How Nonlinear Modeling Improved Understanding of a Hydrometallurgical Leaching Process

Development of quality mathematical models fit for industrial production processes, particularly leaching, has been considered to be very difficult. However, the results of a recent project illustrate that newer nonlinear modeling techniques have clearly improved the situation.

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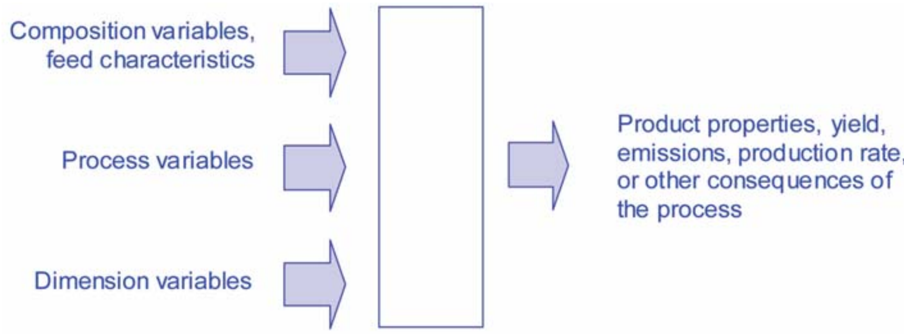
Mineral leaching processes are often quite complicated even if only one or two chemical reactions cause the leaching. The reactions are usually heterogeneous and can be mass-transfer limited or reaction-rate limited. At nickel products producer Norilsk Nickel Harjavalta Oy, the main reaction in the leaching process is a three-phase chemical reaction, and there are a few other reactions occurring in parallel leaching metals other than nickel. Such processes cannot be modeled practically by phenomenological modeling. A large number of variables affect the leaching rate, and therefore, the yield of the process. Empirical and semi-empirical modeling approaches do not need deep knowledge of the phenomena occurring in the process; it is sufficient to measure the variables of interest. Conventional empirical modeling employs linear statistical techniques, primarily linear regression and its variants. However, most industrial processes do not tend to be very linear. Therefore, nonlinear empirical or semi-empirical modeling is almost always a better alternative to linear techniques.

This article describes the experience of developing nonlinear models of a leaching process used by Norilsk Nickel Harjavalta Oy in Harjavalta, Finland. Theoretical issues are also discussed, followed by a brief explanation of how the nonlinear models were implement-

The Norilsk Nickel Harjavalta Oy plant in Finland.

ed in software suitable for use by plant operators.

Norilsk Nickel Harjavalta Oy has years of experience in producing high-quality nickel products, including both metals and chemicals, and several of its products are produced by innovative and efficient production processes developed in-house. The company's product portfolio is diverse, its products have applications in several industrial sectors and are exported to practically all parts of the world from the Harjavalta plant. Even so, its production processes are in continuous development.



A typical model configuration for process development.

The Process Development Problem

Any production process can be made more efficient with better quantitative knowledge of the effects of process variables and feed characteristics on the consequences of the process.

Different industrial processes have different characteristics—different objectives, variables, constraints, raw materials or micro-organisms. The process may be a batch process, a continuous process or a fed-batch one. However, some things are common to process development of various kinds of processes. A product needs to be produced with a given process, from specified raw materials such that the resulting product properties satisfy some conditions, typically upper and lower limits.

$$a_1 < \text{property } 1 < b_1$$
$$a_2 < \text{property } 2 < b_2$$
$$a_3 < \text{property } 3 < b_3$$
$$\ldots$$
$$a_n < \text{property } n < b_n$$

For development of many kinds of industrial processes, product concentrations, concentrations of undesired side-products and viscosity, for example, can be considered to be the product properties, where the products are the materials (liquid, solid, gas, slurry) resulting at the end of the process. Besides these constraints, there also are limits on other variables. Process variables such as temperatures, pressures, flow rates or pH stirring, for example; and feed characteristics such as concentrations in the feed and particle sizes also have upper and lower limits. The objective of process development is usually to determine the best values of the feed characteristics and process variables such that the product properties are within desired limits, and preferably, a production economic variable (e.g., production rate, raw material consumption, energy efficiency, purity, number of defects or emissions, to name a few) is maximized or minimized. The same methodology can be applied to a wide variety of processes.

The degrees of freedom may differ in different cases. Sometimes there may be no control over the raw material or feed characteristics, and the only degrees of freedom may be the process variables within certain limits. Sometimes, different amounts of feed materials may be degrees of freedom.

The problem looks somewhat similar from the process modeling point of view for a wide variety of industrial processes. From the process modeling point of view, the product properties are consequences of feed characteristics, process variables and dimension variables, as summarized in the figure above.

These relations, however, tend to be complicated for most industrial processes in general, and mineral leaching processes in particular. Mathematical modeling can be performed in various ways, and different ways are suitable in different situations. Attempts at physical modeling lead to modest accuracies in predicting most of the interesting consequences of leaching like product purity and energy consumption, partly because they require plenty of assumptions and simplifications, and partly because of lack of knowledge of mass transfer characteristics and reaction kinetics of several components in leaching. Empirical and semi-empirical models, on the other hand, have neither of these limitations. All that is needed is sufficient amount of production data with a fair variation in the variables of interest.

Nonlinear Modeling

Nonlinear modeling has been successfully utilized by many sectors of industries for a variety of purposes[1,2], particularly for process development involving metallurgy[3-5], polymers[6], plastics processing[7,8], ceramics[9], concrete[10], pulp, paper and board, power generation[11], semiconductor processing[12], water treatment, chemical production[13], biotechnology[14] and food processing. Yet, overall industry awareness of these techniques is still very limited.

Nonlinear modeling can roughly be defined as empirical or semi-empirical modeling which takes at least some nonlinearities into account. Nonlinear models can be static or dynamic. Nonlinear modeling can be performed in many ways. The simpler ways include polynomial regression and linear regression with nonlinear terms. Nonlinear regression is useful in some situations. The form of the nonlinearities, however, has to be specified in these older techniques. The newer techniques of nonlinear modeling are based on free-form nonlinearities. They include series of basis functions, splines, kernel regression, feed-forward neural networks, etc. Feed-forward neural networks are a set of efficient tools for nonlinear modeling, particularly because of their universal approximation capability.[15]

Why Nonlinear Modeling?

Mathematical models represent knowledge of quantitative effects of relevant variables in a concise and precise form. They can be used instead of experimentation if they are reliable enough. Mathematical models also permit the user to carry out various kinds of calculations such as optimization, which can be used to determine suitable values of process variables. Mathematical modeling can be performed in various ways, and different ways are suitable in different situations.

It is not possible to use physical modeling in every situation. Even if it is possible, physical models tend to compute the output more slowly than empirical or semi-empirical models. Development of physical models is time consuming. Nonlinear modeling tends to be expensive, but physical modeling usually costs even more. Physical models involve assumptions and simplifications. Thus, empirical modeling is often a better alternative.

Traditional empirical modeling is based on linear statistical techniques. But, nothing in nature is absolutely linear, so it helps to take nonlinearities into account rather than ignore them. If the range of variables is small, linear techniques are sometimes sufficient. New techniques of nonlinear modeling based on artificial neural networks allow us to approximate nonlinearities without specifying in detail the nonlinearities to be accounted for. They allow for free-form nonlinearities, unlike linear and nonlinear regression methods.

For this work, we used an empirical approach based on feed-forward neural networks, since plenty of reliable production data was available from the plant. Such networks are a set of efficient tools for nonlinear modeling, particularly because of their universal approximation capability.

Feed-forward Neural Networks

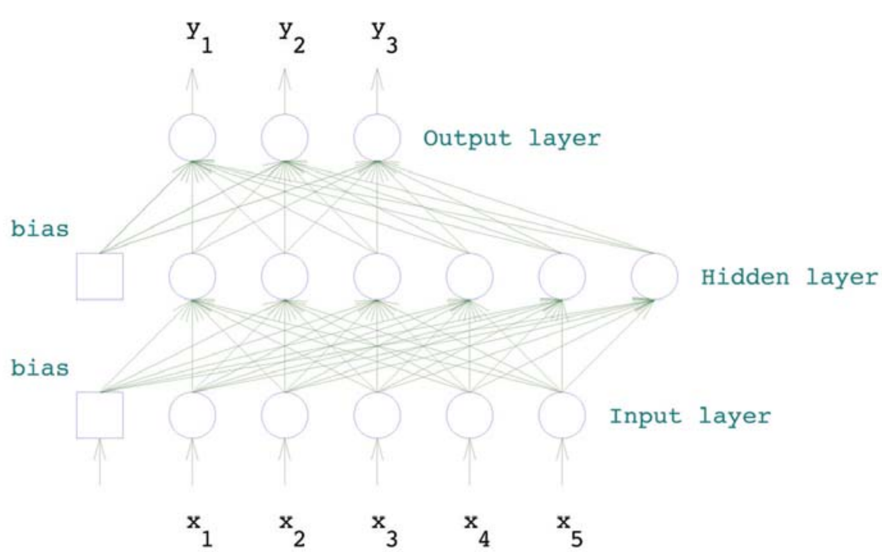
Feed-forward neural networks consist of neurons or nodes, which are calculation units. These neurons are arranged in layers, and the connections between neurons are in the forward direction only; i.e., from the input layer toward the output layer, as shown in the figure below. The input layer has as many neurons as the number of input variables and usually the neurons in the input layer serve only to provide the value to several neurons in the layer above it. There can be layers between the input and the output layers, which are called hidden layers. The neurons in the hidden layer normally have some nonlinearity. In most situations, only one hidden layer is used.

The output of each neuron i in a feed-forward neural network is given by

$$z_i = \sigma\left(\sum_{j=0}^{N} w_{ij} x_j\right)$$

where the activation function σ(a) is often the logistic sigmoid, given by

$$\sigma(a) = \frac{1}{1+e^{-a}}$$



A typical feed-forward neural network.

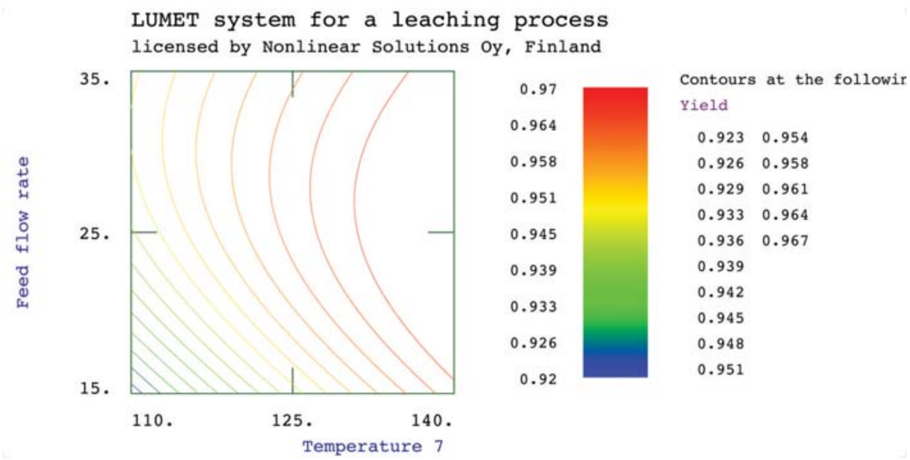
The incoming signals to the neuron are x_j, and w_{ij} are the weights for each connection from the incoming signals to the i^{th} neuron. The w_{i0} terms are called biases. This results in a set of algebraic equations which relate the input variables to the output variables. For each observation (a set of input and output variables), the outputs can be predicted from these equations based on a given set of weights. The training procedure aims at determining the weights which result in the smallest sum of squares of prediction errors. There are a number of well-known methods for achieving this, which is basically an optimization problem; we generally use the Levenberg-Marquardt method. It is also possible to combine neural networks with physical models or other empirical models, which often lead to better solutions.

Quality of Nonlinear Models

Many people claim to be able to develop nonlinear models in the form of neural networks or others. A large number of people can offer impressive user interfaces that hide the details of the models inside. However, not many people can solve real-world problems. Very few are able to produce industrially usable systems of good quality. Fewer are consistently successful in every project they agree to undertake. The result is that there is a wide variation in the quality of nonlinear models.[2] How do you know which models are good and which models are not? In other words, what are the characteristics that you look for in a good nonlinear model?

The simple answer is that 'the proof of the pudding is in the eating': A good model has to work. There is, of course, more to it than that. A good model for industrial purposes has to be reliable. Accuracy is secondary. A good industrial model has to be robust and easily updatable. Models should have some transparency, and the simpler the better.

A good model efficiently treats all the important nonlinearities. Reliability, robustness, simplicity, maintainability often come at the cost of accuracy and efficient treatment of nonlinearities. These conflicting demands make nonlinear modeling a harder task. That does not leave many people who will offer you all these attributes. Most are satisfied



Contours of yield in terms of feed flow rate and temperature in a certain location in the autoclave.

with claiming accuracy. It is important to insist on highly reliable and robust models because several decisions might be made based on the answers from these models. Considering the possible effects these decisions can have, it becomes quite obvious that the models should be as high quality as possible.

In other words, the quality of a nonlinear model is much more than accuracy, and there is a scarcity of quality of nonlinear modeling today. There are no simple ways of measuring reliability and robustness of nonlinear models. How does one ensure these and other features? Experience and expertise are essential for neural network model development. However, a good software tool also goes a long way by offering a variety of measures that highlight possible undesirable features in the models.

Nonlinear Models for the Leaching Process

For the development of nonlinear models of Norilsk Nickel's leaching process, a large number of variables were identified. Production data from July 9, 2010, to January 22, 2012, were available for use.

The data set contained 53 columns of different variables. Production data tends to be dilute in information and often contains misleading observations. Therefore, only selected observations from this data were taken for model development. Although this work was done carefully, several observations had to be excluded from the 'cleaner' data set during model development work. Nonlinear models were developed for several consequences of the process, including nickel content in the leachate, some impurities in the leachate, nickel content in the other stream and yield.

Implementation of the Nonlinear Models for Efficient Use

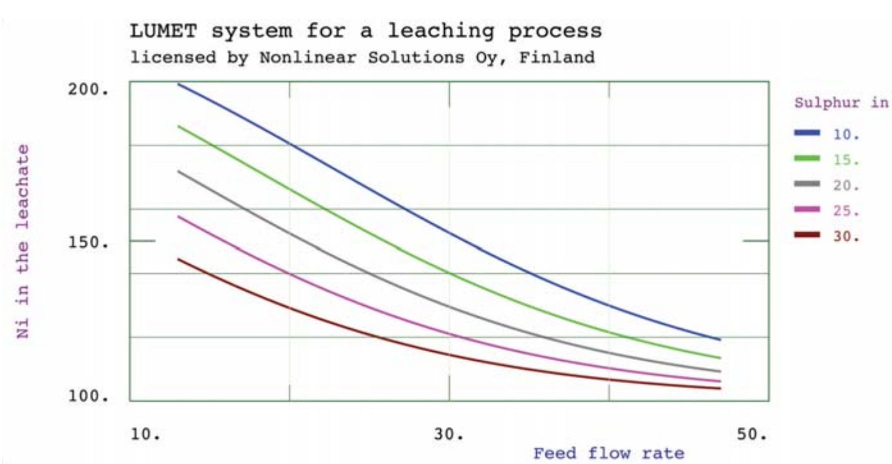
Mathematical models can contain a lot of valuable quantitative knowledge in a concise and a precise manner. Concrete benefits, however, are achieved only if the models are used efficiently, but plant operators cannot be expected to understand nonlinear models—and even most R&D personnel cannot work with the equations of nonlinear models, which tend to be unwieldy and cumbersome for mathematical operations. Therefore, *LUMET* systems have been developed over 15 years with several features which make it easier for the user to utilize the model for several kinds of calculations. *LUMET* systems are a set of software components offering facile use of the models by people unfamiliar with nonlinear modeling. For this leaching process, nonlinear models were implemented in a *LUMET* system.

When implemented in *LUMET* systems, we can use the models to see the individual and combined effects of the input variables on each of the outputs. The accompanying figure illustrates the effect of feed flow rate at different sulphur contents in the feed on nickel content in the leachate. At low sulphur contents in the feed, nickel content in the leachate is more sensitive to the feed flow rate. The figure below shows contours of yield in terms of feed flow rate and temperature in a certain location in the autoclave. One can see that there is an optimal feed flow rate which varies with that temperature.

Some input variables have desirable effects on some outputs while having undesirable effects on other outputs. These and such other conflicting objectives make it a challenging task to determine the best ways of operating the autoclave. *LUMET* systems make that task easier.

Boosting Business Competitiveness with Nonlinear Modeling

Any process operation can be made more efficient with better quantitative knowledge of the effects of process variables and feed characteristics on the consequences of the process. These relationships, however, tend to be complicated for most industrial processes.



Effect of feed flow rate on nickel in the leachate for different values of sulphur in the feed.

Nickel cathodes, briquettes and powder.

Nonlinear modeling is a relatively new technology which helps production units derive more from their equipment and raw materials while also improving their control over product properties. Industries usually collect a lot of production data that is unused or underutilized—data that can contain valuable information which can be extracted by nonlinear modeling. If used effectively, nonlinear modeling can add to a company's competitiveness.

Nonlinear modeling can contribute much to mining and mineral processing. New technologies come up from time to time which affect production economics, and open up new possibilities. Those companies that utilize new technologies effectively have an edge over those that do not. Nonlinear modeling is expensive compared with linear statistical techniques, but as experience shows time and again, the benefits clearly outweigh the costs.

Scientists and engineers can perform better process development with less experimentation effort by using nonlinear modeling. Deriving maximum mileage from a reactor or separation equipment is an optimization task, for which it is necessary to have detailed quantitative knowledge of its operation. Such knowledge can be summarized in the form of nonlinear empirical or semi-empirical models describing the effects of process variables and feed characteristics. It has become feasible to utilize this new technology in practice.

Development of quality mathematical models fit for industrial production processes, particularly leaching, has been considered to be very difficult. However, newer nonlinear modeling techniques have clearly improved this situation, as results from this work demonstrate. Because these nonlinear models can be quite complicated, and technical personnel generally aren't experts on optimization techniques, a simple tool has been devised bringing these new possibilities within the reach of engineers and scientists.

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