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Using machine learning and artificial intelligence methods to study the current-voltage characteristics of membrane systems

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ABSTRACT

The aim of the investigation is the mathematical modeling of processes that take place in electro membrane systems (EMS). The article is devoted to the use of machine learning and artificial intelligence methods for a theoretical study of the current-voltage characteristic (CVC) of membrane systems, taking into account space charge, electroconvection, forced convection, non-catalytic reaction of dissociation/recombination of water molecules, as well as taking into account the presence and absence of spacers. We have created new artificial intelligence systems, namely neural networks trained by modern machine learning methods, for the numerical study of CVC. The creation of neural networks allowed using prediction to obtain the CVC for a wider range of input parameter values than with the help of currently available numerical algorithms.

1. INTRODUCTION

Electro membrane systems (EMS) is widely used for purification, separation, enrichment, desalination and concentration of liquid and gas mixtures. EMS are used in chemical, petrochemical, food technology, biotechnology and pharmacy. The current-voltage characteristic (CVC) is an important integral characteristic of the process of transfer of salt ions in EMS in the desalting channel of an electrodialysis machine. The article examines the CVC for the calculation of which, a 2D mathematical model of non-stationary transfer of 1:1 electrolyte in potentiodynamic mode is formulated and numerically solved. Based on the Gauss theorem, using a mathematical model, a formula for calculating CVC was derived, resistant to random errors, which made it possible, given certain parameter values, for example, the initial speed of forced convection, initial concentration, to stably calculate CVC [Kov-20]. Each calculation of the CVC for given values of the specified parameters, using mathematical models, has significant

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computational difficulties and takes large time resources. The CVCs are calculated in a limited range of parameters, for a small set of data, which entails the loss of some important characteristics of the mass transfer process.

It should be noted that without the use of the latest mathematical methods and models, such as machine learning methods and artificial intelligence systems, it becomes more and more problematic to move forward in the development of the theory and application of membrane systems, since models are becoming more and more complex and become so complex that the compilation of algorithms and numerical solutions, engineering calculations of membrane systems are made disproportionately time-consuming, expensive, multiscale, as shown by V. Pham, Z. Li, J. White, J. Han and other foreign researchers [Pham-12, Kim-16].

Artificial intelligence systems have shown their effectiveness in various fields of science and technology, including in electrochemistry for such tasks as modeling membrane separation [Nie-95], variable operation control of a simple seawater reverse osmosis plant [Cab-17]. Modeling and optimization of desalination for an air gap membrane using an artificial neural network was presented in [Kha-12]. Forecasting models for analyzing the efficiency of an industrial-scale membrane distillation unit for desalting brines are described in [Gil-18]. However, the study and prediction of CVC of membrane systems by machine learning and artificial intelligence methods has not yet been conducted.

We were faced with the task of developing a neural network model for CVC modelling, which would significantly save computation time. The neural network model for modelling CVC was created in the Google Colab development environment using the Python programming language.

2. ANALYSIS OF CVC BEHAVIOR DEPENDING ON VOLTAGE

Let's look at the CVC chart shown in Fig. 1. The ordinate axis indicates the current output normalized to Leveque current $\left(I_{av}/I_{\lim}\right)$ [Kov-Nik-24]. The abscissa axis indicates the voltage, in volts [Kov-20, Kov-21, Kov-Che-24]. A gradually increasing voltage is applied to the system and when we obtain a normalized system current equal to unity, this means that the limit state has been reached $\left(I_{av}/I_{\lim}=1\right)$.

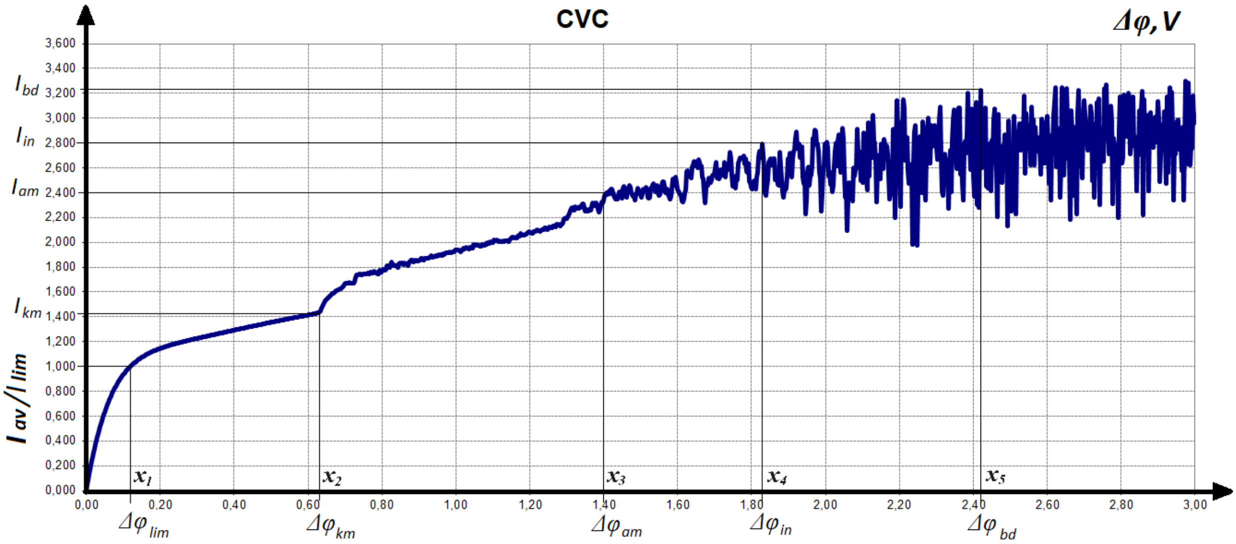

Fig. 1 Current-voltage characteristic of an electromembrane channel formed by anion-exchange and cation-exchange membranes, calculated using a two-dimensional model described in detail in [Kov-21]

Let's call the point corresponding to the limiting current $x_1 = \Delta\varphi_{\lim}$. This is the first point that will need to be obtained when predicting CVC using the neural network we developed. After the point x_1 corresponding to the limit state, the system reaches a limiting plateau, which continues until the point $x_2 = \Delta\varphi_{km}$. This point x_2 corresponds to the first rise in the current-voltage characteristic $\left(I_{km}\right)$, which is associated with the beginning of electroconvection at the cation-exchange membrane [Kov-22]. The next point $x_3 = \Delta\varphi_{am}$ corresponds to another rise in CVC associated with the onset of electroconvection at the anion-exchange membrane.

Next comes the point $x_4 = \Delta\varphi_{in}$ corresponding to the beginning of the interaction of electroconvective vortices at the cation-exchange and anion-exchange membranes and the beginning of chaos. On the one hand, there is intense mixing, and it would seem that this should improve the performance and, according to all the forecasts of CVC scientists, linear growth should be observed, but in fact, stagnation and a change in trend are observed. This is where the destructive processes of dissociation/recombination of water molecules begin [Kov-Nik-24, Kov-Che-24]. Desalting slows down. The tension begins to act on the water molecules. Thus, the voltage is wasted, that is, to break a strong water molecule into OH^- and H^+ ions (this process is called dissociation). And just as positive and negative ions are drawn to the electrodes and want to pass through the membranes, they are just as strongly drawn to each other, and the reverse process begins - recombination. As a result, the system spends energy on breaking the water molecule, and not on desalting the solution.

The dissociation/recombination process is quite destructive. It damages the membranes themselves, expends a huge amount of energy, and so on. However, another destructive phenomenon has recently been discovered and theoretically justified - space charge breakdown [Kov-20, Kov-21]. When the voltage in the system increases, after some time, phenomena similar to the shooting of a charge from one membrane to another begin to occur. Experimental studies have shown that as soon as the shooting began, i.e. with increasing voltage supplied to the system, the current output of the purified (desalted) solution did not increase.

After point x_5, strong CVC fluctuations are clearly visible in Fig. 1 - this is precisely the period when breakdowns of space charges begin. Breakdown is a phenomenon that is similar to lightning, only it occurs in microchannels between membranes. After passing through the breakdown, the vortices die out, then grow again, and so on.

3. SIMULATION OF CVC BEHAVIOR BY THE CREATED NEURAL NETWORK

At first step we are calculated CVC for creation of training, control and test samples for neural networks. The calculation of CVC based on the use of the Gauss theorem for a two-dimensional channel (2D) [Kov-20] was made with help of Comsol Multiphisics. The input parameters of the system were supplied to the input: the initial concentration of the solution, the rate of supply of the solution into the channel, the length and width of the desalting channel, the potential jump (sweep speed), the diffusion coefficients of cations and anions, transfer numbers, calculation time and the size of the storage step for constructing the CVC. In addition, information about spacers - their quantities and forms (Spacers in the intermembrane space are obstacles, flowing around which the fluid flow changes its direction). All spacers were considered non-conducting. Information about the accounting for dissociation/recombination reactions of water molecules was taken into account. 42 SMS values were calculated for each set of input parameters. They served to create of training sets, with help of which 42 CVC points were predicted. They were then again supplied to the network input, etc.

The method of teaching with the Adam teacher was used. The output included tables of ready-made CVC values, as well as the following data: points $(x_1,1),(x_2,I_{km}),(x_3,I_{am}),(x_4,I_{in}),(x_5,I_{bd})$. Selection of architecture, topology, structure and type of neural networks showed that the best way to model CVC is to use a combination of convolutional and recurrent layers, since thanks to them, local structures of the graph behavior are tracked, and their sequence is also taken into account. The use of convolutional layers in neural network architecture allows one to track local structure in the input data. In the case of current-voltage characteristics, they allow the identification of special areas, such as peaks or dips that indicate anomalies or unusual behavior.

The use of recurrent LSTM (Long Short-Term Memory is a type of recurrent neural network) layers in the architecture makes it possible to take into account the sequence of changes in the graphs of current-voltage characteristics. Also, LSTM layers are capable of storing information for a long time. This allows the model to take into account dependencies over a long period of time. Thus, it was this combination of layers that led to more accurate results in predicting current-voltage characteristics. The results of CVC modeling using the created neural network are presented in Fig. 2.

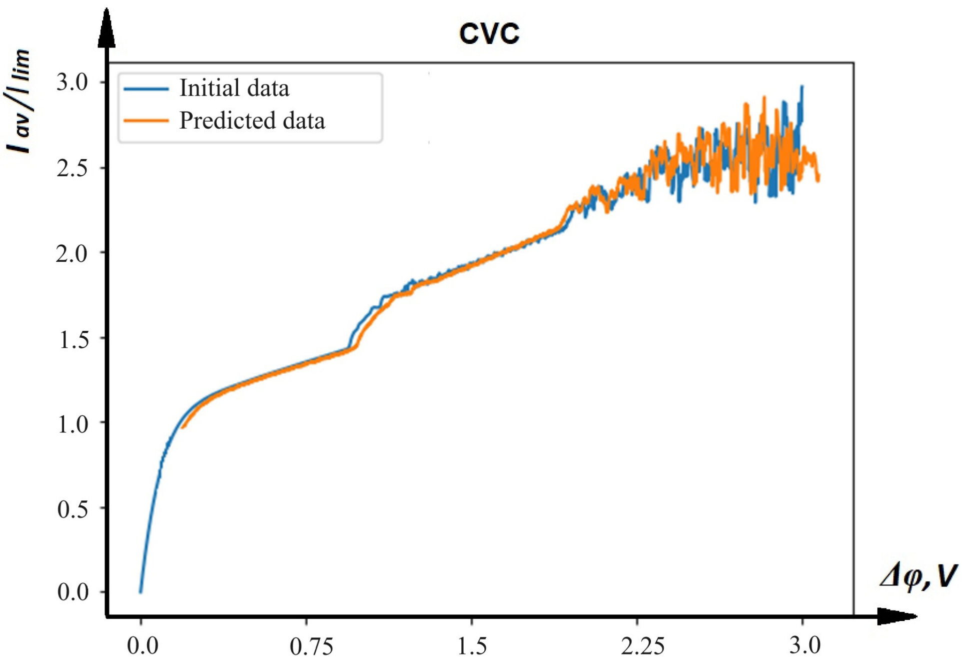

Fig. 2 Modeling CVC behavior using the created neural network

From Fig. 2 you can see that the model predicts the behavior of the current-voltage characteristics graph quite well. We can also say that the model does a good job of predicting points that signal transitions to different states of the system.

To evaluate the performance of the neural network, cross-validation was used to objectively evaluate the model's ability to generalize to new and unknown data. Its use is particularly useful since the amount of data was limited. For the one shown in Fig. 2 example of calculating CVC using a neural network, the root mean square error is 0.00012, the mean absolute error is 0.0098, MAPE (mean absolute percentage error) is 1.37. This suggests that the model predicts the behavior of the graph quite well on the selected test sample.

The neural network was shown to work well on different input values, which made it possible to work with different input data to predict current-voltage characteristics. Also, computational efficiency guarantees the ability to quickly predict CVC.

4. CONCLUSIONS

To summarize, we can conclude that to simplify the calculations of current-voltage characteristics, you can use the neural network created in this study for modeling CVC, which simulates the behavior of CVC and significantly saves time and computing resources. During the work, about 10 different neural network architectures were developed and tested and the best neural network was selected for modeling CVC behavior, including convolutional, recurrent and LSTM layers with the best predictive results on test samples.

A software product was created with which you can carry out numerical calculations in the Comsol Multiphysics environment of any two-dimensional models of the EMS desalting channel and create a database for various two-dimensional models of electromembrane systems, including taking into account diffusion, migration, convective transport, electroconvection, spacers of different shapes and sizes, dissociation/recombination and space charge breakdown. The obtained data is used to train the created neural network that models the behavior of CVC.

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