Prediction of the properties anhydrite construction mixtures based on neural network approach

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Abstract. The article considered the question of applying the backstop modeling mechanism from the components of anhydrite mixtures in the process of managing the technological processes of receiving construction products which based on fluoranhydrite.

1. Introduction

In the hydrogen fluoride production process the by-product is formed as a result of decomposition of fluorspar. It is known as acid fluoride or technogenic anhydrite. Acid fluoride isn't often used in chemical production. It is usually landfilled as waste or dumped in waters whereas this product can replace gypsum in traditional production.

Mainly technogenic anhydrite is used in construction to produce anhydrite binder, cement mixes, plasticizers and more complex building products such as slagblocks, gypsum sheets and profile building products [1-7].

It is known that unlike gypsum hardening of acid fluoride, cement takes longer time, and products obtained from waste have higher strength than the very high-grade gypsum. Another advantage of technogenic anhydrite is its low cost and excellent hygienic properties.

The main component of anhydrite construction mixtures is Synthanite (S-10), the composite which contains 98,5% wt. acid fluoride (AF-10) and 1,5 % wt. potassium sulfate. Potassium sulfate is used for accelerating gelation and strengthening. Sulfanol is a combination of sodium salts. It is also introduced at the mixture to improve water fastness and frost resistance of anhydrite products. Depending on the purpose of anhydrite production it is required to prepare anhydrite construction mixtures which are different in mineral composition. It provides the manufacturing of products having desired strength, water fastness and frost resistance. It is difficult and time consuming task to select anhydrite concrete mixture components in composition depending on its purpose to produce construction products with desired properties.

Acceleration and optimization of the decision-making process on the selection of anhydrite concrete mixture components in composition and refining properties of the resulting construction products is possible through modeling by artificial neural network (ANN). As in our case, some processes of mixing components and their interaction are not linear and the research base is not...
enough, the data are incomplete and noisy so the obtained artificial neural networks model are the most suitable for the task [13-15].

The uniqueness of this approach lies in its ability to train and memorize during the data processing. In the training examples forming it is necessary to take into account all the parameters that can affect the network output. It is required to prepare a sufficient amount of data which describe the experimental field and are not in conflict. One of the important properties of the neural network is the ability to generalize. It provides new properties using the pre-trained model.

The object under study in modeling neural networks is anhydrite concrete composition. Its main components are technogenic anhydrite (TA-10), Synthanite (S-10), sulfanol and inert (silicic acid anhydride). During properties prediction modeling of anhydrite construction mixtures it is required to complete the following tasks:
- to explore the primary components and their influence on the properties of anhydrite construction mixtures;
- to choose the methods of creating and training neural networks;
- to select the composition of construction mixtures with provision for the mixing time and depending on the required performance of construction products.
- to provide and study the algorithms and properties prediction procedure of concrete construction mixture;

2. Data for the modeling
A number of experiments were carried out and the changing data of technogenic anhydrite grade strength (TA-10) and Synthanite (S-10), depending on the percentage of water-soluble calcium sulfate were obtained. Results of the experiments are shown in Table 1.

Table 1. Effect of water-soluble calcium sulfate content on grade strength of anhydrite materials.

| №  | The content of water-soluble calcium sulfate % Wt. | Grade strength of TA-10 MPa | Grade strength of Synthanite S-10 MPa |
|----|---------------------------------|---------------------|----------------------------------|
| 1  | 12                              | 1,4                 | 4,5                              |
| 2  | 16                              | 2,0                 | 5,5                              |
| 3  | 18                              | 2,5                 | 7,5                              |
| 4  | 20                              | 3,0                 | 9,0                              |
| 5  | 22                              | 3,5                 | 10,0                             |
| 6  | 24                              | 4,0                 | 13,0                             |
| 7  | 28                              | 4,4                 | 16,0                             |

The obtained construction samples characteristics were examined for technogenic Synthanite of grade strength 7.5 MPa and 4.5 MPa depending on the content percentage of sulfanol in the mixture: σ strength (MPa); water resistance coefficient K (%); frost resistance coefficient K (cycles (pc)) (Table. 2).
Table 2. Effect of sulfanol on water and frost resistance of anhydrite materials.

| №  | S – 10, MPa | Sulfanol % Wt | σ, MPa | Water resistance coefficient K | Frost resistance coefficient K Cycles (pc) |
|----|-------------|---------------|--------|-------------------------------|----------------------------------------|
| 1  | 7,5         | 0             | 7,5    | 55                            | 15                                     |
| 2  | 7,5         | 0,005         | 7,4    | 60                            | 18                                     |
| 3  | 7,5         | 0,01          | 6,9    | 93                            | 25                                     |
| 4  | 7,5         | 0,02          | 6,7    | 83                            | 19                                     |
| 5  | 7,5         | 0,05          | 6,4    | 80                            | 17                                     |
| 6  | 7,5         | 0,1           | 5,6    | 75                            | 16                                     |
| 7  | 7,5         | 0,2           | 3,8    | 65                            | 14                                     |
| 1  | 4,5         | 0             | 4,5    | 50                            | 13                                     |
| 2  | 4,5         | 0,005         | 4,44   | 56                            | 15                                     |
| 3  | 4,5         | 0,01          | 4,14   | 75                            | 21                                     |
| 4  | 4,5         | 0,02          | 4,0    | 73                            | 17                                     |
| 5  | 4,5         | 0,05          | 3,8    | 72                            | 16                                     |
| 6  | 4,5         | 0,1           | 3,4    | 68                            | 14                                     |
| 7  | 4,5         | 0,2           | 2,3    | 55                            | 12                                     |

Also, constraints of anhydrite samples strength were obtained depending on the mixing time of the anhydrite mixtures (Table 3) and the amount inert (silicic acid anhydride) content in the mixture (Table 4).

Table 3. Effect of stirring time on strength anhydrite solutions and concretes.

| № n/n | The mixing time of the anhydrite solution (turbulent mixer), N = 680 rpm), min. | Strength of anhydrite samples after aging for 28 days, MPa | Mixing time for anhydrite concrete (laminar mixer), N = 120 rpm), min. | Strength of anhydrite samples after aging for 28 days, MPa |
|--------|--------------------------------------------------------------------------------|----------------------------------------------------------|--------------------------------------------------------------------------------|----------------------------------------------------------|
| 1      | 1,0                                                                             | 3,8                                                      | 3,0                                                                          | 4,0                                                      |
| 2      | 1,25                                                                            | 4,5                                                      | 3,5                                                                          | 4,6                                                      |
| 3      | 1,5                                                                             | 5,0                                                      | 4,0                                                                          | 4,9                                                      |
| 4      | 1,75                                                                            | 5,1                                                      | 4,5                                                                          | 5,1                                                      |
| 5      | 2,0                                                                             | 5,1                                                      | 5,0                                                                          | 5,1                                                      |

The dependences of the strength of anhydrite samples and the amount of inert in the mixture were also obtained (Table 4).
Table 4. Effect of silicic acid anhydride content on anhydrite samples strength.

| №  | Inert (silicic acid anhydride) | The inert content in anhydrite mixture, % wt. | σ, MPa 1 day | σ, MPa 3 days | σ, MPa 5 days | σ, MPa 7 days |
|----|-------------------------------|---------------------------------------------|--------------|--------------|--------------|--------------|
| 1  | SiO₂                          | 0                                           | 3.0          | 7.2          | 8.9          | 9.0          |
| 2  |                               | 1.0                                         | 3.4          | 7.6          | 9.2          | 9.5          |
| 3  |                               | 3.0                                         | 2.5          | 5.6          | 6.8          | 7.0          |
| 4  |                               | 5.0                                         | 2.3          | 5.1          | 6.2          | 6.4          |
| 5  |                               | 7.0                                         | 2.2          | 4.9          | 6.0          | 6.1          |

As you can see from the tables, the data are very different and also have different measuring units. For implementing the neural network modeling it is necessary to bring data to a common standard to be able to process them.

To do this, the procedure of data normalization is applied with the help of simple exponential 1:

$$X = \frac{x}{\sum_{n=1}^{n} X_{i}}$$

where x – the original value; X – the input value.

The normalized values are listed in the Table 5.

Table 5. Normalized values.

| S–10, MPa | Sulfanol, wt. | σ, MPa | Water resistance coefficient |
|-----------|---------------|--------|-----------------------------|
| 1.25      | 0.00          | 1.48   | 0.80                        |
| 1.25      | 0.09          | 1.46   | 0.88                        |
| 1.25      | 0.18          | 1.36   | 1.36                        |
| 1.25      | 0.36          | 1.32   | 1.36                        |
| 1.25      | 0.91          | 1.26   | 1.26                        |
| 1.25      | 1.82          | 1.11   | 1.11                        |
| 1.25      | 3.64          | 0.75   | 0.75                        |
| 1.25      | 0.75          | 0.75   | 0.75                        |
| 1.25      | 0.75          | 0.75   | 0.75                        |
| 1.25      | 0.75          | 0.75   | 0.75                        |
| 1.25      | 0.75          | 0.75   | 0.75                        |

3. The choice of neural network architecture

To simulate the properties of the resulting building products, a two-layer artificial neural network with the Levenberg-Marquardt algorithm with back error propagation training is used, which is the standard way of learning the neural network. Its advantage is in minimizing the root-mean-square deviations of the current output and the desired output of the network. The inputs of the neural network are the values of the components of anhydrite concrete, and the yields are the indices of the obtained characteristics of anhydrite products.

One of the layers of the network is hidden. To determine the number of neurons in the hidden layers of neural networks, we use formula 2 to calculate the number of synaptic weights N_w in a multilayer network

$$\frac{N_y Q}{1 + \log_2 (Q)} \leq N_w \leq N_y \left(\frac{Q}{N_x} + 1\right) \left(N_x + N_y + 1\right) + N_y$$

(2)
where $N_y$ is the dimension of the output signal; $Q$ is the number of elements in the set of training examples; $N_w$ is the required number of synaptic connections; $N_x$ is the dimension of the input signal.

In our case,

$$12.5 \leq N_w \leq 277$$

The number of neurons $N$ of the hidden layer of the network is defined by the formula 3:

$$N = \frac{N_w}{N_x + N_y}. \quad (3)$$

Knowing the minimum and maximum values of the synaptic weights of the network, according to formula 3, the number of neurons of the hidden layer is within [0; 8].

4. Neural network training

For the formation and training of a neural network in the MATLAB R2015a environment, experimental normalized values were used. The data are represented in the form of a matrix of dimension 8 * n, where n is the number of input parameters. At the output, a matrix will also be obtained, but with a dimension of 1 * n, the exponent in this matrix will reflect the obtained values when modeling the properties of substances.

For the forecasting, a neural network model was used with back propagation of the error and the number of neurons in the hidden layer was 8, and the number of learning epochs was 100 (Figure 1).

![Figure 1. The structure of the artificial neural network.](image)

The adequacy of the obtained neuronet model of the substance was verified from known experimental strength data. The verification showed that the modeling error does not exceed 1%. The result of the network is shown in Table 6.

| №  | Experimental data | Modeling results | Prediction error, % |
|----|-------------------|------------------|---------------------|
| 1  | 0                 | 0.0001731        | 0                   |
| 2  | 0.08              | 0.07988          | 0.15                |
| 3  | 0.215             | 0.21395          | 0.49                |
| 4  | 0.055             | 0.055126         | 0.23                |
| 5  | 0.40583           | 0.3735           | 7.97                |
| 6  | 0.41667           | 0.41584          | 0.2                 |
| 7  | 0.7133            | 0.71519          | 0.26                |
| 8  | 0.94583           | 0.94309          | 0.29                |
| 9  | 0.165             | 0.16501          | 0.006               |
| 10 | 0.30167           | 0.30145          | 0.94                |
| 11 | 0.418             | 0.41924          | 0.3                 |
| 12 | 0.695             | 0.69             | 0.72                |
Also, the Performance graph (Figure 2) allows you to assess the accuracy of training. This graph shows the dependence of the standard deviation on the iteration of training. The schedule is constructed for three sets of data: training, validation and test - training stops when the error for the validation set of data ceases to decrease.

![Figure 2. Chart Performance.](image)

5. Conclusion
The presented modeling of the forecasting system for the properties of anhydrite mortar mixtures based on INS will allow determining the required strength values of building products depending on the ratio of initial components of the anhydrite mixture. Successful training in INS suggests that by changing the ratio of the original components, it can also predict the water and frost resistance characteristics of the product and determine how the mixing time affects its strength characteristics.

Thus, neural network modeling of the forecasting system for the properties of anhydrite mortar mixes provides ample opportunities for construction industries when making production decisions, saving time and financial resources for additional research and testing, and minimizing the human factor.

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