

# Calculation of optimal flow of ionite during water treatment in the column of continuous action

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**Abstract.** In the article an algorithm for calculating the continuous ion exchange column is proposed. By analogy with the calculation of the optimal phlegm number of the rectification column this algorithm takes into consideration depreciation charges for capital costs associated with the size of the column and working capital associated with the consumption of ionite and its regeneration. This algorithm can be used to calculate depreciation charges for capital costs related to column sizes and working capital regarded to ionite consumption and regeneration. Examples of ionite consumption calculation at typical and proposed algorithms of calculation and technological and geometric parameters used in column of water purification from sodium cations are given. Thus, in a typical calculation, when the water being purified from sodium cations moves in the ideal displacement mode and the excess of ionite is 1% of its minimum consumption. The optimal ionite consumption corresponding to the minimum of capital costs and working capital, which requires an increase in the ionite consumption by 5.6% of its minimum consumption. In this case the cost of ion exchange increases by 4.5%. It confirms the recommendations for industrial operation and design of ion exchange columns and increases the minimum ionite consumption by 1÷10%. The continuous ion exchange column was calculated including the longitudinal diffusion. Necessity of the further increase of the ionite consumption with regard to the longitudinal diffusion is shown. In the article an example of the ion exchange process calculation in comparison with the typical one, when the displacement mode for the treated water is ideal, is given. Similar equations for the dependences of the concentration of extracted ions in the purified solution and ionite granules are proposed if the equilibrium dependence is described by a linear equation. The working line is dependent on the concentration of the extracted ions in an ionite and on their concentration in the purified water, first, because of a jump in concentration at the inlet and a concave shape of the working line (the latter is usually a straight one in case of the mass-transfer processes) reduces the local and average driving forces of mass-transfer process significantly. It leads to increasing of the moving layer height of the ion exchanger in the column 2 times, and can lead to crossing the line of equilibrium by reducing the concentration jump at the entrance. Consequently, it is necessary to increase ionite consumption by more than 18% compared to its minimum consumption.

## 1 Introduction

Engineering calculations of ion exchange column geometric and technological parameters must be carried out taking into consideration energy and resource savings. The main cost of working capital is the consumption of ionite while the capital costs usually depend on the size of ion exchange column.

Standard algorithms for calculating continuous ion exchange columns are known to be based on calculations of basic mass exchange processes (rectification, absorption, adsorption and extraction), on determination from material balance with regard to equation of minimum flow rate of reflux, sorbent or extractant and their increase from several percent (ion exchange consumption) up to several tens of percent (in sorption and extraction processes) and even several times, that is,

hundreds of percent (in the process of rectification) [1-8].

Attempts are made to take into account the flow pattern (e.g., longitudinal diffusion) and its effect on column sizes [9-15], but the economic costs associated with working capital (ionite consumption and regeneration) and with the depreciation charges for capital costs and their minimization are neither considered nor calculated at typical algorithms.

The purpose of the work is to determine the function of costs minimization for the shock absorption depending on the size of the column and on the working equipment depending on the flow rate of the ionite and its regeneration, as well as the effect of longitudinal diffusion on technological parameters and geometric dimensions of the ion-exchange column.

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## 2 The calculation of the ionite columns

According to the articles [1, 16, 17] described minimization function "C" can be represented as a function

$$C=V+aG_x, \quad (1)$$

where  $V$  is the column volume,  $G_x$  is the ionite consumption, and  $a$  is the weight coefficient of the relationship between depreciation charges for capital expenditures proportional to the column volume and working capital proportional to the ionite consumption.

Tables 1 and 2 show the initial, reference data and calculated parameters of a continuous ion exchange column for removing sodium cations from water, calculated using the standard algorithm and the formula (1). A typical algorithm for calculating an ion exchange column with the specified initial data is presented in the article [18].

**Table 1.** Initial and reference data, calculation parameters of a continuous ion exchange column for removing sodium cations from water.

№	Parameter	Value
1	2	3
<u>Initial data</u>		
1	Productivity on the water $q_v$ , m <sup>3</sup> /hour	1.5
2	Initial concentration of ions in water $\bar{C}_H$ , mol-equiv/m <sup>3</sup>	4.35
3	Final concentration of sodium cations $\bar{C}_K$ , mol-equiv/m <sup>3</sup>	0.2175
4	Full exchange capacity of the ionite (cation exchanger KU-2) $x_0$ , kg/kg	0.11
5	Molecular weight of extracted ions (sodium cations) $M$ , kg/kmole	23
6	Bulk specific volume of the dry ionite $v_0$ , m <sup>3</sup> /kg	$3 \cdot 10^{-3}$
7	The equivalent diameter of the granules of the ionite $d$ , m	$0.9 \cdot 10^{-3}$
8	Bulk density of wet swollen ionite $\rho_H$ , kg/m <sup>3</sup>	800
9	The equilibrium constant of the ion exchanger (cation exchange resin KU-2) $K_P$	1,2
10	The porosity of ion exchanger layer $\epsilon_0$ , m <sup>3</sup> /m <sup>3</sup>	0,4
11	The solution density $\rho_B$ , kg/m <sup>3</sup>	1000
12	Viscosity of water $\mu$ , P/sec	$10^{-3}$
13	Diffusion coefficient of ionite in water $D_v$ , m <sup>2</sup> /sec	$1,17 \cdot 10^{-9}$
14	Array of standard column diameters $D_{a(i)}$ , m	Reference data
15	The effective diffusion coefficient of the extracted ions inside the grains of the ionite (internal diffusion) $D_x$ , m <sup>2</sup> /sec	$2,3 \cdot 10^{-10}$
16	The initial concentration of extractable ions in the granules of the ionite after regeneration $x_H$ , kg/kg	$5 \cdot 10^{-3}$
17	Weight ratio of the relationship between depreciation and working capital (formula 1) $a$	0,14
<u>Calculation parameters</u>		

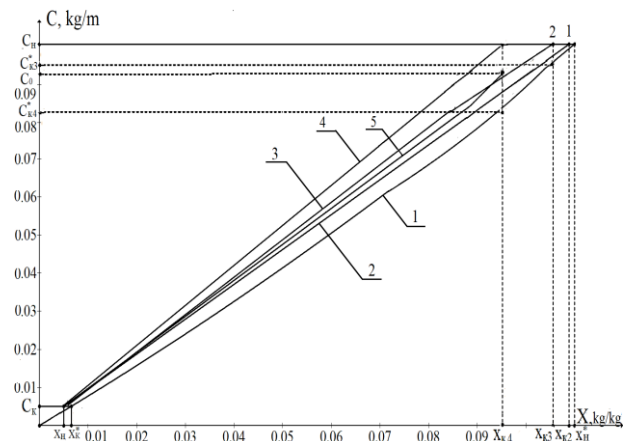
1	Initial concentration of extracted ions in water $C_n$ , kg/m <sup>3</sup>	0,1
2	Final concentration of recoverable ions in water $C_k$ , kg/m <sup>3</sup>	$5 \cdot 10^{-3}$
3	The apparent density of the moist swollen ionite pellets $\rho$ , kg/m <sup>3</sup>	1333,3
4	Archimed's number of ionite granules $A_r$	2383,8
5	Reynold's number for the granules of the ionite $R_e$	1,436
6	Calculated rate of deposition of ionite granules in water $v$ , m/sec	$1,595 \cdot 10^{-3}$
7	Rated diameter of a column $D_{ap}$ , m	0,576
8	The standard diameter of the column $D_{ac}$ , m	0,6
9	Working fictitious speed of water in the column $v_p$ , m/sec	$1,474 \cdot 10^{-3}$
10	The Reynold's number in the standard column for granules of the ionite $R_{ep}$	1.327
11	The solution density $\rho_B$ , kg/m <sup>3</sup>	1000
12	Viscosity of water $\mu$ , P/sec	$10^{-3}$
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10	The Reynold's number in the standard column for granules of the ionite $R_{ep}$	1.327
11	Prandtl number for water to be treated $P_r$	854.7
12	Nusselt's number $N_u$	14.67
13	Mass transfer factor for external diffusion $\beta_y$ , m/sec	$1.91 \cdot 10^{-5}$

14	Volume coefficient of a mass transfer $K_b$ , 1/sec	$7.63 \cdot 10^{-2}$
15	Apparent density of dry ionite $\rho_u$ , kg/m <sup>3</sup>	555.6
16	Average concentration of recovered ions in water $C_c$ , kg/m <sup>3</sup>	$3.17 \cdot 10^{-2}$
17	Equilibrium concentration of recovered ions in the ion granules corresponding to their average concentration in water $x_c^*$ , kg/kg	$3.936 \cdot 10^{-2}$
18	Average tangent of the angle of inclination of the equilibrium line $g_r$ , $\frac{kg/m^3}{kg/kg}$	1.24
19	Bio criterion characterizing ratio of external and internal diffusion of extracted ions (if it < 1 - limiting stage is external mass transfer) $B_i$	$5.415 \cdot 10^{-2}$
20	The equilibrium coefficients of the Langmuir equation $a, b$	1.319 1.999
21	Equilibrium concentration of extracted ions in ion corresponding to their initial concentration in water $x_H^*$ , kg/kg	0.11
22	Equilibrium concentration of extracted ions in ion corresponding to their final concentration in water $x_K^*$ , kg/kg	$6.53 \cdot 10^{-3}$
23	Working final ion concentration in the granules at the outlet of the column $x_K$ , kg/kg	0.1089
24	Minimum flow of an ionite $G_{xm}$ , kg/hour	1.358

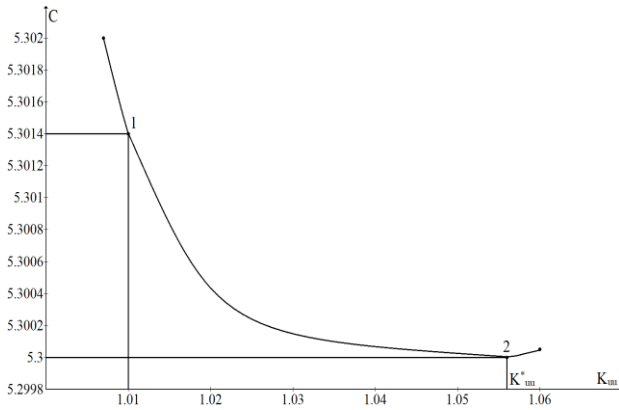
**Table 2.** Comparison of parameter values for the structure of the fluid flow corresponding to the ideal displacement with regard to the longitudinal diffusion. from water.

№	Parameter	Typical algorithm	formula (1)	Regarding the longitudinal diffusion
1	2	3	4	5
1	The working flow of the ionite $G_x$ , kg/hour	1.372	1.434	1.61
2	The excess ratio of the ionite in comparison with its minimal consumption $K_{uu}$	1.0106	1.056	1.186
3	Transference units number TUN	28.07	12.41	13.71
4	Height of the ionite granule layer moving from top to bottom $H_B$ , m	0.543	0.24	0.265
5	Volume of the	0.153	0.068	0.075

	granule layer in the column $V_{uo}$ , m <sup>3</sup>			
6	The total height of the column $H_o$ , m	1.442	1.140	1.165
7	The total volume of the column $V_o$ , m <sup>3</sup>	0.82	0.329	0.4076
8	Speed of movement of granules from top to bottom in the column $U_x$ , m/sec	$1.7 \cdot 10^{-6}$	$1.7 \cdot 10^{-6}$	$1.7 \cdot 10^{-6}$
9	The residence time of the pellets of the resin in the column $\tau_x$ , sec	121219	150360	321768
10	Residence time of the treated water in the granule layer $\tau_B$ , sec	162.7	179.7	367.9
11	The annual ionite consumption kg/year $G_g$	9878.4	110324.8	11592



**Fig. 1.** Equilibrium (1) and working lines of ionite: 2 - when calculating is made according to the standard algorithm,  $K_{uu}=1.0106$ ; 3 - when calculating is made on the formula (1) minimizing capital costs and working capital  $K_{uu}=1.056$ ; 4 - when ionite flow excess takes place,  $K_{uu}=1.186$ ; 5 - for the diffusion flow structure of the solution to be purified at  $Pe=41.7$ .



**Fig. 2.** Graph of dependence of the minimization function of the capital expenditure amount and working capital on the coefficient of ionite excess consumption in comparison with its minimum value without taking into account longitudinal diffusion; point 1- for a typical calculation, point 2 - according to the proposed formula (1).

### 3 Discussion of calculation results and conclusions

As it is evident from the comparison of the results of calculations of technological and geometric parameters of a continuous ion exchange column using the standard algorithm and the proposed algorithm for optimizing ionite consumption with regard to the minimum capital costs and working capital, the latter requires an increase in ionite consumption from 1.372 kg/hour to 1.434 kg/hour, that is 4.3%. In a year, this increase will be 500 kg/year. However, it is obvious from the graph shown in figure 2, the "C" minimization function is reduced from a value of 5.3014 to 5.3. It leads to a reduction in capital expenditures by 0.026%.

Thus, the proposed algorithm for calculating the optimal ionite consumption with regard to depreciation charges for capital expenditures and working capital confirms the correctness of increasing ionite working consumption compared to its minimum consumption by 1-10%.

Proposed algorithm makes it possible to determine exact value of optimum flow rate of ion exchange column operating in mode of ideal displacement by cleaning solution.

The increase in longitudinal diffusion in the liquid phase often requires a greater increase in ionite consumption compared to the ideal displacement mode. It can be explained by a jump in the concentration at the entrance of the liquid phase flow in the column. A decrease in  $C_H$  to  $C_0$ , in this case, can lead to a value of the concentration of  $C_0 < C_K^*$  and the intersection of the working line and the equilibrium one (Fig.1). This is what happened in this case. Only an increase in the ionite flow rate from  $G_X=1.434$  kg/hour to 1,61 kg/hour, i.e. an excess of its flow rate from 5,6% to 18,6% in comparison with the minimum flow rate, allows the ion exchange process to be carried out in case the entire working line is under equilibrium line (Fig.1).

A response curve was taken on a laboratory column with ionite granules. Its dispersion was  $\sigma^2=0.048$

[19,20]. If the Pecle number of longitudinal diffusion is calculated by the formula

$$\sigma^2 = \frac{2}{Pe} - \frac{2}{Pe^2} [1 - \exp(-Pe)];$$

it is equal to  $Pe=41.7$ .

In Fig.1 a graph of the working line (line 5) is shown. It has a jump in the input concentration from  $c_H= 0.1$  kg/m<sup>3</sup> to  $c_0 = 0.0928$  kg/m<sup>3</sup> and the working line obtained by solving a non-uniform differential equation of the second order [10-14]

$$\frac{d^2c}{dh^2} = Pe \frac{dc}{dh} + k\tau_s Pe(c - c^*), \quad (2)$$

when the equilibrium line can be approximated by the equation

$$c^* = \frac{x}{A}, \quad (3)$$

In this case, the deviation from the equation  $c^* = \frac{x}{A - Bx}$  does not exceed 6%.

The analytical solution of the differential equation (2) with regard to the formula (3) has the form

$$c = c_1 \exp(r_1 h) + c_2 \exp(r_2 h) + Q, \quad (4)$$

The coefficients  $c_1$ ,  $c_2$  and  $Q$  are found from the boundary conditions

$$\begin{cases} h=0, & c_0 = c_1 + c_2 + Q; \\ g_0 = c_1 r_1 + c_2 r_2 \end{cases} \quad u \quad \begin{cases} h=1, & c = c_K; \\ g_K = 0 \end{cases}, \quad (5)$$

and the equation of the working line takes the form

$$x = x_H + (q_v/G_x)(c - c_K) - (q_v/G_x)g/Pe, \quad (6)$$

where  $g=dc/dh$  – is the concentration gradient of the extracted component from the purified solution and  $h$  is the dimensionless height.

According to the results of calculations and the graph of the working line (Fig.1, line 5) the working line not only does not reduce the concentration of extracted ions at the input  $c$  from  $c_H$  to  $c_0$  due to a jump in concentrations due to longitudinal diffusion, but it also has a concave appearance (that is, the working line is no longer straight), which further reduces the local and average driving force of mass transfer. It leads to an increase in the number of transfer units, the average residence time, and the required height of the moving ionite layer.

Thus, the calculation presented in the article takes into account that the flow mode of the liquid phase does not correspond to an ideal displacement, but to a longitudinal diffusion. It changes the position of the working line significantly, firstly, shifting it towards the equilibrium line at the entrance and reducing the double-acting force of the mass transfer process. Secondly, it requires an increase in the ionite consumption compared to the ideal displacement. At the same time, the proposed

calculation of the optimal ionite consumption, considering capital costs and working capital, allows us to calculate the ionite consumption accurately and reduce the cost of the ion exchange process. Thus, it is advisable to replace the standard algorithm for calculating the ion exchange column with its exact calculation considering the formula (1) and longitudinal diffusion.

## References

- [1] K.F. Pavlov, *Examples and tasks for the course of processes and devices of chemical technology: study guide for University students* (576, 2013).
- [2] A.S. Timonin, *Engineering-ecological reference book* (Volume 1, 917, 2003).
- [3] A.S. Timonin, *Engineering-ecological reference book* (Volume 2, 884, 2003).
- [4] A.G. Kasatkin, *Basic processes and devices of chemical technology: study guide for University students* (784, 2008).
- [5] A.I. Rodionov, V.N. Klushin, N.S. Torocheshnikov, *Environmental protection Techniques: for students, higher educational* (519, 1989).
- [6] O. Levenspiel, *Engineering design of chemical processes* (624, 1969).
- [7] D. Perry, *Handbook of chemical engineers* (504, 1968).
- [8] V.V. Kafarov, M.B. Glebov, *Mathematical modeling of basic processes in chemical production* (400, 1991).
- [9] A.B. Golovanchikov, N.V. Shibitova, D.A. Baev, The removal of anions of chlorine from a solution of caustic soda in the ion-exchange column continuous action, *Izvestia VSTU, Ser. Rheology, processes and devices of chemical technology*, **1**, 23-27 (2014).
- [10] A.B. Golovanchikov, O.A. Zalipaeva, N.A. Merentsov, A.A. Kobernik, Adsorption in a continuous column with a diffusive flow structure in the gas phase, *Ecological systems and devices*, **2**, 23-31 (2016).
- [11] A.B. Golovanchikov, O.A. Zalipaeva, N.A. Merentsov, A.A. Kobernik, Influence of the diffusion structure of the liquid phase flow on ion exchange in a countercurrent device of non-discontinuous action, *Water Supply and sanitary engineering*, **3**, 57-63 (2016).
- [12] A.B. Golovanchikov, O.A. Zalipaeva, A.A. Kobernik, N.A. Merentsov, Modeling of ion exchange in a continuous-action apparatus with a diffusion structure of a liquid flow, *Ecological systems and devices*, **10**, 15-23 (2015).
- [13] A.B. Golovanchikov, O.A. Zalipaeva, N.A. Merentsov, *Modeling of sorption processes taking into account the flow structure* (130, 2018).
- [14] A.B. Golovanchikov, N.A. Prokhorenko, N.V. Shibitova, M.D. Romanenko, O.A. Zalipaeva, Simulation of the process of rectification with the account of longitudinal diffusion, *Journal of Physics: Conference Series*, 1-8 (2018).
- [15] N.I. Gilperin, *Structure of flows and efficiency of column devices of the chemical industry* (261, 1977).
- [16] A.B. Golovanchikov, O.A. Zalipaeva, A.A. Kobernik, Modeling of continuous adsorber taking into account energy and resource saving, *Energy and resource saving: industry and transport*, **3**, 36-42 (2018).
- [17] A.B. Golovanchikov, O.A. Zalipaeva, A.A. Kobernik, Calculation of optimal consumption of absorbent taking into account the costs of depreciation and working capital, *Energy and resource saving: industry and transport*, **3**, 27-31 (2018).
- [18] Y.I. Dynarski, *Basic processes and apparatuses of chemical technology: textbook* (750, 2008).
- [19] A.Y. Zakheim, *Introduction to modeling of chemical and technological processes, Mathematical description of processes* (224, 1973).
- [20] A.Y. Zakheim, *Mathematical modeling of the main processes of chemical production* (400, 1991).