Optimizing the Process of Soybean Oil Epoxidation by the means of Artificial Intelligence

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Abstract

The study of the process of soybean oil epoxidation was conducted in solution of hydrogen peroxide H_2O_2 and acetic anhydride $(CH_3CO)_2O$ in the presence of the KU-2×8 catalyst. As a result of the study, experimental data were obtained, which were used for training an artificial neural network. With the help of a trained neural network, it was possible not only to control the epoxidation process at the synthesis stage, but also select the most favorable parameters and conditions of the experiment, and improve the technology for obtaining chemical products.

A new mechanism for calculating the results of epoxidation of mixtures of unsaturated compounds has been developed. It was demonstrated that by the means of this mechanism it is possible to control the epoxidation process at the stage of synthesis of compounds and in this way to improve the technology of obtaining final products of this reaction.

Keywords 1

Neural network, Epoxidation, Optimization, Soybean oil, Peroxide

1. Introduction

The process of deep machine learning used to solve a system of practical problems. This approach is characterized by a high level of information technology, which is determined by the development of modern computer technology [1].

An artificial neural network (ANN) has been used to solve practical problems in various fields, particularly in medicine. The human speech synthesizer was created based on electroencephalograms of patients, on which their utterances were recorded. The materials were analyzed by the multilayer differential neural network method. With the help of a human speech synthesizer, it is possible to predict and express words and fixed expressions that the patient used, but cannot remember during the operation of the synthesizer [2]. An artificial neural network was used to analyze X-ray images, which were used to determine the service life and degree of use of artificial implants and prostheses installed in the patient's body. [3].

In chemistry, an artificial neural network was used to predict the result of a chemical reaction under different conditions and concentrations of catalysts [4,5].

In robotics, ANN is used to calculate the trajectories of automated mechanisms and manipulators, rational consumption of energy carriers and resources. [6].

In the natural sciences, which include mathematics, physics, and mathematical physics, the use of ANN allowed solving classical fundamental equations [7]. They describe real multidimensional systems for which numerical solutions were previously unavailable [8].

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In physics, with the help of neural networks, a mathematical description of the energy transfer phenomenon in the form of electromagnetic radiation became possible. It includes several simultaneous processes: absorption, secondary radiation and scattering [9], as well as the processing of information received from sensors as a result of the identification of substances [10] to solve physical problems of propagation of electromagnetic waves and ultrasound, Neural networks are also used [11]. Neural networks are widely implemented in atmospheric science, remote sensing, and optics[12].

Research is being conducted on the synthesis of solid polymer materials based on soybean oil with mechanical properties that can be used as construction materials.

Green chemistry is entrenched the principle of sustainable development, based on the use of renewable and environmentally friendly raw materials. It ensures biodegradation and reduction of product toxicity during the production of polymers. [13]. Polymers for the production of printing inks were created as a result of the polymerization of soybean oil. Epoxidized oils are used to improve the properties of rubbers, which are a component for obtaining light-sensitive films, packaging materials for baby food and the production of medical materials. [14]. Soybean oil is a raw material used in research of the synthesis of solid polymer materials. They have mechanical properties that allow them for structural materials.

Epoxides are cyclic ethers, metabolites that are often formed by cytochromes as a result of the action on aromatic or double bonds. The site on the molecule that undergoes epoxidation is its site of epoxidation (SOE).

Thanks to artificial neural networks, it is possible to improve the identification of the SOE of the molecule and to choose the best parameters for controlling the epoxidation process at the stage of product synthesis. ANN is a technical software implementation of the biological neural structure of the human brain. The main part of ANN is a system of connections that allow one neuron to form a signal propagation route to other neurons and receive signals in the reverse direction.

The volume of use of epoxidized oils is increasing, which is connected with the intensive production of polyvinyl chloride (PVC) and polymers based on it. Since epoxidized oils are one of the best stabilizers-plasticizers of such polymers. They have advantages over stabilizers of other types. The introduction of an epoxidized stabilizer into the polymer dramatically increases its thermal stability, prevents the decomposition of the polymer under the action of ionizing radiation as well. Their main functions are: hardeners in compositions with various oligomers and stabilizers in PVC compositions. In the paint industry, epoxidized oils are part of paint products based on epoxy, ethercellulosic oligomers, PVC, as well as plasticizers for organodisperse coatings. [15, 16].

Organic peracids are introduced for liquid-phase epoxidation of unsaturated organic substances. [17,18].

2. Experiment

Based on research [19] was proposed to introduce the H_2O_2/formic acid/catalyst epoxidizing system. Organic peracid, is formed during the interaction of H_2O_2 with an organic acid in the presence of a catalyst, is an epoxidizing agent (Fig. 1). In this system, there was no stage of production and release of peracid, while the organic acid remained circulating.

Replacement of the formic acid with a more affordable option were considered. Among the acids, they chose the cheaper one - acetic [20].

It is suggested to use organic acid anhydride instead of organic acid in our research. As a result, the amount of water in the reaction mixture was reduced, and the reaction of peracetic acid was accelerated.

The purpose of the work is to improve the technology of obtaining epoxidized oils. The selection of optimal conditions for the economical production of epoxidized oils, the quality of which meets the standards (Table 1), modification of the production technology of this product.

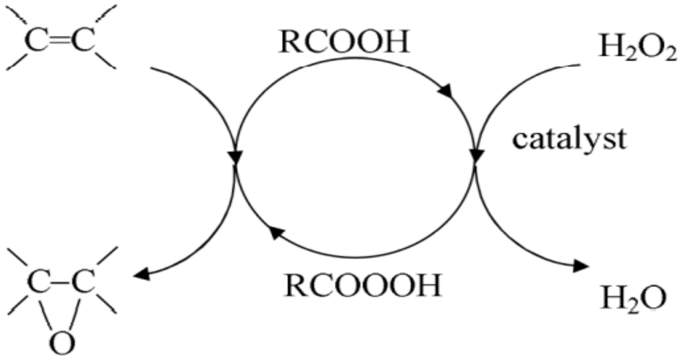

Figure 1: Scheme of epoxidation by H_2O_2/organic acid/catalyst system

Table 1
Quality indicators of epoxidized oils

Physical-chemical indicator	Norm for brands (technical conditions*)		
	ST	SU	C
Epoxy number, % (oxyran oxygen content), not less than	6.5	6.4	6.0
Iodine number, g I2/100 g, no more than	1.5	2.0	8.0

*As stabilizers and plasticizers for PVC-based polymers

Practical value Using a model of the process obtained with the help of a neural network allows control of epoxidized oil during the synthesis stage.

A study of the dependence of the reaction speed of the epoxidation process on:

- Initial concentration of acetic anhydride (AA)
- Initial concentration of hydrogen peroxide
- Initial concentration of ion exchange resin KU-2x8
- Temperature of the process

to establish the optimal concentration of reactants of the epoxidizing mixture, duration of the process, and temperature.

It was experimentally established that at different concentrations of acetic anhydride, hydrogen peroxide, the amount of catalyst, and the duration of the process, the dependence of the epoxide number of epoxidized soybean oil has a complex essence. Increasing the temperature and concentration of the catalyst contributes to the growth of the reaction rate. However, a temperature more than 348K and a catalyst concentration above 15% may decrease the achieved epoxy number.

It is necessary to optimize the conditions for carrying out the process. It is relevant to create a mathematical model and calculate optimal conditions using special methods.

To create the model, the following factors and their limitations were adopted:

- X1 – concentration of acetic anhydride, wt.% $2<x1<9$
- X2 – concentration of hydrogen peroxide 46%, wt.% $25<x2<40$
- X3 - Amount of catalyst, wt.%, $x3<15$
- X4 – temperature, K, $333<x4<353$
- X5 – duration of the process, min, $x5<360$

3. Methods

A sample set was created for neural network training from the array of experimental data obtained. The inputs of the neural network are the conditions of the experiment, and the outputs are the final results, in the form of the acquired properties of substances.

Input parameters:

1. Concentration of AA (normalized)
2. Concentration of H_2O_2 (normalized)
3. Catalyst KU-2×8 (Kat) (normalized)
4. Normalized temperature
5. Normalized reaction time
6. Initial value of Epoxy number (normalized)
7. Initial value of Iodine number (normalized)

For calculations it was accepted that the initial values of the Epoxy and Iodine numbers influence the course of the experiment. The total reaction time for the experimental data sample was within 400 minutes, and the temperature range is 423 - 443 K.

Output parameters:

1. Final value of Epoxy number (normalized)
2. Final value of Iodine number (normalized)

The training of the neural network was carried out on the input experimental data. It were obtained during the epoxidation of soybean oil. For this, 7 input parameters were taken. Their values were normalized to 1. The output layer of the neural network consisted of 2 neurons. As a result, a five-layer network with three hidden layers of 20 neurons each was created (Fig. 2).

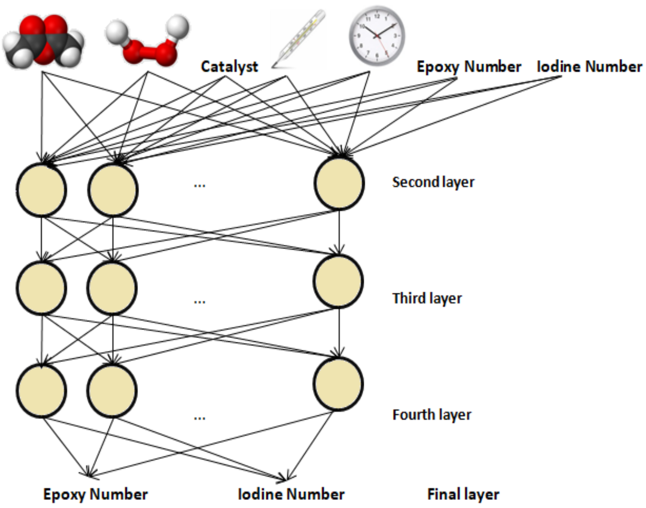

Figure 2: A neural network for data processing obtained during the epoxidation of soybean oil

Neural network training occurs thanks to the mechanism of training with a teacher. The minimum of the error function was determined using the error backpropagation algorithm and the stochastic gradient descent model. The training took place during 1000 epochs.

4. Results and Discussion

As can be seen from Fig. 3, which was obtained after neural network training, an increase in catalyst concentration in the mixture does not lead to a significant change in the growth of the Epoxy number in the first 60 minutes of the reaction. However, during the continuation of the reaction at a higher concentration of the catalyst, the growth of the epoxy number, although it slows down, quickly reached its maximum value. After 1 hour of reaction, at low catalyst concentrations in the mixture, the growth of the Epoxy number stops and is restored around the 4th hour of reaction, at the given concentrations of the substances included in the mixture (see caption under figure 3). Despite the fact that the amount of data and their range of arguments is insignificant, the neural network managed to increase the range of argument values and build a detailed graph, according to which intermediate values were found. It made possible by the neural network's ability to learn. It will be possible to specify this dependence thanks to the replenishment of the database with new experimental data on which the neural network is trained.

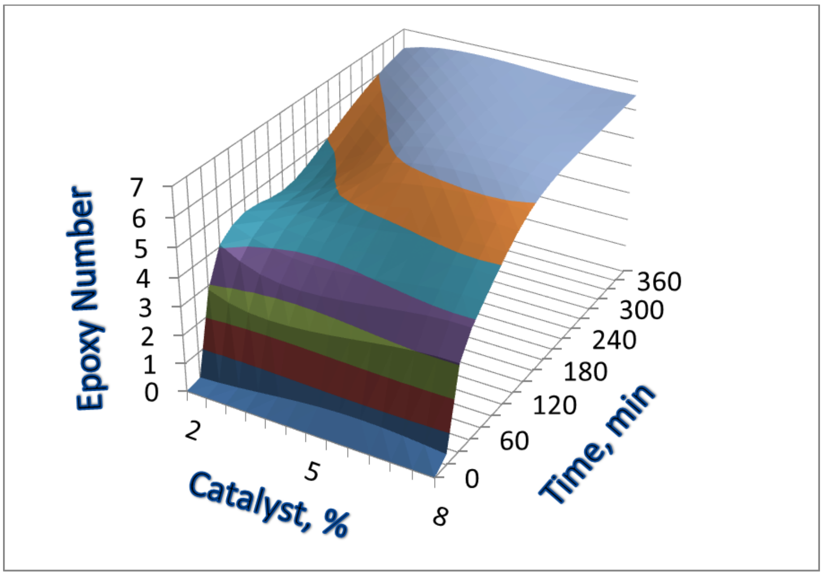

Figure 3: Dependence of the epoxy number on the concentration of the catalyst and the time of the chemical reaction of soybean oil. The calculations were carried out during the interaction of a solution of soybean oil in toluene with the epoxidizing system H_2O_2/acetic anhydride/catalyst Concentration of AA = 5.72 concentration H_2O_2=33.1 wt.%, reaction temperature T=343 K

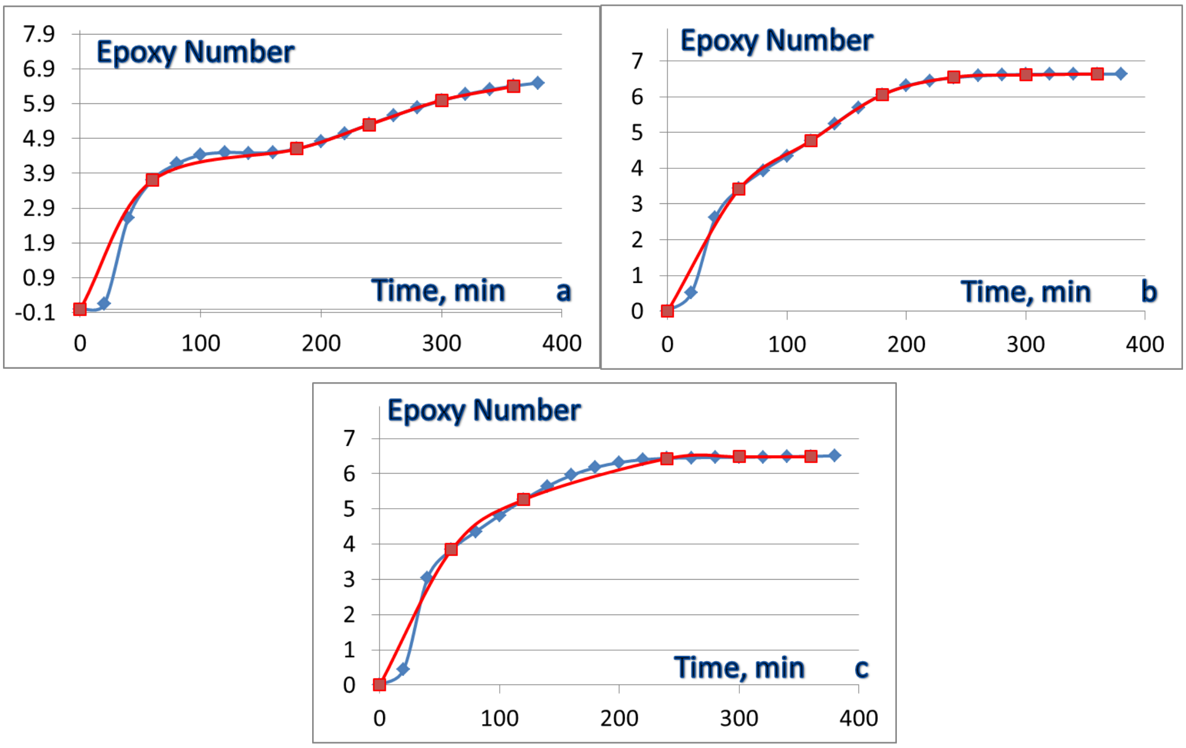

Figure 4: Comparison of dependences of the epoxy number on catalyst concentration and time of soybean oil epoxidation reaction. Experimental data - red lines, and studied (predicted) neural network - blue lines. The calculations were carried out during the interaction of a solution of soybean oil in toluene with the epoxidizing system H_2O_2/acetic anhydride/catalyst. Concentration of AA = 5.72 wt.%, H_2O_2=33.1 wt.%, reaction temperature T=343 K. a - catalyst concentrations in the mixture 2.5 wt.%, b – 5.0 wt.%, c – 7.5 wt.%

The experimental data were compared with the data obtained after training the neural network (Fig. 4). As can be seen, after training, the neural network reproduces the input data with high accuracy and can make experimental predictions beyond the experimental data.

Since the neural network was trained on the intermediate results of the experiment, a bulge appeared at low time limits (Fig. 4a). This convexity is a consequence of the fact that the totality of all input data was considered.

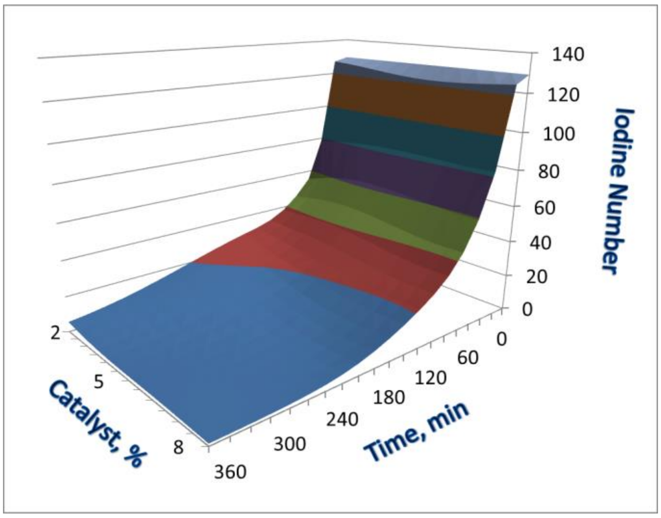

Figure 5: Dependence of Iodine number on catalyst concentration and time of soybean oil epoxidation reaction. The calculations were carried out during the interaction of a solution of soybean oil in toluene with the epoxidizing system H_2O_2/acetic anhydride /catalyst Concentration of AA = 5.72 wt.%, H_2O_2 =33.1 wt.%, reaction temperature T=343 K

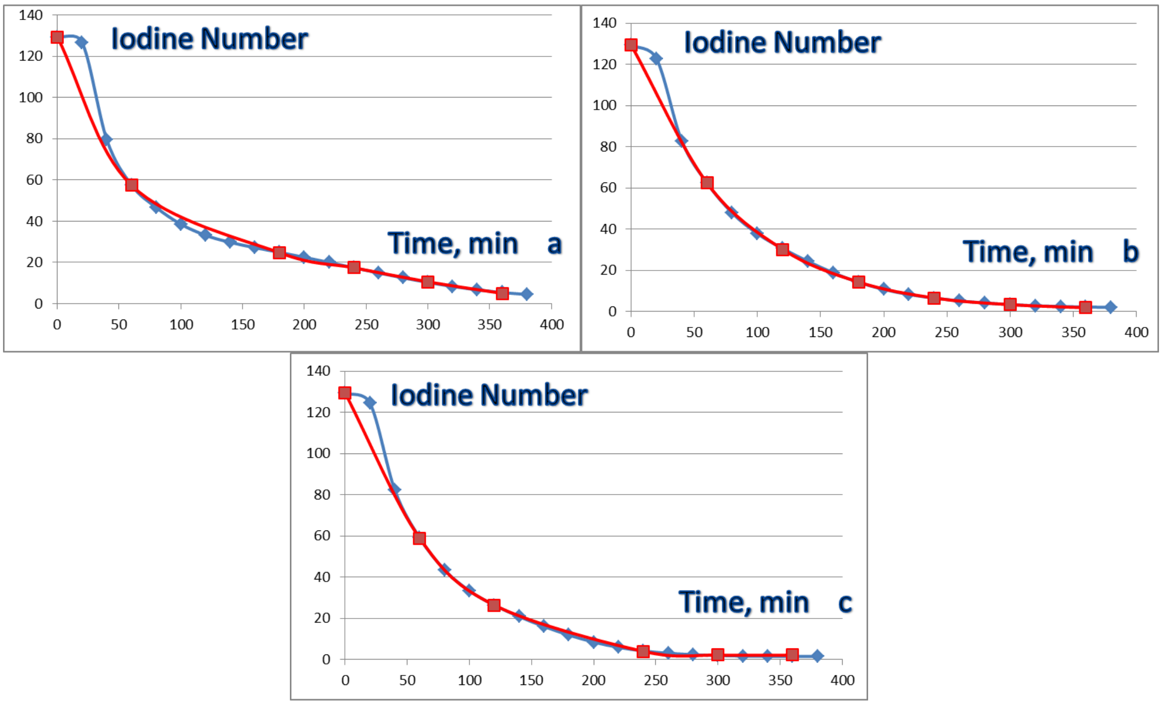

Figure 6: Comparison of dependences of Iodine number on catalyst concentration and time of soybean oil epoxidation reaction. Experimental data - red lines, and studied (predicted) neural network - blue lines. The calculations were carried out during the interaction of a solution of soybean oil in toluene with the epoxidizing system H_2O_2/acetic anhydride /catalyst Concentration of AA = 5.72 wt.%, H_2O_2 =33.1 wt.%, reaction temperature T=343 K. a - catalyst concentrations in the mixture 2.5 wt.%, b – 5.0 wt.%, c – 7.5 wt.%

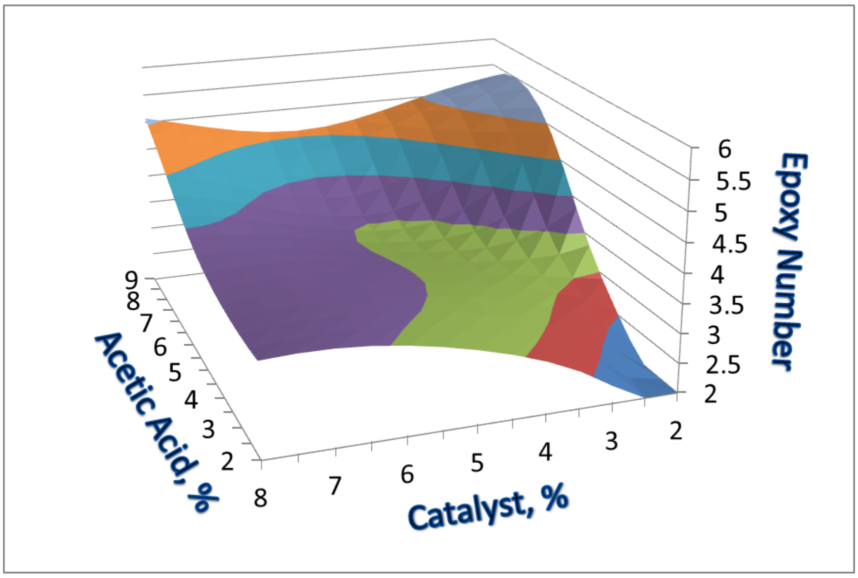

Figure 7: Dependence of the epoxy number on the concentration of AA and the concentration of the catalyst during the epoxidation reaction of soybean oil. The calculations were carried out during the interaction of a solution of soybean oil in toluene with the epoxidizing system H_2O_2/acetic anhydride/catalyst. The concentration of H_2O_2 =33.1 wt.%, the reaction temperature is T=343 K. The reaction time is 60 minutes

As can be seen from Fig. 5, which was obtained after neural network training, an increase in the catalyst concentration does not lead to a significant change in the dependence of the decrease in the ionic number. However, at low concentrations of the catalyst, the decrease in the ionic number is a slightly slower.

As with the Fig. 3 dependence, the data obtained during the experiment are limited by the number and range of argument values. However, as a result of training, the neural network details the dependence of the Iodine number on the selected arguments.

Figure 6, as well as Figure 4, shows a comparison of experimental data with data obtained after neural network training. As a result of the training, the neural network accurately reproduces the experimental data and predicts the result of the experiment based on this data.

Due to the fact that the neural network during training process uses the output functions from seven variables, it becomes possible to see the projections of the calculated functions on the selected axes of the required parameters. The dependence of the epoxy number after a one-hour interval of the epoxidation reaction of soybean oil on the concentration of AA and the catalyst is shown in Figure 7. The duration of the reaction and the concentration of H_2O_2 are constants.

A simultaneous increase in the concentration of AA and the catalyst contributes to the growth of the reaction rate (Fig. 7).

The optimal concentrations of AA and catalyst were calculated to achieve the maximum Epoxy number and minimum Iodine number during the interaction of a solution of soybean oil in toluene with the epoxidizing system H_2O_2/acetic anhydride/catalyst (Fig. 7, 8).

Conditions:

- X2= 33.1 wt.% (H_2O_2)
- X4= 343 K. (reaction temperature)
- X5= 60 minutes (Reaction time).

Optimum values of Epoxy number occur at:

- X1= 8 wt.% (AA concentration)
- X3= 2 wt.% (Catalyst concentration)

Optimum values of Iodine number occur at:

- X1= 9 wt.% (AA concentration)
- X3= 3 wt.% (Catalyst concentration)

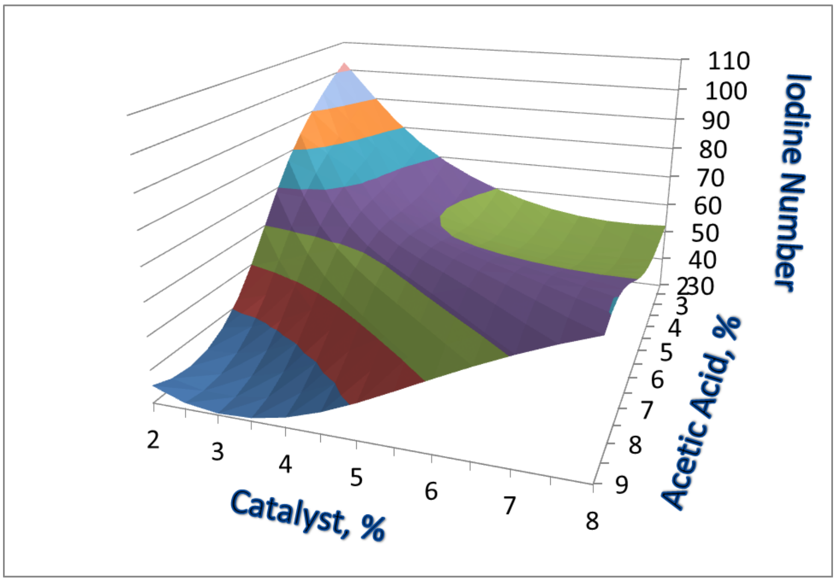

Figure 8: Dependence of Iodine number on AA concentration and catalyst concentration during the epoxidation reaction of soybean oil. The calculations were carried out during the interaction of a solution of soybean oil in toluene with the epoxidizing system H_2O_2/acetic anhydride/catalyst. The concentration of H_2O_2 is 33.1 wt.%, and the reaction temperature is T=343 K. The reaction time is 60 minutes

If we fix the reaction time, temperature and concentration of AA in the mixture, we will get the following dependences presented in Fig. 9, 10.

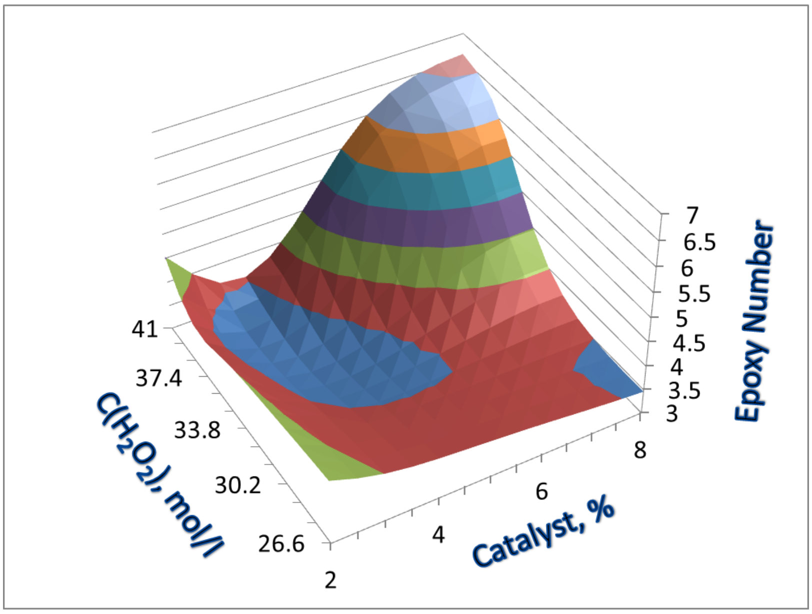

Figure 9: Dependence of the epoxy number on the concentration of H_2O_2 and the concentration of the catalyst during the epoxidation reaction of soybean oil. The calculations were carried out during the interaction of a solution of soybean oil in toluene with the epoxidizing system H_2O_2/acetic anhydride/catalyst. The concentration of AA is 5.72 wt.%, the reaction temperature is T=343 K. The reaction time was 60 minutes.

Simultaneous increase in concentration H_2O_2 and the concentration of the catalyst contributes the increase of the Epoxy number (Fig. 9). The figure also shows a local minimum, which indicates the most suboptimal values of the H_2O_2 concentration and concentrations at which the reaction will proceed very slowly.

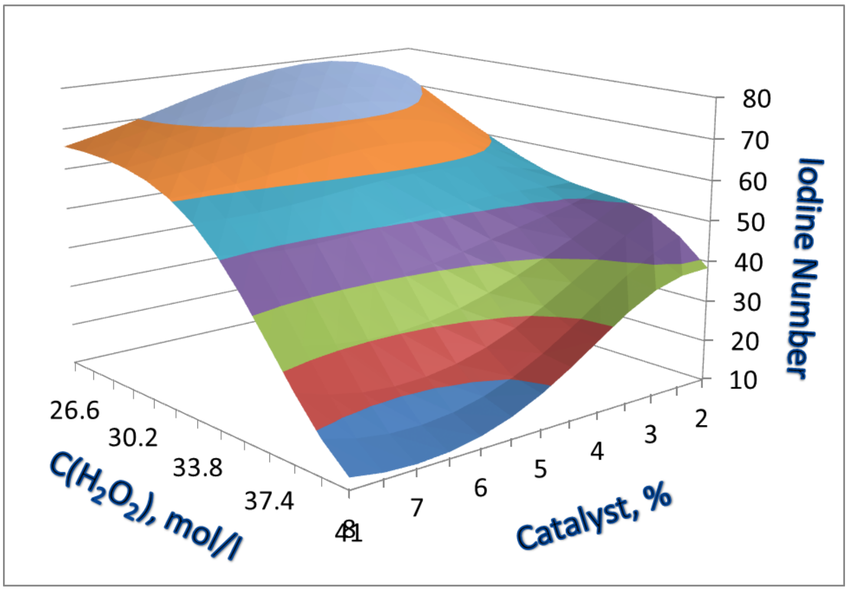

Figure 10: Dependence of the iodine number on the H_2O_2 concentration and the catalyst concentration during the epoxidation reaction of soybean oil. The calculations were carried out during the interaction of a solution of soybean oil in toluene with the epoxidizing system H_2O_2/acetic anhydride/catalyst. The concentration of AA is 5.72 wt.%, and the reaction temperature is T=343 K. The reaction time is 60 minutes

In Figure 10, we have similar dependencies as in Figure 9 for the Iodine number.

As can be seen from the figure, at the maximum concentration (in the selected range) of H_2O_2 and the almost maximum concentration of the catalyst, the Iodine number becomes the minimum value. By analogy with Fig. 8, we calculate the optimal concentrations of) H_2O_2 and the catalyst to achieve the minimum Iodine number during the interaction of a solution of soybean oil in toluene with the epoxidizing system H_2O_2/acetic anhydride/catalyst, we obtain:

Conditions:

- X1= 5.72 wt.% (AA concentration)
- X4= 343 K. (reaction temperature)
- X5= 60 minutes (Reaction time).

Optimum values of Iodine number occur at:

- X2= 40.0 wt.% (H_2O_2)
- X3= 7 wt.% (Catalyst concentration)

5. Conclusions

The process of optimal parameters and conditions selection for the epoxidation process of soybean oil has been presented. As an example of the application of the search method, the dependence of the reaction parameters on the concentration of hydrogen peroxide, acetic anhydride, and the catalyst is demonstrated. The implementation of a neural network showed that even with a small experimental dataset, it is possible to predict the quantitative result of epoxidation, especially, epoxy and iodine numbers. Therefore, the proposed approach makes it possible to more accurately and quantitatively predict the result of the epoxidation reaction of soybean oil.

The optimal conditions for the oil epoxidation process were established using an initial set of specific determined values for the concentration of acetic anhydride, hydrogen peroxide, KU-2x8 catalyst, reaction duration and temperature conditions.

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