from some of the nonlinear models implemented in the processMax+ system. The user feeds in the variables in blue, and the system predicts the three properties.

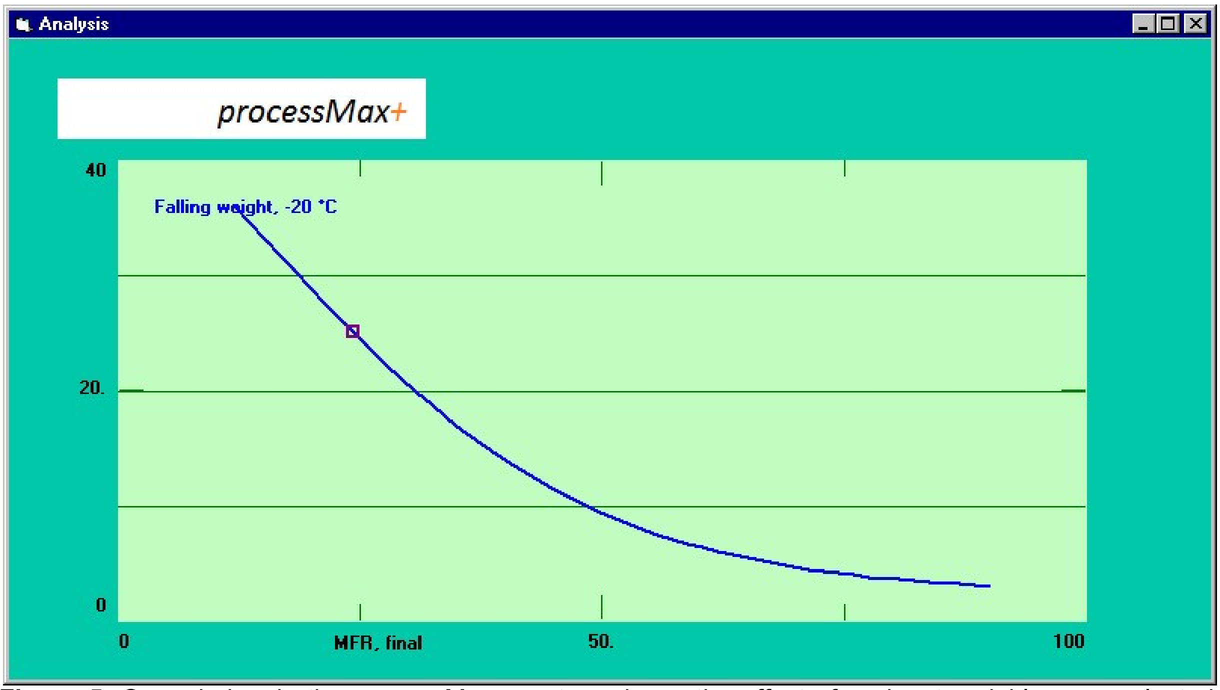

Figure 5. One window in the processMax+ system shows the effect of an input variable on a selected material property.