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Intelligent Computational Methods for Simulation and Analysis of Chemical Processes. A Comparative Review

Cristina Popa*, Otilia Cangea*, Luana Florentina Pascu**

* Universitatea Petrol-Gaze din Ploieşti, Bd. Bucureşti 39, Ploieşti
e-mail: ceftene@upg-ploiesti.ro; ocangea@upg-ploiesti.ro

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Abstract

Advances in computing have facilitated major progress in computational chemistry, model-based process control, and real-time process optimization. Modern computer graphics—including simulations— have greatly enhanced the ability of scientists and engineers to understand and utilize the results of their computations.The paper presents a review of some of the most important results, related to simulation and analysis of chemical processes, obtained by the authors by applying intelligent computational methods. Thus, there are presented and comparatively analized artificial neural network structures that have been succesfully applied both for predictive control systems for catalytic cracking processes and for estimating the extracting time of Au(III) from a hydrochloride solution.

Key words: *chemical processes, simulation, analysis, intelligent computation*.

Introduction

Modeling and simulation are extremely important tools in chemical sciences. The understanding and engineering of complex chemical processes generally rely heavily and increasingly on modeling and computation. Modern computer graphics—including simulations and animations— have greatly enhanced the ability of scientists and engineers to understand and utilize the results of their computations. Recent advances in computing not only have enabled more accurate and reliable calculations, but have also provided new tools for interpreting the output of the calculations [1].

A number of major challenges exist in process systems engineering in which computing will play a major role. These can be grouped by major areas of application, among these Process Control being one of the most important., given the fact that in chemical and petrochemical industry there will always be an increased need for synthesizing plantwide control systems, as well as integrating dynamics and safety functions, achieved through new mathematical and computer science developments.

Progress in this area will require a number of new supporting tools that can effectively handle and solve a variety of mathematical models involving thousands of variables. These supporting tools will require chemical engineers to become acquainted with new advances in numerical analysis and mathematical programming.

Estimating the Extraction Time of Au(III) from Chloride Using Artificial Neural Networks

Hydrometallurgy, or the industry of extracting metals from aqueous solutions, represents a group of industrial processes that have an increasing importance, as a result of decrease of useful mineral content of the deposits. In this context, a very important problem is represented by the extraction time, especially in the case of valuable metals, and by the manner in which one can estimate the complete extraction duration from an initial concentration to a zero concentration.

Estimation of the extraction time of Au(III) from a hydrochloride solution implies acquisition and processing of experimental data, the aim being to elaborate a mathematical model that allows the proper estimation of the time needed to recover a metal by means of a solvent extraction technique. Extraction time estimation is performed using an Artificial Neural Network, whose topology and weights will be computed accordingly.

Acquiring the experimental data for the elaboration and validation of the mathematical model was performed using Au(III) solutions of 10^{-4}M and 2. 10^{-2} M concentrations, in a HCl 1M concentration. For gold recovery from the membrane, it was used a NaCl solution of different concentrations and there have been performed four sets of experimental measurements, using gold solutions of different concentrations and time intervals up to 370 min. The determination of gold concentration has been performed by means of atomic absorption spectrometry [2].

In order to estimate the extraction time of Au(III) from the chloride, a feed forward back propagation neural network with two layers was designed (figure 1). The input of the network is the Au(III) concentration in solution, and the output is considered to be the time corresponding to the respective concentration. The first layer consists of 5 neurons having $f_1(s)$ TANSIG activating functions, that has the nonlinearity and derivability advantages that recommend it for the back propagation algorithm. The second layer consists of a neuron having the $f_2(s)$ PURELIN (linear) activating function [2].

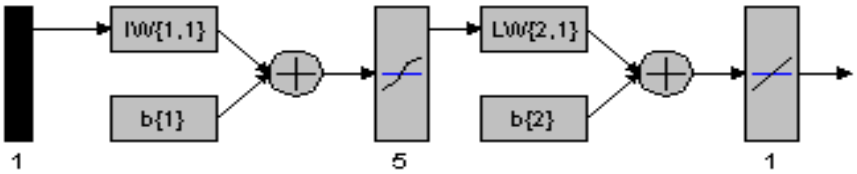

Fig. 1. Neural network block diagram

In order to implement the program, the MATLAB *Neural Network* toolbox graphical interface was used [5]. After training, the IW{1,1} and LW{2,1} vectors, as seen in figure 1, will have the weights of the connections from the input to the 1st layer, respectively from the 1st layer to the 2nd layer, b{1} and b{2} being the biases corresponding to the layers. For the selection of the training set, one analyses the available experimental data that consists of 4 measurement sets (Table 1), having the graphical representation displayed in figure 2 [2]. The 3rd set of experimental data is used for the training process. The input values are given in the *c*3 concentrations vector, and the desired output values are presented in the *t*3 time vector, as follows:

*c*3 = 39.8400 27.4800 21.2200 15.8800 12.2000 7.0200
*t*3= 0 60 120 180 240 360

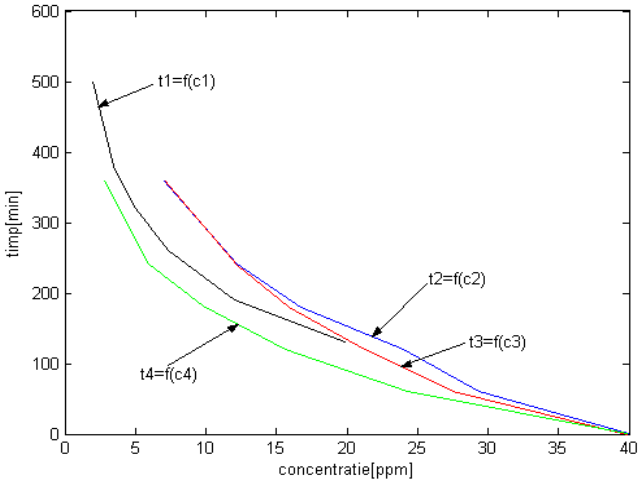

Fig. 2. Experimental data graphical representation

Table 1. Experimental data measurement sets

Set	Concentration[ppm]	Time moments [min]	Set	Concentration[ppm]	Time moments [min]
1.	19.834	0	3.	39.84	0
	12.02	60		27.48	60
	7.29	130		21.22	120
	5	190		15.88	180
	3.43	250		12.2	240
	2.01	370		7.02	360
2.	39.92	0	4.	39.82	0
	29.38	60		24.24	60
	24	120		15.64	120
	16.72	180		9.8	180
	12.18	240		5.91	240
	6.98	360		2.82	360

The neural network response, in comparison with experimental data, presented in Figure 3 [2], is generated as *t*3*r* =60.7786 114.9237 181.8307 243.2525 358.3540

The network is tested for the concentrations set:

40 39 38 37 36 35 34 33 32 31 30 29 28 27 26 25 24 23 22
21 20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0

The results of the neural network testing are:

0.3510 3.5959 7.0563 10.7466 14.6820 18.8787 23.3541 28.1267 33.2163 38.6437
44.4315 50.6036 57.1853 64.2038 71.6882 79.6692 88.1797 97.2549 106.9321
117.2511 128.2544 139.9872 152.4979 165.8378 180.0617 195.2280 211.3989 228.6407

247.0241 266.6242 287.5213 309.8008 333.5535 358.8765 385.8729 414.6526 445.3325 478.0373 512.8995 550.0603 583.7761

and the graphical representations of these results, in comparison with experimental data, are presented in figure 4 [2].

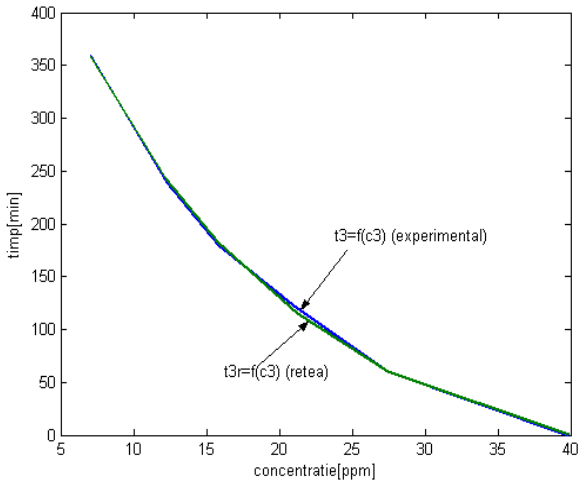

Fig. 3. Neuralnetwork response presented in comparison with experimental data

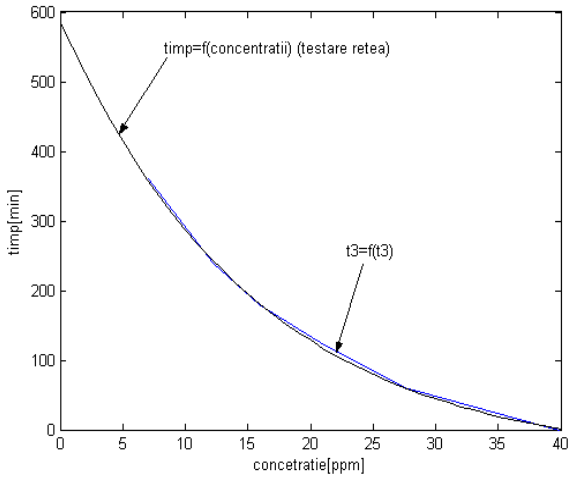

Fig. 4. Results of the neural network testing, in comparison with the 3rd experimental data set

The conclusion is that using the neural network, one can estimate the complete extraction duration from an initial concentration to a zero concentration, even if, practically, the last value can not be accurately experimentally determined.

Neural Network Predictive Control System for a Catalytic Cracking Process

Considering the value of the obtained products, the catalytic cracking plant represents one of the most important parts of a refinery. It ensures the conversion of heavy fractions into gasoline, Diesel oil or rich olefins gases, that are used in petrochemical industry or for private consumption.

In this respect, one may emphasize the fact that neural networks are often used in designing control structures that can be applied to chemical processes.

A suggestive example, presented in figure 5, is represented by the neural network-based control structure for the catalytic cracking process described in paper [3]. This structure has three components, that are: *the process, the neural network-based process model and the optimization module.*

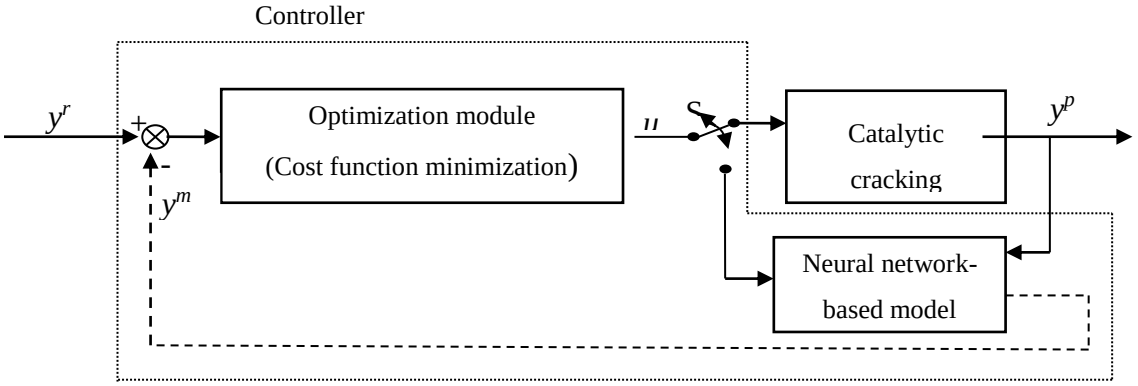

Fig. 5. Neural network-based predictive control structure

The significance of the annotations in Figure 5 is: y^r – the reference of the predictive controller; y^m – the output estimated by the neural network; u – the command to the process or to the neural network-based model; y^p – the controlled output.

In order to design and simulate the neural network, the authors have used one of the facilities of SIMULINK *Neural Network Predictive Control*toolbox [5], that is *Process Identification*, and designedand implemented a simulator of the cracking process, presented in figure 6.Thus, the *Reactor* block represents the plant model, connected to the *NN Predictive Controller* block. The *NN Predictive Controller* block signals are connected as follows:

- *Control Signal* is connected to the input of the *Reactor* model;
- The *Plant Output* signal is connected to the *Reactor* block output.
- The *Reference* is connected to the *Ts_ref* signal.

The required stages for designing the controller are:

- *Developing a data base for training the neural network* –using the process simulator, one applies a random signal, having variable amplitude and frequency, to the process input. The prediction error between the plant output and the neural network output is used as the neural network training signal.
- *Determining the neural network structure* – one usually recommends, for process controlling-applications, feed-forward networks with a single hidden layer. The hidden layer of the neural network was designed with 7 neurons, as presented in the graphical interface displayed in figure 7, that indicates the main parameters of the network architecture and the training data for plant identification.
- *Validating and training of the neural network* – considering the data base, only 80% of the recordings are used for neural network training, the rest being required for network validation. A Levenberg-Marquardt training algorithm was used, of a backpropagation type. The number of training epochs for the neural network, as well as the number of neurons from the hidden layer, were settled by tests and performed until the resulted error,related to the output of the process and the output of the neural network, was considered satisfactory.

The authors configured **Plant Identification**in order to design the neural network plant model, that predicts future dynamics of the plant outputs. The optimization algorithm uses these predictions in order to determine the control inputs that optimize future performance. The plant model neural network has one hidden layer, as shown previously. The authors have selected the

size of this layer -7, the number of delayed inputs – 2, and delayed outputs -2, and the training data and parameters, as seen in figure 7. There are displayed the graphical representations associated to neural network validation of the controller structure for the riser-reactor subprocess.

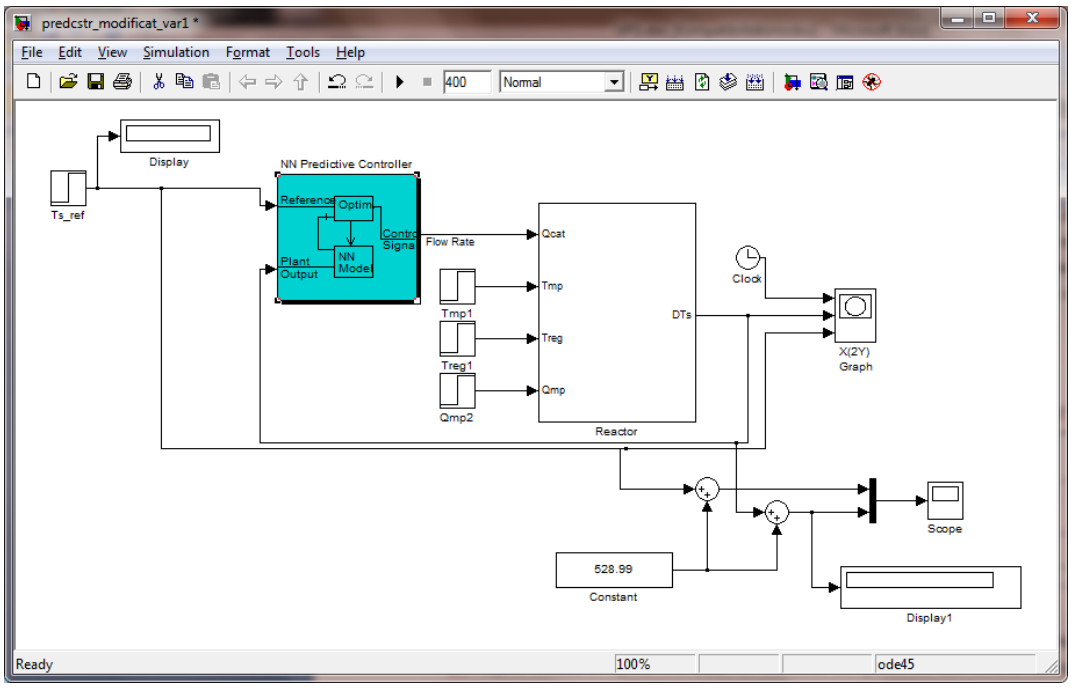

Fig. 6. The simulator of the neural network-based predictive control structure for the reactor subprocess

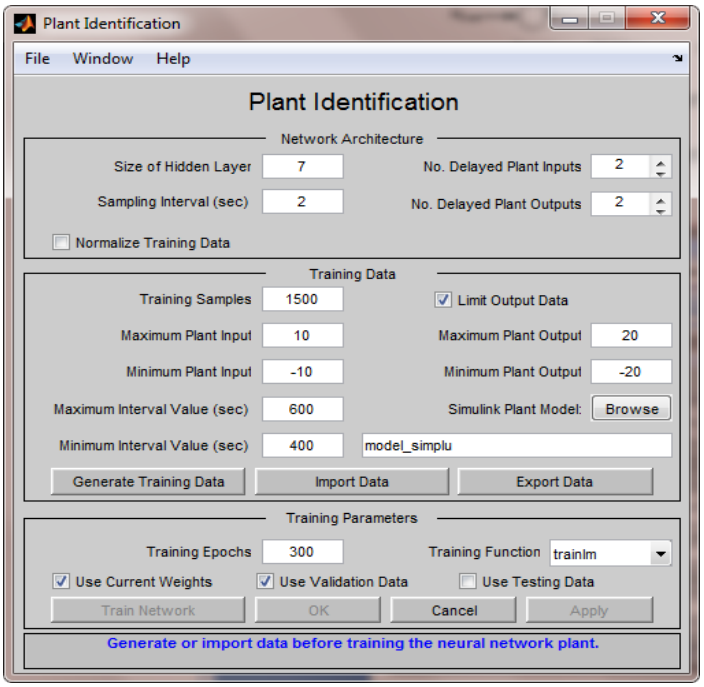

Fig. 7. Plant identification graphical interface

The results of the stage of validating and training of the artificial neural network are presented in Figure 8. Thus, the graphical representations emphasize the output of the SIMULINK plant

model (Output process), the Neural Network model output (Output NN), one step ahead prediction, and the resulted difference between plant output and NN model output (Errors).

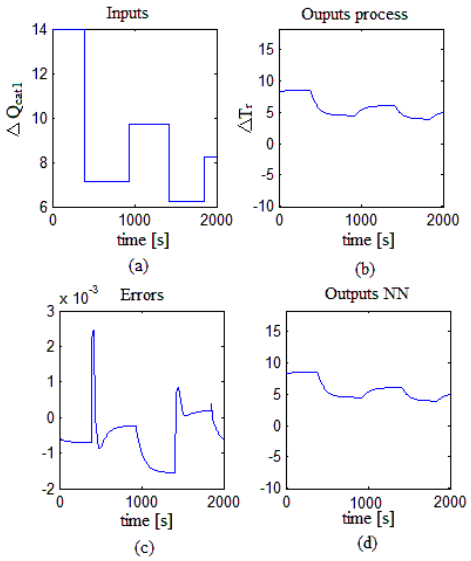

Fig. 8. Graphical representations associated to neural network validation of the controller structure for the riser-reactor subprocess

Conclusion

The paper presents a comparative review of two of the most important results, related to simulation and analysis of chemical processes, obtained by the authors by applying intelligent computational methods. The topic belongs to the scientific research area of the authors having a significant experience, with important results, that led to the interest and opportunity of developing the proposed subject.

In this respect, there are presented and comparatively analysed two artificial neural network structures, both of feedforward back propagation type, that have been successfully applied in different approaches. Thus, the authors presented the results obtained by designing a predictive control system for catalytic cracking processes using an artificial neural network. The results of the simulator in a steady–state regime have proved a typical behaviour of the fluid cracking process. Both the temperature in the reactor and the feedstock concentration decrease exponentially compared to the spatial coordinate associated to the riser. The gasoline concentration confirms an optimum value for the height of the riser.

This new research is comparatively presented related to a similar neural network structure, used for estimating the extracting time of Au(III) from a hydrochloride solution. In this case, on the base of a measurement set and without any prior information regarding the system structure and characteristics, the neural network successfully replaces the overlong timing of data acquisition process, being capable of simulating the process operation and to determine the intervals from an initial, assigned concentration, to a final one.

On the other hand, MATLAB is strongly recommended for applications specific to experimental data processing by its graphical properties and resources, as well as for the facilities of its dedicated toolboxes, such as the *Neural Network Predictive Control* toolbox. Thus, the *Process Identification* facility, from the *Neural Network Predictive Control* toolbox, uses a neural network model of a nonlinear plant to predict future plant performance.

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Metode de calcul inteligent pentru simularea şi analiza proceselor chimice. O abordare comparativă

Rezumat

Lucrarea prezintă o abordare comparativă a unora dintre cele mai importante rezultate referitoare la simularea şi analiza proceselor chimice, obţinute de către autori prin aplicarea metodelor de calcul inteligent. In acest sens, sunt prezentate şi analizate comparativ două structuri de reţele neuronale artificiale, ambele de tip feedforward back propagation, care au fost utlizate cu succes în abordări diferite, atât pentru proiectarea unor sisteme de reglare predictive pentru procesele de cracare catalitică, cât şi pentru estimarea timpului de extracţie a Au(III) dintr-o soluţie hidrocloridă. De asemenea, Process Identification, din cadrul Neural Network Predictive Control toolbox-MATLAB, permite utilizarea unui model al procesului de tip retea neuronala artificiala care poate oferi predictii referitoare la performanţele şi comportarea sistemului.