Modelling technological process of ion-exchange filtration of fluids in porous media

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Abstract. Solution of an actual problem related to the process of filtration and dehydration of liquid and ionic solutions from gel particles and heavy ionic compounds is considered in the paper. This technological process is realized during the preparation and cleaning of chemical solutions, drinking water, pharmaceuticals, liquid fuels, products for public use, etc. For the analysis, research, determination of the main parameters of the technological process and operating modes of filter units and for support in managerial decision-making, a mathematical model is developed. Using the developed model, a series of computational experiments on a computer is carried out. The results of numerical calculations are illustrated in the form of graphs. Based on the analysis of numerical experiments, the conclusions are formulated that serve as the basis for making appropriate managerial decisions.

1. Introduction

The technological process (TP) for filtering and cleaning the chemical (spinning) solutions, drinking water, pharmaceuticals, liquid fuels, juices and other solutions from gel particles and heavy ionic compounds is usually realized by ionic and multilayer filters.

Therefore, the correct and rational organization of control of operating modes of filtering units and machines allows us to significantly reduce the operating costs and improve the quality of the final output product as a whole.

Various (in physical and mechanical properties) filters and filter partitions are used in filtering liquid solutions and suspensions. The efficiency of filtering equipment is largely determined by filtering partitions, by means of which the separation of the solid particles from the liquid or gas, gel particles, ions from the solution and other accompanying elements is carried out.

It should be noted that the study of the process of filtering ionic suspensions, the determination of the main parameters of the process under consideration and their change ranges for the purpose of controlling it at functioning objects are difficult due to the following factors:
- the data collection of the process takes a long time;
- it is necessary to conduct experiments in the laboratory, which takes a lot of labor and time;
- it is difficult to find the relationship between the parameters of the filter and the TP by the limited experimental sample.

Analysis of the undertaken studies has shown that the process of ion exchange filtration of liquid solutions is affected by a number of internal and external parameters with different specific weights. Deviation of these parameters from the norm value leads to qualitative and quantitative changes of
discussed TP as a whole. Therefore, the definition of the main parameters and their ranges of change is one of the main issues in the theory of research and management of the technological process.

The process under consideration can be divided into two main parts:

- extraction by mechanical filtration of gel particles and impurities from liquid solutions fed to the unit column;
- dehydration of ionic impurities by means of the ion exchange filter.

To realize these tasks, it is advisable to use the methods of mathematical modeling and the computational experiment, which are implemented in the form of software and algorithmic tools taking into account new information technologies and the capabilities of modern computer technology.

Taking into account the above, the process of ion exchange filtration of liquids must be considered as a mechanical separation of impurities and gel particles from the solution and as ion exchange filtration.

Experimental studies have shown that a number of parameters with different specific weights influence the process of filtering liquid solutions. In this connection, it is necessary to comprehensively investigate this process with the use of a mathematical model of the object and to conduct a computational experiment on a computer to determine the conditions for the most complete filtration of liquids from impurities and heavy ions.

Nevertheless, the analysis of scientific publications has shown the presence of certain gaps in studying the TP [1-6]. This paper presents an investigation of certain gaps. In particular, the colmatage of gel particles in the pores of filtration partition of the unit at various depths during ion exchange filtration of solutions through a porous medium with variable porosity of the filter.

2. Problem statement

In mathematical model derivation of the process of ion exchange filtration of liquids through a porous medium, it is assumed that in the filtering process, the gel particles settle in the pores uniformly over the entire thickness of the filtering partition. However, theoretical and experimental data show that the degree of colmatage of gel particles from the filter surface at different depths is not the same. Since the ion exchange process occurs over the entire thickness of the ion exchanger, the solution of the problems taking into account the degree of colmatage at different depths of the ion exchange filter is of particular interest.

To derive a mathematical model of the process of filtering a liquid through a porous medium, the dimensionless variables are introduced:

\[ \bar{W} = \frac{W}{W_0}, \quad q = \frac{H_0}{\mu W_0} P, \quad \bar{n} = \frac{n}{N_0}, \quad \bar{x} = \frac{x}{H_0}, \quad \bar{t} = \alpha x, \quad \bar{\alpha} = \frac{PF}{\mu}, \quad \bar{\theta}^{(3)} = \frac{\theta^{(3)}}{\theta^{(1)}}, \quad \bar{\xi} = \frac{\xi}{\theta^{(1)}}, \quad \bar{\theta} = \frac{\theta}{\theta^{(1)}}. \]

Equations of two-phase media are used and the system of partial differential equations in a dimensionless form is obtained [7-8]:

\[ \frac{\partial \bar{W}}{\partial \bar{t}} + \bar{R} \frac{\partial \bar{W}}{\partial \bar{x}} - \frac{\bar{W}}{\bar{x}} = \frac{F}{H_0^2} \left( \frac{\partial q}{\partial \bar{x}} + \frac{\partial^2 \bar{W}}{\partial \bar{x}^2} - \frac{H_0 F}{H_0^2 \left( 1 - \bar{\theta}^{(3)} \right) (1 - \bar{\xi}^2)} \right); \]

\[ \frac{\partial \bar{\theta}}{\partial \bar{t}} + \bar{R} \frac{\partial \bar{\theta} \bar{W}}{\partial \bar{x}} = 0; \]

\[ \frac{\partial \bar{\theta}^{(3)}}{\partial \bar{t}} = k_1 \left( k_2 + \bar{\theta}^{(3)} \right) \frac{\partial \bar{\xi}}{\partial \bar{t}}; \]

\[ \frac{\partial \bar{\xi}}{\partial \bar{t}} = \lambda_1 (\theta - \bar{\xi}); \]

\[ \frac{\partial n}{\partial \bar{t}} + \bar{R} \frac{\partial n \bar{W}}{\partial \bar{x}} + \frac{\partial N}{\partial \bar{t}} = a_0 \frac{\partial^2 n}{\partial \bar{x}^2}; \]
\[
\frac{\partial N}{\partial \tau} = \beta \alpha \left( n - \frac{a_1 N}{a_2 - bN} \right). \\
\] 

(6)

with corresponding initial and boundary conditions:

\[
\begin{align*}
W &= 1, \quad \theta^{(3)} = 0, \quad \theta = e^{-h_{x}}, \quad \xi = 0, \quad (\tau = 0); \\
W &= 1, \quad \theta = 1, \quad (x = 0); \\
\frac{\partial W}{\partial x} &= \varphi, \quad (x = 1); \\
n(x, 0) &= 0, \quad N(x, 0) = 1; \\
n(0, \tau) &= 0, \quad n(1, \tau) = \frac{n_0}{N_0} = n^0.
\end{align*}
\]

(7)

(8)

3. Solution method

It is not possible to analytically integrate system (1) - (8). To solve the problem, using the Samarsky-Fryazinov vector scheme, a numerical algorithm is developed based on the finite-difference approximation of differential operators on difference algorithms, as well as a software tool for performing a computational experiment on a computer [8].

4. Discussion of results

To carry out the computer experiments on a computer, a corresponding software tool has been developed to determine the main parameters of the process and their ranges of change. The results of numerical calculations are shown in the form of graphs (Figures 1-5).

![Graph](image)

**Figure 1.** Change in the filtration rate of the solution with time.
It can be seen from numerical calculations that the passage rate of the suspension through the porous medium exponentially decreases with time (Fig. 1). By computational experiment, it is established that at the initial stages of the process, the filtration rate of the suspension through the porous medium reduces moderately, and when the filtering time is \( t \geq 10.06 \) hours it decreases exponentially with time. The decrease in the rate of suspension filtration is related to the process of colmatage of gel particles in the pores of filter partition and to the formation of a layer of sediment on the filter surface. The increase in suspension concentration mainly occurs in the upper layers of the filter. With the passage of filtering time, the suspension concentration increases in the deep layers of the filtering partition.

Basing on the results of numerical experiments (Figures 2 and 3), it is evident that the rate of exchange in sorbent and the solution changes with the change in a barodiffusion coefficient.

**Figure 2.** Change in exchanging ions in solution with time: 1- at \( D_\delta=3 \times 10^{-6} \); 2 - at \( D_\delta=3 \times 10^{-5} \).

**Figure 3.** Change in concentration of exchanging ions in sorbent with time:
1- at \( D_\delta=3 \times 10^{-6} \); 2 - at \( D_\delta=3 \times 10^{-5} \).

This is especially noticeable at the initial stages of this process (at \( t = 1-6 \) h). Due to a decrease in the concentration of exchanging ions in the solution, the concentration of exchanging ions in the sorbent increases (Fig. 3).

Numerical calculations have shown that in solving the mass transfer problem with the colmatage of filter pores by gel particles, despite the fact that the filtering partition is not completely saturated with ions, the filter unit is not switched over in time. This effect is explained by the fact that gel particles by
the colmatage ion exchanger filter somehow "isolate" the grains of the ion exchanger and thus represent the contact with the liquid phase. Changes in the volume of liquid solutions passing through the filtering column are shown in Fig. 4.

![Figure 4. Increase in volume of filtrate passing through filter column.](image)

According to Fig. 4, at the initial stages of the filtration process, the rate of solution passage increases linearly with time. When \( t > 10 \), the increase in liquid passage becomes imperceptibly lower, and when \( t > 16 \) h, it almost approaches zero.

![Figure 5. Increase in pressure in filtering column with time: (1- calculated data, 2 - experimental data).](image)

Numerical computer calculations have shown that the main indicator that affects the halt time of the filter is the hydraulic pressure formed inside the filtering chamber of the unit (Fig. 5). It is seen from Fig. 5 that it grows exponentially with time. Numerical calculations have established that the growth of hydraulic pressure depends on the particle colmatage rate in the pore space of the filter, the pores dimensions in filter partition, and the degree of clogging of fed liquid.

To validate the adequacy of the developed TP model, the calculated data are compared with experimental data (Fig. 5).

An analysis of numerical calculations has shown that at initial stage of the filtration process (when \( t = 4-5 \) h), the output concentration of suspended gel particles in the solution will decrease imperceptibly, and when \( t = 5 \) h, it decreases exponentially. A sharp decrease in the particles concentration in the solution is due, firstly, to the saturation of filter pores with gel particles, and secondly, to an increase in the thickness of the sediment layer on the surface of the filter. The resulting sediment layer, in turn, acts as a filter. As follows from the results of experiments, the time of clogging of filter pores with gel particles depends on the passage rate and the initial concentration of the filtrate,
as well as on gel particles diameters in the solution. The rate of precipitation of gel particles in filter pores when $t = 3$ h will increase exponentially. The complete saturation of the pores of filtering column occurs at filtration time of $t = 10.5$ h.

From the analysis of conducted experiments, it follows that output concentration $\theta^{(3)}$ of suspended particles in the filtrate decreases with time. This is due, firstly, to the fact that the formed sediment layer and its repacking under the influence of surface pressure force on the surface of the unit further serves as a filter and, secondly, the filling of the filter pores with suspended particles occurs, which prevents the passage of gel-particles through the filter. At a filtration time of $t = 10$ h, value $\theta^{(3)}$ will be 0.01.

5. Conclusion

Thus, a mathematical model and a numerical algorithm are developed to carry out a complex study of the process of ion exchange filtration of liquids through a porous medium with specified operating conditions of the filtering unit and physical and chemical properties of ionic solutions.

By numerical calculations it has been stated that the rate of suspension filtering over the depth of filtering partition decreases sharply on the upper layers of the filter, and then it remains constant over the depth of filtering partition, depending on filter thickness and gel particles diameters in the suspension. With the increasing filter thickness, the rate of filling the porous space of filtering partition with gel particles decreases, and due to the increase in the resistance force, the filtering rate and the filter operation time decrease, while value $\theta^{(3)}$ of suspended particles in the filtrate decreases exponentially with time.

As a result of colmatage of suspended particles in the pores of the ion exchanger filter, the rate of ion exchange and the duration of the filter operation decrease. The theoretical (calculated) switching time in the absence of suspension concentration in water is 16.6 hours, with the addition of concentration 0.0001, the switching time is 15.1 hours, with a concentration of 0.0003 - 13.7 hours. In the presence of concentrations, the average design switching time is 16.2 hours. Calculations performed to distribute the concentration of citric acid salts with time have shown that the theoretical slip time without suspension concentration is 21 minutes; with the addition of suspension concentration, it is 17 minutes and the practical slip time is 25 minutes.

The theoretical and experimental saturation time without suspension concentration is 110 minutes, and with suspension concentration - 93 minutes. It should be noted that in solving the mass transfer problem with colmatage at a given time, the adsorption process ceased; however, the concentration of the ion exchanger is not fully saturated. This effect is explained by the fact that gel particles by colmatating the ion exchanger filter, somehow "isolate" the grains of the ion exchanger and thus represent the contact with the liquid phase.

Computational experiments are performed under various modes of filtration of ionized liquid solutions, heavily contaminated suspensions and others, and it is established that the rate of ion exchange in sorbent and solution changes with the change in the barodiffusion coefficient.

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