Construction of a catalytic reaction mathematical model using a perceptron with one hidden layer

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Abstract. Mathematical models were developed for homogeneous catalytic reaction between alcohols with dimethyl carbonate by least squares method, using a perceptron with one hidden layer and on the basis of the law of mass action. The relative error in deviation of the calculated values from the experimental data is minimal when using the perceptron model with one hidden layer.

1. Introduction

Artificial neural networks consist of formal neurons and connections between them. In fig. 1 shows an illustration of a formal neuron [1].

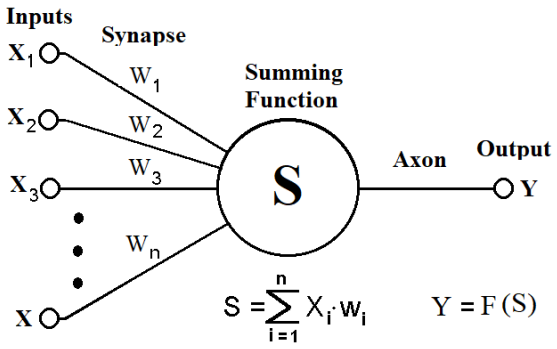

Figure 1. Structure of a formal neuron.

Perceptron - one of neural network models. A neural network consists of an input layer (n inputs), a hidden layer (m formal neurons) and an output layer (k outputs). Learning of the neural network occurs at the time of error and by changing the weights at the inputs to the neurons. Neural networks of back propagation - a tool for finding patterns, prediction, qualitative analysis. The name, backpropagation networks, was obtained from training algorithm used, in which the error propagates from the output layer to the input layer, i.e., in the direction opposite to the signal propagation direction during normal network operation. The back propagation neural network consists of several layers neurons, with each neuron of layer i connected with each neuron of the i + 1 layer, that is, it is a fully connected neural network [2].

The main advantages of reverse propagation neural network are: solving problems with unknown laws, resistance to noise in the input data, adapting to changes, potential ultrahigh performance, as well as fault tolerance in hardware implementation of the neural network.

The main disadvantages are: a long computation, difficulty in understanding the work, the means to perform

2. Object of study

In the neural network are applied to describe the experimental data obtained during the reaction between dimethyl carbonate (DMC) with alcohols in the presence of metal catalysts [3-5]. The reaction belongs to the field of "green chemistry". DMC has shown its need as an effective substitute for existing toxic reagents, in particular phosgene and methyl halides. Using metals of complex catalysts, in particular octacarbonyl diobalt ($Co_2(CO)_8$) and hexacarbonyl tungsten ($W(CO)_6$) [1], allowed the reaction to be triggered at 150–200°C.

In [3], experiments are carried out under different conditions: different temperatures, different initial amounts of catalyst. The previously obtained mathematical model [4-6] describes these conditions. The mathematical model was developed on the basis of the law of mass action (1) [7, 8].

$$\frac{dx_i}{dt} = \sum_{j=1}^{J} v_{ij} w_j (k_j (k_j^{\,0}, E_j, T), x_i), i = 1,..., I \qquad (1)$$

with initial conditions: at $t=0$, $x_i(0)=x_i^0$; where t – reaction time, min; v_{ij} – stoichiometric coefficients; J – amount of stages, x_i– concentration of substances participating in the reaction, mol/L; I – amount of substances; w_j – rate j-th stage, 1/min; k_j– constant velocity stage (reduced), 1/min; E_j, – energy activation stages, kcal/mol; T – temperature, K; k_j^0 – preexponential factors, 1/min.

The numerical values of pre-exponential factors and activation energies are given in [4, 5]. In fig. 2 shows experimental data (points) and calculated values (curve) according to model (1) for the target reaction product $ROCO_2Me$ ($R = C_6H_{13}$) at a temperature of 180°C, the initial amount of catalyst is 3 mmol.

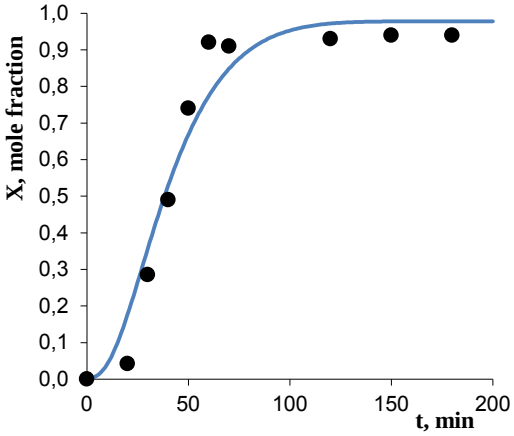

Figure 2. Experimental data (points) and calculated values (curve) by model (1) for $ROCO_2Me$ ($R=C_6H_{13}$), T = 180°C, initial amount of catalyst 3 mmol.

Relative error deviations of the experimental data from the calculated values in model (1) is 10%. In addition to obtained kinetic curves for the constructed model (1), it was proposed to use description of the curves by the method of least squares and using the trained neural network.

3. Least squares approximation

When studying the experimental data for $ROCO_2Me$ using the least squares method [9], it was obtained that the points are best described by function (2)

$$x=0.3213*\text{arctgt}(t) + 0.3346 \qquad (2)$$

In fig. 3 shows the experimental data (points) and calculated values (curve) according to model (2) for the target reaction product $ROCO_2Me$.

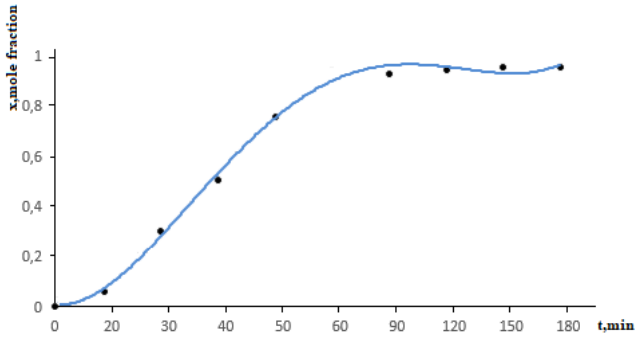

Figure 3. Experimental data (points) and calculated values (curve) by model (2) for $ROCO_2Me$ ($R=C_6H_{13}$), T = 180°C, initial amount of catalyst 3 mmol.

Approximation error was about 14%. Approximation error exceeded an error on the basis of the law of mass action. Thus, it was decided to abandon the use of the method of least squares.

4. Approximation data using a trained neural network

Experimental data were processed using a perceptron [10-12]. For this task, one hidden layer of the neural network is sufficient. At the point of the input layer is fed at temperatures from 20°C to 180°C. This layer approximates the received data, sends data to the second layer. On the second layer, the selection of coefficients occurs, the description of which satisfies the specified values. Due to the second layer, the weights of synapses are trained (at the second layer). The model obtained has the form (3)

$$x=th(t*2.863+2.422048566)*(1.605724575)-0.8255. \quad (3)$$

In fig. 4 shows the experimental data (points) and calculated values (curve) according to model (3) for the target reaction product $ROCO_2Me$.

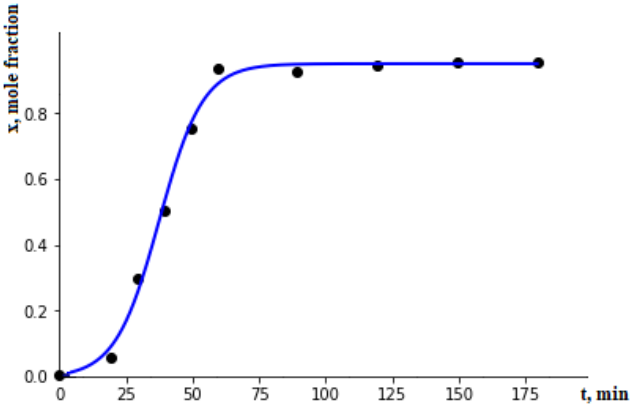

Figure 4. Experimental data (points) and calculated values (curve) by model (3) for $ROCO_2Me$ ($R=C_6H_{13}$), T = 180°C, initial amount of catalyst 3 mmol.

Using model (3), the relative error was 5–7%. In the future, it is planned, when training a neural network, to bring the percentage of error to 1%.

5. Results and discussions

Mathematical modeling was carried out in three different ways: the law of mass action; least square method; perceptron with one hidden layer.

With increasing data, the mathematical model will describe the experimental data with an increasing approximation error. The neural network being trained will be improved according to various experimental data. In the future, it is planned that the neural network will describe a large amount of incoming data. Increase the accuracy of calculations. Based on this neural network, models of homogeneous and heterogeneous catalytic reactions will be developed.

6. References

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