Development of a neural network to control the process of cleaning the pyrolysis fraction from acetylene compounds

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Abstract. The process of purification of the pyrolysis fraction from acetylene compounds is one of the stages in the production of butadiene. The efficiency of purification of the pyrolysis fraction many factors. Artificial neural networks are selected for the development of a process control system due to the fact that they are fault tolerant. In a neural network, information is distributed throughout the network, which means if a neuron fails, the behavior of the network will be changed slightly, the behavior of neurons will change, but the network itself continues to function successfully.

It is necessary to develop a neural network to control the process of purification of the pyrolysis fraction from acetylene compounds. To minimize the loss of butadiene, it is proposed to use a more efficient control system that will take into account the optimal ratio of butadiene to acetylene and the flow rate of the fraction, which significantly affect the yield of butadiene. As a result of the training, a neural network was obtained which, without reconfiguring the connection weights, generates output signals when any set of input signals from the training set is fed to the network input.

1. Introduction
The process of purification of the pyrolysis fraction from acetylene compounds is one of the stages in the production of butadiene. The efficiency of purification of the pyrolysis fraction from acetylene compounds and the selectivity of the reaction are affected by the volumetric feed rate of the fraction, the mass concentration of butadiene before hydrogenation, the mass content of alpha-acetylene compounds, the content of pure acetylene, and hydrogen consumption.

For the effective management of the described multiply connected process, it is necessary to develop a multidimensional control system that takes into account the mutual influence of all parameters of the technological process. To solve this problem, the authors set the task to develop a multidimensional control system that can take into account the mutual influence of parameters using neural networks developed in the Matlab software package.

Artificial neural networks are used to control technological processes as a regulator of multidimensional and multiply connected dynamic objects, they are also used to develop and study methods for solving various problems in economics, medicine, robotics, etc. Artificial neural networks are selected for the development of a process control system due to the fact that they are fault tolerant.

In a neural network, information is distributed throughout the network, which means if a neuron fails, the behavior of the network will be changed slightly, the behavior of neurons will change, but the network itself continues to function successfully [1-3].
2. Process description

1,3-butadiene is obtained at the separation unit of the butylene-butadiene fraction (BBF) using a copper-ammonia solution. Copper with alpha-acetylene hydrocarbons forms explosive copper acetylenides, and the total mass fraction of alpha-acetylene hydrocarbons in BBF should not exceed 0.02 wt.%

For this purpose, BBF, previously purified by distillation from heavy hydrocarbons and dried in an azeotropic drying column, is purified from acetylene hydrocarbon impurities by selective catalytic hydrogenation.

The technological scheme of the hydrogenation unit is shown in figure 1.

The butylene-butadiene fraction entering the acetylene hydrocarbon hydrogenation unit is cooled in the refrigerator (T₁ heat exchanger) and sent to the posed catalytic hydrogenation reactors (P₁, P₂, P₃).

In each reactor loaded with 1.5-1.6 tons of PD catalyst. The composition of the feed to the hydrogenation unit is presented in table 1.

| Component              | Composition (%) |
|------------------------|-----------------|
| Isobutane              | 3.8—4.7 wt.%    |
| n-Butane               | 6.8—8.0 wt.%    |
| (α+i)-Butylene         | 37.8—30.9 wt.%  |
| ∑β-Butylene            | 3.7—4.3 wt.%    |
| 1,3-Butadiene          | 38.5—46.2 wt.%  |
| Methylallen            | Traces (<0.01)  |
| Ethylacetylene         | 0.06—0.11 wt.%  |
| Vinylacetylene         | 0.9—1.8 wt.%    |

To minimize the loss of butadiene, it is proposed to use a more efficient control system that will take into account the optimal ratio of butadiene to acetylene and the flow rate of the fraction, which significantly affect the yield of butadiene.

After the third reactor, where the hydrogenation reaction is carried out, the BBP is sent to a separator, from where the gas fraction is returned to the process, and the liquid, purified from acetylene hydrocarbons, is collected in a tank.

The main technological indicators of the selective hydrogenation process are presented in table 2.
Table 2. The main technological indicators of the process of selective hydrogenation.

| Parameter                                                                 | Value         |
|----------------------------------------------------------------------------|---------------|
| BBF consumption for hydrogenation, t/h                                      | 8—14          |
| Hydrogen consumption, m³/h                                                 | 120—540       |
| Temperature, °C                                                            | 10—14         |
| The sum of acetylene, wt.%, in the original BBF                            | <1.9          |
| The sum of acetylene, wt.%, in purified BBF                               | <0.02         |
| The ratio of H₂/acetylene, mol/mol                                         | 8—12          |
| The loaded catalyst in the reactor, mass t                                 | 1.5—1.6       |
| The loaded catalyst in the reactor, volume, m³                             | 1.2—1.3       |
| BBF volumetric feed rate, h⁻¹                                              | 2.38—4.16     |

3. Neural network development
It is necessary to develop a neural network to control the process of purification of the pyrolysis fraction from acetylene compounds.

NN development was carried out in the Matlab environment. When solving the problem, the MatlabNeuralNetworkToolbox package was used.

The process of constructing a neural network model can be divided into 4 main stages:

- Data processing and preparation: the formation of a training sample, determining the range of parameter changes, data rationing.
- Selection of the type and architecture of the neural network: selection of the type of neural network suitable for solving the problem.
- Construction and training of a neural network.
- Model verification: model verification on a test sample.

4. Data processing and preparation
You must create a table with a training dataset. It will consist of 20 values.

In a multidimensional system of this process, it is necessary to take into account the following input and output parameters for controlling the technological process of purification of the pyrolysis fraction:

Input parameters:

- loading of raw materials in D-8 - G_in, t/h;
- the concentration of butadiene before hydrogenation C_C₄H₆_in, % wt.;
- the mass content of alpha-acetylene C_ac_in, % wt.;
- the content of pure acetylene in the fraction C_C₂H₂_in, % wt.;
- the hydrogen flow rate supplied to the lower part of the hydrogenation reactor, G_H₂_in, m³/h.

Output parameters:

- the concentration of butadiene after hydrogenation C_C₄H₆_out, % wt.;
- the mass content of alpha-acetylene compounds after hydrogenation C_ac_out, % wt.
Table 3. The training data set.

| N | G_in | C_{C_6H_6_in} | C_{C_4H_6_out} | C_{ac_in} | C_{C_2H_2_in} | C_{ac_out} | G_{H_2_in} |
|---|-----|---------------|----------------|-----------|---------------|------------|------------|
| 1 | 9   | 41.23         | 38.41          | 1.09      | 0.04          | 0.029      | 140        |
| 2 | 9   | 41.23         | 38.41          | 1.09      | 0.04          | 0.029      | 145        |
| 3 | 9   | 38.73         | 36.79          | 1.18      | 0.04          | 0.025      | 145        |
| 4 | 9   | 38.73         | 36.79          | 0.97      | 0.04          | 0.012      | 150        |
| 5 | 9   | 37.78         | 34.5           | 0.81      | 0.04          | 0.014      | 150        |
| 15 | 8   | 41.69         | 37.95          | 1.18      | 0.03          | 0.02       | 125        |
| 16 | 8   | 40.16         | 37.84          | 0.98      | 0.03          | 0.02       | 125        |
| 17 | 8   | 40.16         | 37.84          | 0.98      | 0.03          | 0.04       | 120        |
| 18 | 8   | 40.16         | 37.84          | 0.98      | 0.03          | 0.022      | 130        |
| 19 | 8   | 39.2          | 36.83          | 1.02      | 0.03          | 0.019      | 130        |
| 20 | 8   | 36.9          | 34.22          | 0.88      | 0.03          | 0.005      | 130        |

5. The choice of the type and architecture of neural networks

The structure of neural networks has a great influence on the characteristics of the output parameter, this is determined by the location and number of interneuron connections in the hidden layer, which the user needs to configure when training artificial neural networks. The choice of the number of neurons in the hidden layer is decided based on the experimental results of training and testing artificial neural networks. The required number of neurons in the hidden layer was established, and it is 3. The neural network consists of two layers: 1 - the hidden layer, 2 - the output layer (figure 2).

Network training will be carried out using a modified error back propagation algorithm: trainFcn = 'trainbr'. This algorithm determines two “streams” in the network. The input signals move in the forward direction, resulting in an output signal from which the error value is determined. The magnitude of the error moves in the opposite direction, as a result, the weights of the network links are adjusted [4-6].

The maximum number of epochs of training is defined, which determines the number of epochs (time interval) after which training will be stopped: net.trainParam.epochs = 10000. The criterion for graduation is set - the deviation value of each parameter at which the learning will be considered completed: net.trainParam.goal = 0.0000001.

Next, the data is divided into a training set (Training), a test set (Validation), which are used to evaluate the generalizing properties of the network and stop training when the generalization stops.
improving and on the test set (Testing), which does not affect the training, but employees to check for data that was not used in network training:

- A complete set of data for the development of a neural network consists of 29 values.
- Sets the number of data for training – 20. net.divideParam.trainRatio = 20/29.
- Sets the number of data to check – 6. net.divideParam.valRatio = 6/29.
- Sets the number of data for the test – 3. net.divideParam.testRatio = 3/29.

6. Building and training a neural network in Matlab

Next, the implementation and training of the neural network in Matlab is carried out. To do this, open the data editor, click the “Import data” button and download the data for training the neural network. The input data of the neural network is called input, and the output is output. After pressing the Enter key, training of the neural network will begin.

At the end of the network training process, a window for completing the training process appears, which displays: the algorithm parameters and the network training method - Bayes method, the number of iterations performed - 258, the training time spent - 7 seconds, the number of errors that go beyond - 0, the mean square error - 8.7141·10⁻⁵ (figure 3).

![Figure 3. The root-mean-square error.](image)

![Figure 4. Network learning graphs.](image)
The learning function uses early stopping as a means of combating retraining. MeanSquaredError (MSE) is a network performance function, it shows the performance of parameters in accordance with the mean square error [7-8].

Figure 4 shows the graphs of the training status - TrainingState. The “valfail” graph shows the change in error on the control set. As can be seen from the graph, no changes are observed. The “gradient” graph decreases, it shows the change in the gradient of the functional of the learning error by the network weights. The graph “mu” reflects the change in the learning parameter \( \mu \), as can be seen from the figure, no changes in the parameter are observed.

As a result of the training, a neural network was obtained which, without reconfiguring the connection weights, generates output signals when any set of input signals from the training set is fed to the network input.

7. Neural network test
For testing a neural network, 5 values are supplied to the input using the command `sim(net,[x1;x2;x3;x4;x5])`.

| G_in (x1) | C_C4H6_in (x2) | C_C2H6_out (x3) | C_ac_in (x4) | C_C2H2_in (x4) | C_ac_out (x5) | G_H2_in (x5) |
|-----------|----------------|-----------------|--------------|----------------|---------------|--------------|
| 9         | 40.56          | 37.62           | 1.1          | 0.07           | 0.02          | 180          |
| 9         | 40.56          | 37.62           | 1.1          | 0.07           | 0.024         | 175          |
| 9         | 40             | 36.87           | 1.1          | 0.054          | 0.02          | 180          |

Performing this operation for the first line of input parameters of table 4 leads to the following results: the concentration of butadiene after hydrogenation \( C_{C_4H_6} = 37.6199 \) wt.%, the mass content of alpha-acetylene after hydrogenation \( C_{AC} = 0.0155 \) wt.%. Performing this operation for lines 2 and 3 of the input parameters of table 4 leads to the following results of the concentration of butadiene after hydrogenation \( C_{C_4H_6} = 37.6198 \) and \( 36.8715 \) wt.% accordingly, the mass content of alpha-acetylene after hydrogenation \( C_{AC} = 0.0155 \) and \( 0.0139 \) wt.% respectively.

8. Conclusion
As a result of testing, output values are obtained that have a minimum absolute error of 0.01 and a relative 0.0267%. It follows that the parameters of the neural network are selected correctly.

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