Complex Process Modeling using Mathematical Models and Neuronal Network Models.

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Abstract:
The following paper present elaboration of: complex mathematical models of processes, mathematical models and neuronal networks simulation using Matlab 5.3 program and, last but not least, conclusions on the simulation with artificial neuronal networks results.

Key words: math model, neuronal networks, modeling;

1. INTRODUCTION

Generally, a fundamental feature of the technical systems is complexity. Heterogeneity, distributed and charted structure, the presence of the human element, the non-linear character of interactions, the uncertainty of the data and, last but not least, the insufficiency of models are the main criteria which fundamentally determine the manner of approach in the synthesis and analysis of the present systems.

Modeling is a study method of certain processes and phenomena by the substitution of the real object of research. The model is the main investigation instrument in the knowledge of the real world. The main problem of any abstract model consist in its adequacy in the case of the formal model, respectively in its similitude, if we speak about physical models. Thus, the importance of the model is directly proportional with the dimensions of systems and the complexity of processes.

The mathematical model of the process is represented by the relationship between the input and ouput variables of the process.

A simple illustrative example could be the case of a heat exchanger.

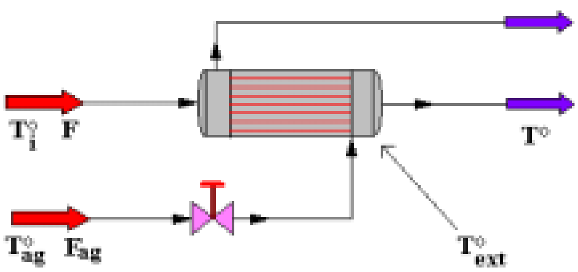


Figure 1. Heat exchanger.

In which the exit temperature from the exchanger may be written as being a function of the following shape:

$$T^0 = f(T_i^0, T_{ag}^0, F, T_{ext}^0, F_{ag}, t) \qquad (1)$$

In order to evidence the complexity of the mathematical modeling of a system we performed a case of study on a vinyl chloride synthesis reactor.

The modeling of the reactor which obtains the vinyl chloride was carried out by analytical modeling and by modeling on the basis of neuronal networks.

2. ANALYTICAL MODELING OF THE REACTOR:

Mathematical models could be: dynamic mathematical models and steady state mathematical models.

Dynamic models are used in the design activity: the establishment of the automatic control system structure and complexity; optimal choice of the controler parameters; the establishment of optimal, adaptive or multi-variable control strategies.

The stady state models are used in the research-pilot activity; the determination of processes development mechanisms; computer simulation of processes behavior in various situations, thus saving time, money and work.

A mathematical model contains: energy conservation law, momentum (impulse) conservation law and mass conservation law.

2.1. Energy conservation law:

In accordance with (e.g. [2]), for a plug flow reactor, the energy conservation law is:

$$\frac{\partial}{\partial t}\left(\rho\, c_p\, T^0\right)+\frac{\partial}{\partial z}\left(V\rho\, c_p T^0\right)+kC_A\cdot\Delta H_r+\frac{4K_T}{D}\left(T^0-T^0_{ag}\right)=\frac{\partial}{\partial z}\left(k_T\frac{\partial T^0}{\partial z}\right) \quad (2)$$

Simplifying assumptions:

- The reactor works in stady state. Terms from the energy conservation law expression which contains a component depending on time become zero.
- Removal speed of the components from the reactor is very high. The diffusions term from the equation becomes zeros.
- The chemical reaction takes place with a higher speed.

According to the simplifying assumptions the energy conservation law becomes:

$$\frac{\partial}{\partial z}\left(V\rho\, c_p T^0\right)+kC_A\cdot\Delta H_r+\frac{4K_T}{D}\left(T^0-T^0_{ag}\right)=0 \quad (3)$$

2.2. Impulse conservation law

The second Newton's law expresses that the sum of forces exercised upon the system is equal to rate of variation of momentum (quantity of movement) of the system.

$$\vec{F}=m\cdot\vec{a} \qquad \sum_{j=1}^{N}F_{ij}=\frac{d}{dt}\left(mv_i\right) \quad (4)$$

Simplifying assumptions:

- The reactor works in stady state. Terms which depend on time become zero.
- The molecules from the same element of volume have the same speed.

According to the simplifying assumptions the second law of Newton, for a reactor, becomes (e.g. [2]):

$$\frac{P}{S_r}-F_r=0 \quad (5)$$

Where F_r is the friction force between the reaction mass and wall reactor.

The upper equation, for a plug flow reactor is: (e.g. [3])

$$dP/dz=\left(rez\_hid\right)\cdot\left(\rho_{gaz}w^2/(2D\cdot 1.013\cdot 10^5)\right) \quad (6)$$

2.3. Mass conservation law.

$$\dot{x}_{CV}=\frac{\dot{x}^0_{CV}+\eta}{1-\eta} \qquad \dot{x}_{HCl}=\frac{\dot{x}^0_{HCl}+\eta}{1-\eta} \qquad \dot{x}_{imp}=\frac{\dot{x}^0_{imp}+\eta}{1-\eta} \quad (7)$$

$$\eta = \frac{-\left[X_{CV}^{0} + X_{HCl}^{0} + \frac{K_f}{K_V p}(1-A)\right]}{2\left(\frac{K_f}{K_V p}+1\right)} \pm \frac{\sqrt{\left[X_{CV}^{0} + X_{HCl}^{0} + \frac{K_f}{K_V p}(1-A)\right]^2 - 4\left(\frac{K_f}{K_V p}+1\right)\left(X_{CV}^{0} + X_{HCl}^{0} + A\frac{K_f}{K_V p}\right)}}{2\left(\frac{K_f}{K_V p}+1\right)} \qquad (8)$$

2.4. The modeling results using matematical models.

Using the Matlab 5.3 progam we obtained the next results:

Figure 2 and figure 3 presents the temperature and the conversion variation from plug flow reactor depending on reactor length and its diameter.

Figure 4 and figure 5 presents the temperature and the conversion variation in the plug flow reactor depending on reactor length and impurites fraction.

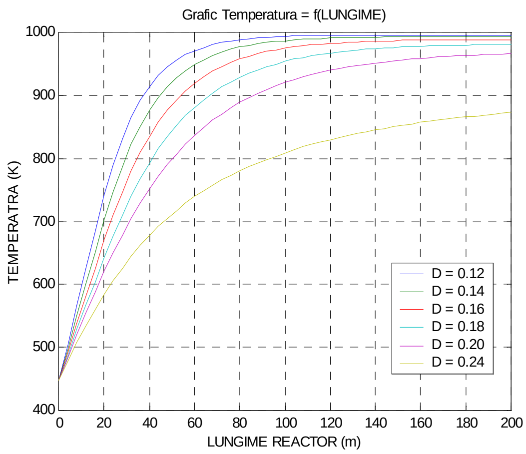


Figure 2

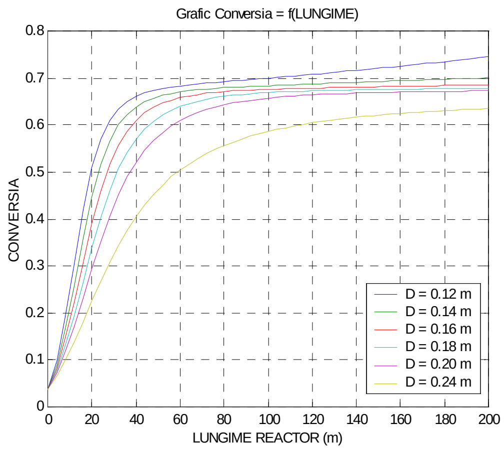


Figure 3

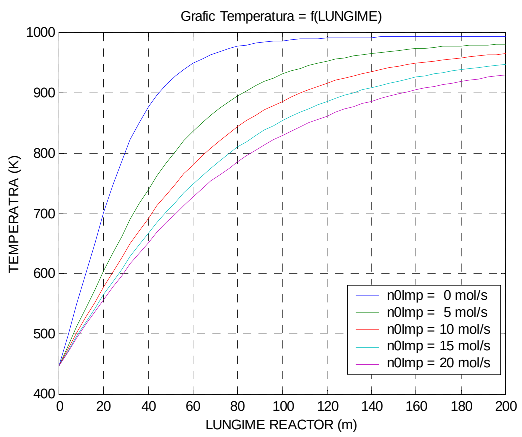


Figure 4

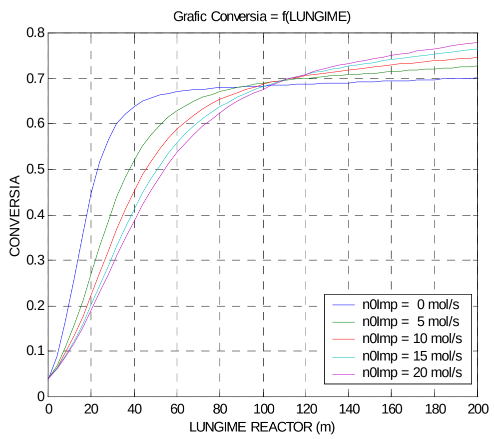


Figure 5

Analysing the influence of all the inputs on the outputs we choose the next conditions for process:

n0DCE = 186 mol/s, n0CV = 0 mol/s, n0HCl = 0 mol/s, n0Imp = 20 mol/s;

D_{react} = 0.14 m, T_{perete} = 627 °C, P_i = 20 atm, T_i = 448 K.

The results obtained by mathematical model are:

- exit temperature from reactor: 794K
- exit pressure from reactor: 21,7 atm
- final conversion: 60%
- reactor length: 200m

3. REACTOR MODELING BY ARTIFICIAL NEURAL NETWORKS.

The artificial neural networks (ANN) have as the main point of inspiration the nervous system.

The organization unit of the nervous system is the neuron, a cell which shows a number of entries, dendrites and an exit, axon, by means of which it is interconnected with other neurons.

An artificial neuronal network is made out of a multitude of knots in which the artificial neurons are located; the neurons are linked by non-linear elements. Each entry has a certain weight which represents the importance the impulse.

The most important characteristics of the artificial neuronal networks are:

1. The capacity to learn. The neuronal networks do not need powerful programs, they are merely the result of the training on the set of data.
2. The capacity of generalization. If they were trained appropriately, the networks are capable of giving correct answers aslo for different entries than those with which they were trained, as long as they are not too different, the ANN automatically generalize.
3. The capacity of synthesis. The artificial neuronal networks may make decisions or draw conclusions when they are facing complex information or irrelevant or partial noises.

The neuronal general model for an artificial neuron is (e.g.[6]):

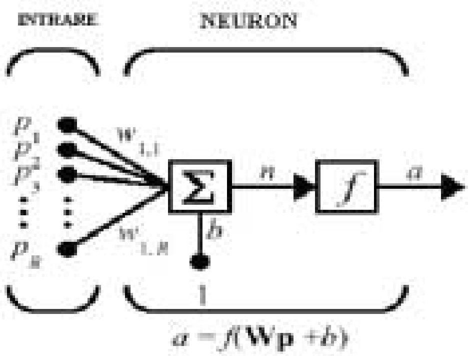


Figure 6. Artificial neuron.

$p_1, p_2, ..p_R$ – represent the values of inputs;

$w_1, w_2, ...w_{1,R}$ – represent the weight which multiply every inputs;

b – bias;

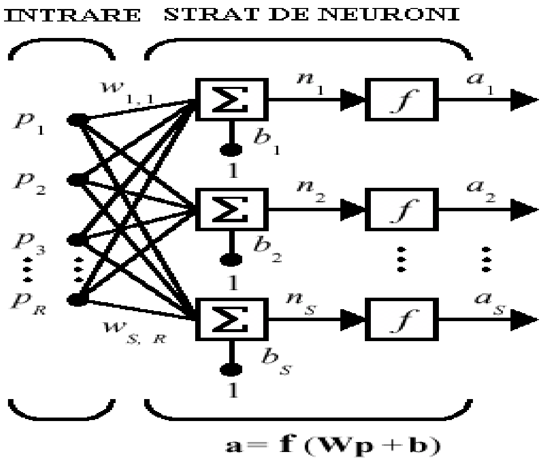
$$n = w_{1,1}p_1 + w_{1,2}p_2 + \dots + w_{1,R}p_R + b \quad (9)$$

Function f is the transfer function, and she gave off the output from neuron.

The transfer function can several forms:

- "hardlim" function;
- "purelin" function;
- "logsig" function;
- "tansig" function;

A general neuronal network model (e.g. [6]):



The neural feedforward networks is a complex, compound by artificial neurons organized on levels between which have are weight connections, the connection between neurons is only one way and top-down.

For higer performances and more complex problems could be create feedforward multilavel networks.

Figure 7. Neuronal network.

3.1. The modeling results using neural networks.

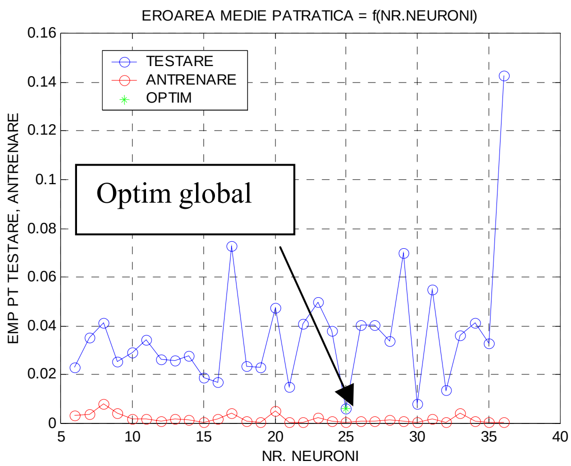


Figure 8. Square Means Error variation depending on neurons number in the hidden layer.

A network with 25 neurons the hidden layer gives the minimal square mean error. The correlation coefficient (R value) between the network response and the target was:

- for test data : 1.0032;
- for training data: 1.0001;

The choosen network has the square mean error: 0.0061621 for test data and 0.00029838 for training data.

$$ERR = RSP - REZ \quad ; \qquad ERMP = \sum_{i=1}^{N} (ERR^2) \qquad (10)$$

Where:
ERR – error obtained in training and test stage;
RSP – neuronal network answer appling of training and test data;
REZ – the result suply conversion function, is the right answer by RNA;
ERMP – square mean error for training data and test data;
N – Grups number of test data: 320;

Training data and test data are obtain with the conversion function which has the form given in (11):

$$\eta\left(T, p, \dot{X}^0_{HCl}, \dot{X}^0_{CV}, \dot{X}^0_{A''}\right) \qquad (11)$$

The difference between network answer and mathematical model computation for test data is given in (figure 9) ; the same difference but for training data (figure 10);

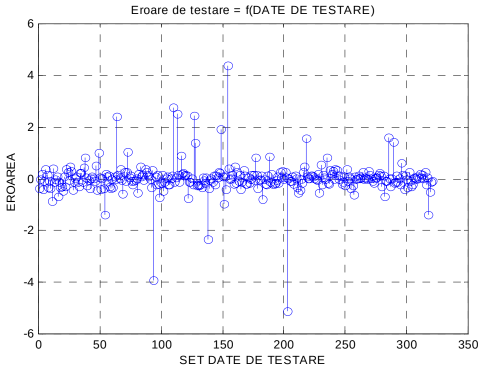


Figure 9.

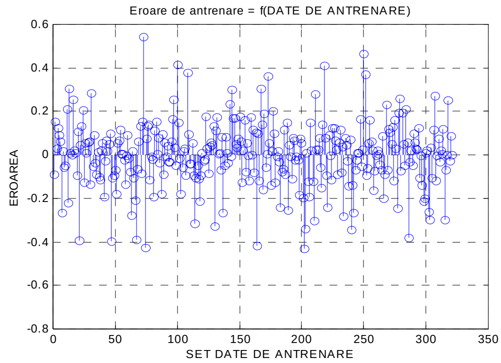


Figure 10

4. CONCLUSIONS ON THE SIMULATION WITH ANN RESULTS:

Out of the above figure one may observe that the error on every set test or training data is located within the interval [-6, +6]% which is an acceptable level of errors. Their great majority, 50%, are placed into a field of [-3, +3]% both for the training and for the test data. Carrying our a regression, using the postreg function of the Matlab 5.3 program, a regression for training coefficient of R=1 was obtained, and for the test phase was obtained the coefficient R=0.999. (e.g.[6])

The ANN is capable of supplying the correct conversion at the exit of the synthesis reactor of the vinyl chloride, it has a very good capacity of data interpolation, a finding which may be reached also during tests. The ANN works to when into the reactor, there are reaction products from a separation system not adequately operated, represented by values different from zero of the molar fractions of the vinyl chloride and of the hydrochloric acid.

Modeling by ANN is used in the cases when there are no data on the reaction kinetics, or the mathematical model may not describe to a satisfactory extent the behavior of the studied process. A great disadvantage of the neuronal networks is the necessity of having many data sets, a fact which may be a serious disadvantage in the case of a real installation. A network trained for given process may not be transposed for another process, so they are used just locally, adapted to a single process and the results cannot be transposed on other processes too. Thus a neuronal network is not a solution for a class of general problems.

5. BIBLIOGRAPHY:

[1]I. Velea Gh. Ivănuş *„Monomeri de sinteză”* Ed. Tehnică, Bucureşti 1989;

[2] Şerban Agachi *„Automatizarea proceselor chimice”* Ed. Casa cărţii de stiinţă, Cuj-Napoca 1994;

[3] C. F. Pavlov, P. G. Romankov, A. A. Noskov *„Exerciţii şi probleme la cursul de procese şi aparate în industria chimică”* Ed. Didactică şi Pedagogică, Bucureşti 1966;

[4] Gavril Toderean, Mircea Costeiu, Mircea Giurgiu *„Reţele Neuronale Artificiale”* Ed. Casa de Editură Albastră, Cluj-Napoca, 1995;

[5]The Mathworks Inc. *„Matlab. The language of tehnical computing. Using Matlab”* Version 5.3 COPYRIGHT 1984 - 1999 by The MathWorks, Inc.;

[6]The Mathworks Inc. *„Neural Network Toolbox for Use with Matlab, Users Guide”* versoin3.0. COPYRIGHT 1992 - 1998 by The MathWorks, Inc.;

[7]The Mathworks Inc. *„Simulink. Dynamic System Simulation for Matlab. Writing S-Function”* Version 3.0. COPYRIGHT 1998 by The MathWorks, Inc.;