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# Mathematical Description and Algorithm for Solving the Model of the Ionite Regeneration Process in the Ion Exchange Method of Water Softening

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***Abstract:*** *Based on the modern representation of the water softening process by the ion exchange method, modeling was carried out, an algorithm was developed and the ionite regeneration process was calculated in a water softening plant with a fixed ionite layer. To solve the system of equations of the model, special, but simple enough for use in engineering calculations, techniques and methods have been developed and applied. The constructed model and its solution algorithm can be used to predict the process of ionite regeneration in an ion exchange apparatus. It can also be used to calculate the time of the ionite regeneration process.*

***Keywords:*** *modeling, sorption, regeneration, water softening, ion exchange method, ionite layer, clarified water, cationite, anionite, water hardness, sorbent height, kinetic and equilibrium dependencies, overshoot concentration.*

## Introduction

The conditions for stopping the regeneration of the sodium-cationite filter depend on many factors, such as the concentration of ions in water, the concentration of ions in the ion exchange layer, the length of the ion exchange layer, and others. Usually, the ion exchange layer can be regenerated when the length of the ion exchange layer reaches a certain limit, which depends on the concentration of ions in the water (the hardness of the filtrate reaches 50% of the hardness of the source water) [1]. Also, some ion-exchange materials have the ability to autoregenerate when properly installed and configured.

The technology of cationite regeneration consists of the following operations: loosening, regeneration and washing.

Cationite regeneration is carried out to restore the ion-exchange properties of the ion-exchange mixture. Cationite is an ion-exchange agent that absorbs and removes impurities from water, such as hardness, salts and other undesirable substances [2]. During the ion exchange process, the activity of the cationite decreases, which leads to the loss of its ion exchange properties. Therefore, in order to maintain the ion-exchange properties of cationite, it is necessary to periodically regenerate it. Ionite is regenerated with 8% sodium chloride solutions according to a direct-flow scheme:

$CaR_2 + 2NaCl = 2NaR + CaCl_2$

Cationite regeneration usually occurs when its activity falls below a certain level [3]. This usually happens after a sufficient amount of impurities has collected in the water, which the cationite can no longer remove. Some systems have set activity limits that, when triggered, require cationite regeneration. In other systems, regeneration is performed according to a specific schedule. For example, weekly or monthly.

The washing of the ionite material is carried out in order to clean it from the impurities present on it. Washing allows you to remove salts and other harmful impurities from the ionite material that accumulate on the surface of the ionite material during the ion exchange process. Washing helps to keep the ionite material in good condition and improve its performance. It also helps to prevent clogging of the ionite material and improve the quality of the treated water [4].

Let's make a mathematical description of the ionite regeneration process in the apparatus, the scheme of which is shown in Fig.1.

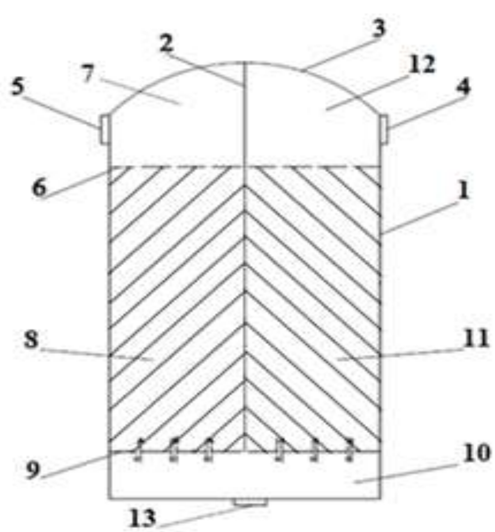


**Fig. 1**. The scheme of operation of the device at the stage of regeneration:

1 - housing; 2 - partition; 3-cover; 4,5,13- fittings; 6,9 - upper and lower switchgear; 7,8,10,11,12 – chambers;

A layer of cationite is located in chamber 11. Cationite is a spherical grain with a diameter of $2r_0$. A layer of anthracite is loaded into chamber 8. During ionite regeneration, exchange tanks are used to preserve the ionite's ionic properties and increase system performance. During the regeneration of this type of filters, the regenerating solution is fed through the fittings 4 and 5 through chambers 12 and 7 into chambers 8 and 11, passes through a layer of strong acid cationite (CU-2-8) and anthracite into chamber 9, and is removed through the fitting 13.

After regeneration, the process of flushing through the fittings 4 and 5 follows in the same order as during regeneration.

The model of the regeneration process was based on the following assumptions:

- he speed of the ion exchange process is limited by both external and internal diffusion;
- he one-dimensional flow of the liquid phase in the apparatus depends only on the x coordinate;
- the change in the concentration of the solution is a function of the average velocity of the liquid phase, only the longitudinal mixing and mass transfer process between the ionite and the solution, the equilibrium of which is described by the equation of the linear Henry isotherm;

The mathematical description of the process, based on the accepted assumptions, consists of the following equations:

material balance:

$$\varepsilon\frac{\partial C}{\partial \tau}+(1-\varepsilon)\frac{\partial \overline{C}_{med}}{\partial \tau}+v\varepsilon\frac{\partial C}{\partial x}=D_n\varepsilon\frac{\partial^2 C}{\partial x^2} \qquad (1)$$

an equation reflecting the kinetics of diffusion into a spherical particle:

$$\frac{\partial \overline{C}}{\partial \tau}=\overline{D}_{ef}\left(\frac{\partial^2 \overline{C}}{\partial r^2}+\frac{2}{r}\frac{\partial \overline{C}}{\partial r}\right) \qquad (2)$$

the equations of the nonlinear Henry isotherm:

$$\overline{C}_p=\Gamma C \qquad (3)$$

an equation reflecting the relationship of the local concentration of a substance in the solid phase with its average value

$$\overline{C}_{med}(\tau)=\frac{3}{r_0^3}\int_0^{r_0} r^2\overline{C}(\tau,r)dr \qquad (4)$$

The mathematical description includes initial and boundary conditions:

$$C(\tau,x)\big|_{\tau=0}=C_0 \qquad (5)$$

$$C(\tau,x)\big|_{x=0}=C_{in} \qquad (6)$$

$$\left.\frac{\partial C(\tau,x)}{\partial x}\right|_{x=H}=0 \qquad (7)$$

$$C(\tau,r)\big|_{\tau=0}=\overline{C}_0(r) \qquad (8)$$

$$\left.\frac{\partial \overline{C}(\tau,r)}{\partial r}\right|_{r=r_0} = \frac{\beta}{\overline{D}_{ef}}(C - C_b) \qquad (9)$$

$$\left.\frac{\partial \overline{C}(\tau,r)}{\partial r}\right|_{r=0} = 0; \qquad (10)$$

To solve this mathematical description, as in the case of the sorption process, the ionite layer along the entire height of the apparatus is divided into elementary layers each with a height of $h = H/\eta$. The time of the technological process will look like sequentially connected time intervals [5].

The second component of equation (1) determines the amount of runoff depending on the ion exchange adsorption process, and it can be replaced by an equation in the form of a finite difference:

$$\frac{\partial \overline{C}_{med,i}}{\partial_\tau} = -\frac{\overline{C}_{med,i}(\tau_j + \Delta_\tau) - \overline{C}_{med,i}(\tau_j)}{\Delta_\tau} = \overline{Kc}_{ij} \qquad (11)$$

For this equation, the index j determines the number of the time interval, and the difference between the time intervals is defined as $\Delta\tau = \tau_{j+1} - \tau_j$.

Solution of a system of equations (2) – (4) reflecting the kinetics of diffusion into a spherical particle, the nonlinear Henry isotherm and an equation reflecting the relationship of the local concentration of matter in the solid phase with its average value, taking into account the initial and boundary conditions (equations (8) – (10) by analogy with solving the problem of determining the thermal conductivity of spherical bodies the forms, provided that the concentration of the target component is unevenly distributed, make it possible to determine the amount of runoff in the following form:

$$\frac{a_0 - \overline{C}_{med,i}}{a_0} = \frac{a_0 - \overline{C}_{0i}}{a_0} \sum_{n=1}^{\infty} B_n \exp\left(-\mu_n^2 \frac{\overline{D}_{ef}\tau}{r_0^2}\right) \qquad (12)$$

In equation (11), the value of $B_n$ is calculated by the formula

$$B_n = \frac{6(\sin\mu_n - \mu_n \cos\mu_n)^2}{\mu_n^3(\mu_n - \sin\mu_n \cos\mu_n)} \qquad (13)$$

where $\mu_n$ are the roots of the equation

$$\mathrm{tg}\mu = -\frac{1}{\frac{\beta r_0}{\overline{D}_{ef} G} - 1}\mu$$

The joint solution of the material balance equation with the equations of the initial and boundary conditions (5) – (7), taking into account the equation determining the amount of runoff, allows the determination of a ratio that allows calculations to be made to determine the spatiotemporal change in the concentration of the regenerating solution when it passes a stationary ionite layer.

In order to facilitate the solution of equation (11), we introduce symbols in the form of dimensionless quantities:

$$N = \frac{C_{in} - C}{C_{in}}; \qquad N_0 = \frac{C_{in} - C_0}{C_{in}}; \qquad \overline{N}_{med} = \frac{a_0 - \overline{C}_{med}}{a_0}; \qquad \overline{N}_0 = \frac{a_0 - \overline{C}_0}{a_0};$$

$$G = \frac{a_0}{C_{in}} \frac{1-\varepsilon}{\varepsilon}; \qquad L = \frac{D_\pi - r_0^2}{\overline{D}_{ef} h^2}; \qquad M = \frac{v r_0^2}{\overline{D}_{ef} h}; \qquad Bi_m = \frac{\beta r_0}{\overline{D}_{ef} G};$$

 

$$Fo = \frac{\overline{D}_{ef}\tau}{r_0^2};\ z = \frac{x}{h}\ (0 \le x \le h);\ \xi = \frac{r}{r_0} \qquad (14)$$

After entering the above symbols, equation (11) can be rewritten in the following wording:

$$\frac{\partial \overline{N}_{med}}{\partial Fo} = \frac{\overline{N}_{med}(Fo) - \overline{N}_{med}(Fo + \Delta Fo)}{\Delta Fo} = -\overline{Kn_j} \qquad (15)$$

where

$$\overline{Kn_j} = \frac{r_0^2}{\overline{D}_{ef}}\overline{Kc_j}$$

As a result of the transformations carried out , the mathematical model of the ionite regeneration process can be written as follows:

$$\frac{\partial N}{\partial Fo} + G\overline{Kn_j} = L\frac{\partial^2 N}{\partial z^2} - M\frac{\partial N}{\partial z} \qquad (16)$$

$$\mathrm{N(Fo,z)}\Big|_{z=0} = N_{in} \qquad (17)$$

$$\mathrm{N(Fo,z)}\Big|_{Fo=0} = N_0 \qquad (18)$$

$$\frac{\partial N(Fo,z)}{\partial z}\Big|_{z=1} = 0 \qquad (19)$$

Based on the above relations, we will solve the nonlinear, inhomogeneous differential equation of the material balance (16) with initial and boundary conditions (17) - (19).

Based on the accepted designations (14), we transform equation (16) to the following form:

$$\varepsilon\left(\frac{\partial}{\partial\tau}N(\tau,r)\right) + \frac{(1-\varepsilon)\left(\frac{\partial}{\partial\tau}\right)}{r_0\varepsilon} = \frac{Dpr_0^2\left(\frac{\partial^2}{\partial z^2}N(\tau,z)\right)}{Defh^2} - \frac{vr_0^2\left(\frac{\partial^2}{\partial z}N(\tau,z)\right)}{Defh} \qquad (17)$$

Based on the Fourier method, we will look for a solution to equation (17) in the form of the following series:

$$N(\tau,r) := \sum_{n=1}^{\infty} N_n(\tau)\sin\left(\frac{\pi nz}{h}\right) \qquad (18)$$

Assuming that the function C(τ,x) can be decomposed into a Fourier series with respect to the variable x, we substitute the relation (19) into the equation (17).

$$N(\tau,r) := \sum_{n=1}^{\infty} N_n(\tau)\sin\left(\frac{\pi nz}{h}\right) \qquad (19)$$

As a result, we obtain the following relation:

$$\varepsilon\left(\sum_{n=1}^{\infty}\left(\frac{d}{d\tau}N_n(\tau)\right)\sin\left(\frac{\pi nz}{h}\right)\right) + \frac{(1-\varepsilon)\left(\frac{\partial}{\partial\tau}Nsp(\tau,x)\right)}{r_0\varepsilon} =$$

$$= \frac{Dpr_0^2\left(\frac{\partial^2}{\partial z^2}N(\tau,z)\right)}{Defh^2} - \frac{vr_0^2\left(\frac{\partial^2}{\partial z}N(\tau,z)\right)}{Defh} \qquad (20)$$

From this equation follows:

$$\frac{d}{d\tau}N_n(\tau) + \frac{DefN_n(\tau)\pi^2 n^2}{h^2} = 0 \qquad (21)$$

The solution of this equation in general form can be represented as the following relation:

$$N_n(\tau) = \_Cle^{-\frac{Def\pi^2 n^2\tau}{h^2}} \qquad (22)$$

 

Based on conditions (17) - (19), it is possible to deduce the initial conditions for $N_n(\tau)$ when τ=0. Then the solution satisfying the initial $N_n(\tau)=0$ conditions of equation (21) can be presented in the following form:

$$N_n(\tau) := \int_0^{\tau} \tau e^{-\frac{Def\pi^2 n^2(\tau-t)}{h^2}} dt \qquad (23)$$

Substituting solutions (23) in a series (18), one can obtain a solution of equation (16) under initial conditions (17) - (19) in the following form:

$$N_n(\tau) := \sum_{n=1}^{\infty} \left( \int_0^{\tau} \tau e^{-\frac{Def\pi^2 n^2(\tau-t)}{h^2}} dt \right) \sin\left(\frac{\pi n z}{h}\right) \qquad (24)$$

If the initial conditions are not equal to zero, it is necessary to add solutions satisfying the initial and boundary conditions of the homogeneous equation to solution (24).

The result can be represented as the following Grin 's function:

$$N_n(\tau) := \int_0^{t} \int_0^{h} G(z,\xi,t,\tau)\, d\xi d\tau \qquad (25)$$

As a result, we get the following function:

$$G(z,zi,\tau,t) := \sum_{n=1}^{\infty} \frac{2e^{\frac{Def\pi^2 n^2(\tau-t)}{h^2}} \sin\left(\frac{\pi n z i}{h}\right) \sin\left(\frac{\pi n z}{h}\right)}{h} \qquad (26)$$

Thus, the solution of equation (16) under initial and boundary conditions is as follows:

$$N_n(\tau) := \sum_{n=1}^{\infty} \frac{2h^2 \sin\left(\frac{\pi n z}{h}\right) e^{\frac{Def\pi^2 n^2(\tau-t)}{h^2}}}{Def\pi^3 n^3(\tau-t)} - \left( \sum_{n=1}^{\infty} \frac{2(-1)^{2+n} \sin\left(\frac{\pi n z}{h}\right) e^{\frac{Def\pi^2 n^2(\tau-t)}{h^2}}}{Def\pi^3 n^3} \right) - \left( \sum_{n=1}^{\infty} \frac{2h^2 \sin\left(\frac{\pi n z}{h}\right)}{Def\pi^3 n^3(\tau-t)} \right) + \sum_{n=1}^{\infty} \frac{2(-1)^{2+n} h^2 \sin\left(\frac{\pi n z}{h}\right)}{Def\pi^3 n^3} \qquad (27)$$

Now let's consider the solution of a nonlinear inhomogeneous differential equation of diffusion kinetics (2) with initial and boundary conditions given in the form of equations (8 - (10).

Using the accepted conditional values, we transform equation (2) to the form:

$$\frac{\partial}{\partial \tau} Nt(\tau,r) = Def \left( \frac{\partial^2}{\partial r^2} Nt(\tau,r) + \frac{2\left(\frac{\partial}{\partial r}\right) Nt(\tau,r)}{r} \right) \qquad (28)$$

As in the previous case, using the Fourier method, we transform the solution of this problem to the form of the Grin function:

$$G(z,zi,\tau,t) := \sum_{n=1}^{\infty} \frac{2e^{\frac{Def\pi^2 n^2(\tau-t)}{h^2}}}{h2} \sin\left(\frac{\pi n r i}{h}\right) \sin\left(\frac{\pi n r}{h}\right) \qquad (29)$$

In this case, the solution of the diffusion kinetics equation (2) with initial and boundary conditions can be written as follows:

$$N_n(\tau,r) := \sum_{n=1}^{\infty} \frac{2h^2 \sin\left(\frac{\pi n r}{h}\right) e^{\frac{Def\pi^2 n^2(\tau-t)}{h^2}}}{Def\pi^3 n^3} - \left( \sum_{n=1}^{\infty} \frac{2(-1)^{2+n} h^2 \sin\left(\frac{\pi n r}{h}\right) e^{\frac{Def\pi^2 n^2(\tau-t)}{h^2}}}{Def\pi^3 n^3} \right) - \left( \sum_{n=1}^{\infty} \frac{2h^2 \sin\left(\frac{\pi n r}{h}\right)}{Def\pi^3 n^3} \right) + \sum_{n=1}^{\infty} \frac{2(-1)^{2+n} h^2 \sin\left(\frac{\pi n r}{h}\right)}{Def\pi^3 n^3} \qquad (30)$$

 

To solve this model, we will use the finite element method - the PDE Toolbox of the Matlab application software package. We denote the packages in the PDE toolbox in the following form:

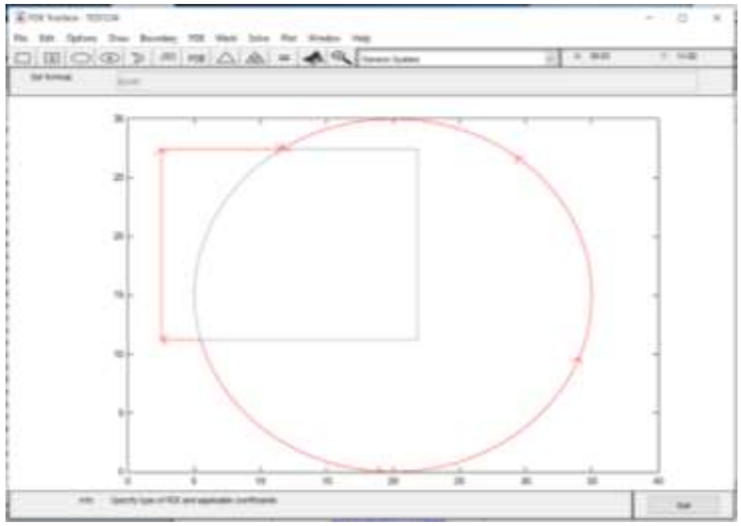

Fig.2. Representation of the model layout in the PDE toolbox.

To determine the interval of possible solutions of the mathematical model (30), we use the Neumann method and introduce the corresponding values:

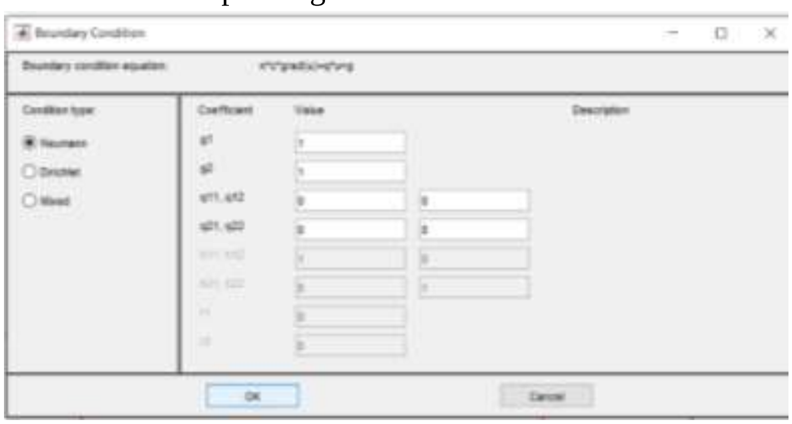


Fig. 3. The method of determining solutions in the PDE toolbox

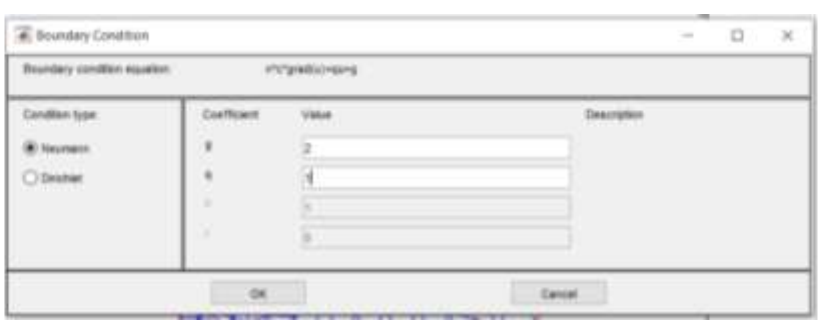


Fig.4. Choosing a solution method in the PDE toolbox

 

To determine the coordinates of the location of possible solutions in the PDE toolbox, it is necessary to enter the appropriate model parameters and determine the following dependencies (Fig.4, Fig.5):

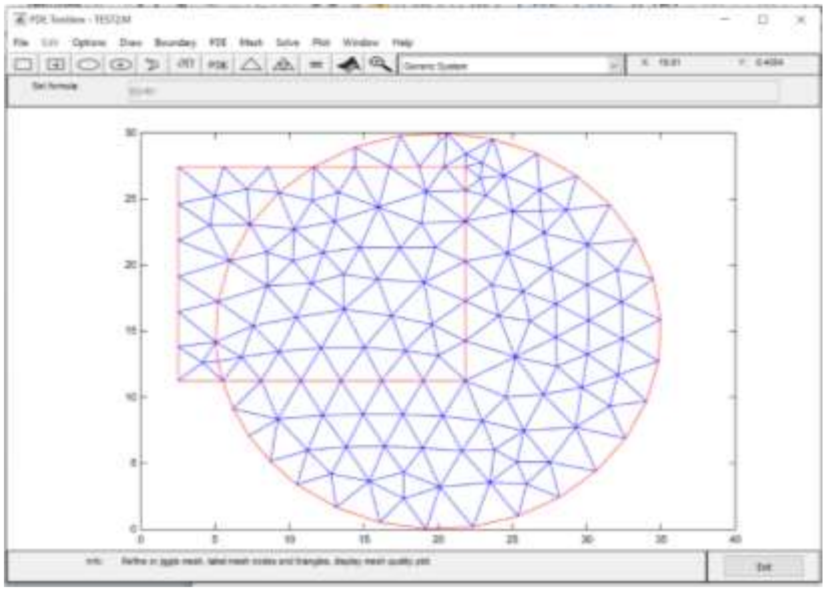

Fig.5. Coordinates of the location of possible solutions in the PDE toolbox

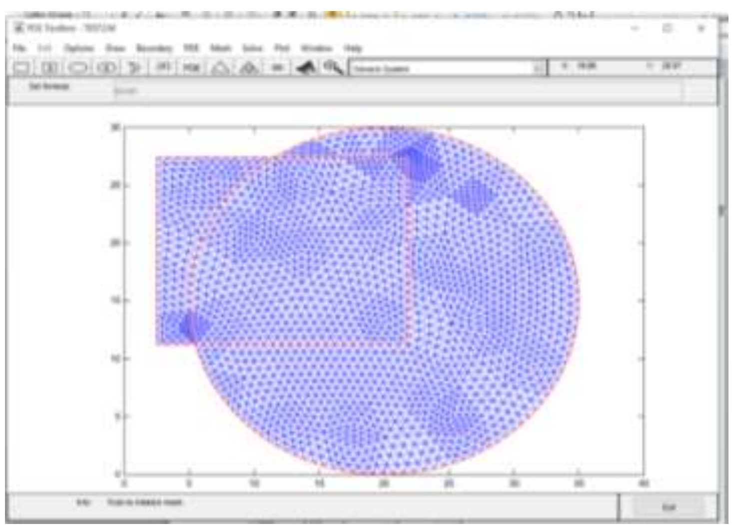

Fig.6. Coordinates of the location of possible solutions in the PDE toolbox

To determine the range of possible solutions according to the Neumann method, coefficients corresponding to the model parameters are introduced:

 

Fig.7. Entering the corresponding coefficients in the PDE toolbox to obtain solutions

After that, in order to clarify the solutions using the Neumann method, we will construct histograms:

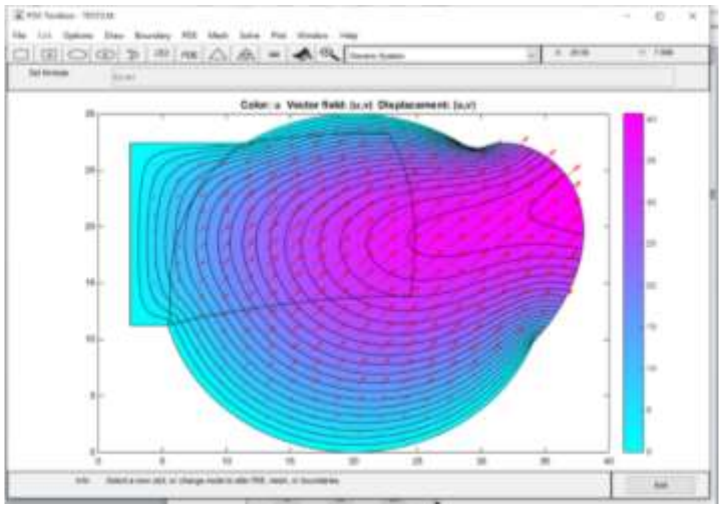

Fig.8. Possible solutions of the model on the PDE toolbox

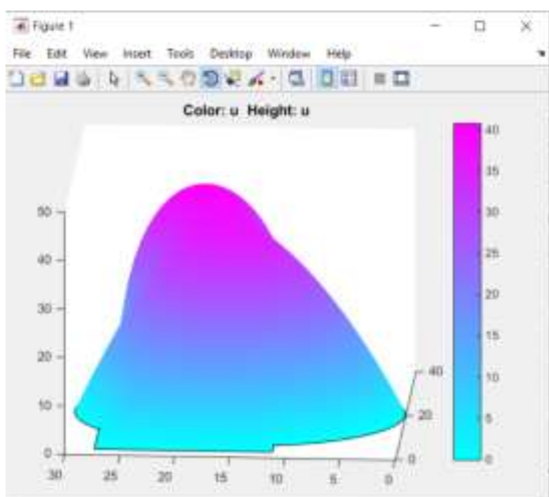


Fig.9. Acceptable model solutions on the PDE toolbox

This means that the permissible solutions of the model are located in the interval (0 – 40) and, as can be seen from Figure 9, the closest values of the permissible solutions are in the interval (25 – 35).

Table 1 shows the values calculated according to the given model and experimental data on cationite regeneration.

 

| Exchange $Na^{+}$ - $Ca^{2+}$ | | | Exchange $Na^{+}$ - $Mg^{2+}$ | | |
|---|---|---|---|---|---|
| Time τ, s | $C/C_{in}$ | | Time τ, s | $C/C_{in}$ | |
| | experiment | calculation | | experiment | calculation |
| 1 | 2 | 3 | 4 | 5 | 6 |
| 240 | 0,680 | 0,678 | 180 | 0,698 | 0,721 |
| 300 | 0,633 | 0,629 | 240 | 0,679 | 0,701 |
| 360 | 0,574 | 0,567 | 300 | 0,644 | 0,679 |
| 420 | 0,492 | 0,479 | 360 | 0,605 | 0,633 |
| 480 | 0,441 | 0,435 | 420 | 0,578 | 0,538 |
| 540 | 0,387 | 0,369 | 480 | 0,546 | 0,515 |
| 600 | 0,293 | 0,283 | 540 | 0,502 | 0,498 |
| 660 | 0,271 | 0,268 | 600 | 0,467 | 0,488 |
| 720 | 0,198 | 0,189 | 660 | 0,413 | 0,449 |
| 780 | 0,143 | 0,147 | 720 | 0,387 | 0,407 |
| 840 | 0,127 | 0,138 | 780 | 0,341 | 0,358 |
| 900 | 0,106 | 0,109 | 840 | 0,305 | 0,327 |
| 960 | 0,098 | 0,101 | 900 | 0,279 | 0,298 |

Table 1
Experimental data and cationite regeneration values calculated according to the developed model

The given experimental and calculated data show that the calculated data satisfactorily correspond to the experimental ones. The standard deviation of the experimental values from the calculated values does not exceed 16%.

A comparative picture of the two parallel experiments is shown in Figures 10 and 11.

 

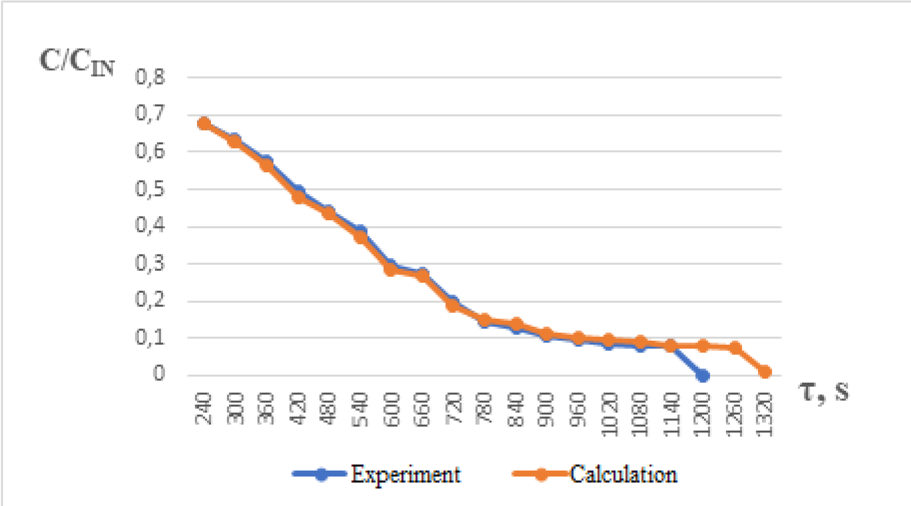


Fig.10. Comparison of experimental and calculated values of regeneration curves $Ca^{2+}$-$Na^{+}$

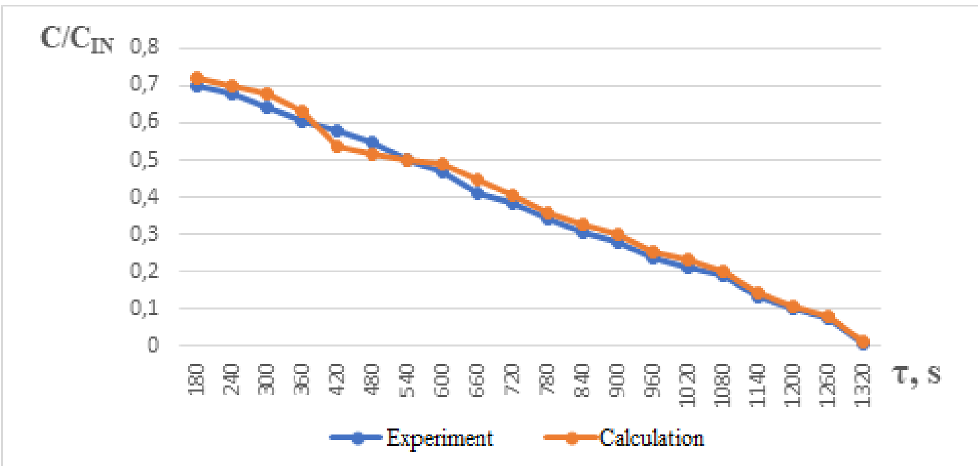


Fig.11. Comparison of experimental and calculated values of regeneration curves $Mg^{2+}$-$Na^{+}$

Summing up the research, it can be stated that an adequate mathematical model of the ionite regeneration process has been developed in a water softening plant with a fixed ionite layer, as eloquently evidenced by the proximity of experimental and model-calculated data, as well as the close coincidence of the curves shown in Figures 10 and 11.

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