Interaction of sorption and hydrodynamic phenomena during water filtration

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Abstract. The paper presents the concept of sorption and surface phenomena, as well as ion exchange. These processes are accompanied by absorption or exchange of ions due to the free energy of the surface layer of the solid phase. It is proposed to consider the process of ion exchange between the solid and liquid phase during filtration. As a solid phase, synthesized loading is used, which is used in various industries. It is noted that the synthesized load has high mechanical strength and chemical resistance. It is indicated that the size and shape of the loading grain affects the ion exchange rate and hydraulic resistance. The dependence taking into account the free energy of the loading surface and the mechanism of ion exchange in the equivalent dependence is given. Technological characteristics of some types of loading are shown. The duration of filtration is determined by the appearance of dissociated ions in the filtrate and depends on the exchange capacity of the load. Static and dynamic exchange capacities are allocated. The relevance, purpose and objectives of the work are formulated. A scheme of fluid motion through the elementary loading layer is proposed for the mathematical description of the process. The increment of substances in the elementary loading layer is described and the conditions of fluid flow around the loading grain of spherical shape are formulated. The reduction of ion concentrations in the elementary layer is mathematically shown. The concentration gradient is obtained as a partial derivative with two variables. The condition of fluid flow around the loading is introduced, based on the processes of hydrodynamics. The flow pattern of the loading elements depends on the Reynolds number. With the help of mathematical and physical analysis, a theoretical dependence was obtained, which relates the initial concentration of the studied substances in water, the metabolic capacity of the load, the hydrodynamic and physical parameters of the flow. The performed theoretical studies allowed to substantiate the conclusions of this work and to formulate a conclusion about the influence of flow hydrodynamics on the change of absorption of substances from water by loading.

Introduction
Sorption phenomena, surface phenomena, as well as their variety - ion exchange are the properties of thin layers of matter at the interface of two media. The absorption of ions or their exchange is due to excess free energy of the surface layer. The structure of the solid phase and its composition affect the physical nature of the phenomenon and can be accompanied by chemical transformations. We consider the sorption process on the example of ion exchange. As the solid phase, we use synthetic resins. Recently, synthetic resins have been used, exchanging both cations and anions in water treatment technologies. In addition, synthetic resins are used for concentration, isolation, removal of ions in solutions in the metallurgical, pharmaceutical, chemical, energy industries [1,2,3].
Synthetic resins have high mechanical strength, chemical resistance and large exchange (sorption) capacity. The sorption capacity of the solid phase is similar to the free energy. The grain size ranges from 0.25 mm to 2.00 mm. The grain size affects the ion exchange rate and the hydrodynamic resistance of the loading layer during filtration. This dependence is represented by inequality

$$d \leq E \geq X$$

where $d$ – grain diameter download;

$E$ – exchange capacity or free loading energy (ionite);

$X$ – hydrodynamic resistance of the ionite layer.

Dissociated ions of the solution are exchanged with the active group of the solid phase by ionites during transportation through the loading, and the active group enters the filtrate. The interaction of the involved components of the cleaning process takes place at the solid - solution interface. If the initial liquid being filtered on ionites has electrolytic properties, then one of the ions of the solution is selectively adsorbed on the loading surface. The mechanism of exchange can be represented as follows

$$A \cdot [T] + a \rightarrow a \cdot [T] + A$$

$$B \cdot [T] + b \rightarrow b \cdot [T] + B$$

where $A$ – active group of the cationite ($H^+, Na^+$);

$B$ – active group of cationite ($OH^-, Cl^-, SO_4^{2-}$);

$a$ – ions are extractable (+);

$b$ – ions are extractable (-);

$[T]$ – solid loading phase.

The exchange according to the above scheme occurs in an equivalent relationship between the exchanging ions [4,5,6].

By origin, ionites can be natural (for example, aluminosilicate Permutite) and synthetic (for example, Polysulfostiro) [7]. Ionites are considered as the solid phase.

The ion exchangers are formed:

1. by types – cation exchange resins, anion exchange resins;
2. by groups – strong acid, weak acid, strong base, weak base;
3. by properties – static exchange capacity, specific volume, selectivity;
4. in structure – grain diameter 0.25 mm – 2.00 mm [8,9,10].

| # | Name, brand | Volume weight, t/m³ | Exchange capacity, g-eq/m³ | Grain size, mm |
|---|-------------|---------------------|-----------------------------|---------------|
| 1 | Sulfonated coal CK-1 | 0.7 | 600 | 1.5 |
| 2 | Ky-2 | 0.71 | 1500 | 1.5 |
| 3 | Amberlight IR-120 | 0.75 | 2000 | 0.6 |
| 4 | Amberlight IRC-50 | 0.5 | 5000 | 0.5 |
| 5 | AH-31 | 0.35 | 1500 | 2.0 |
| 6 | AB-17 | 0.39 | 800 | 0.85 |
| 7 | Amberlight IRA-401 | 0.71 | 800 | 0.85 |
| 8 | Permutit E | 0.6 | 1500 | 2.0 |
| 9 | EDE-10P | 0.45 | 800 | 1.5 |
The average particle size of such ion-exchange resins is 0.2 – 2.0 mm, bulk weight 0.5 – 0.9 t/m$^3$. Under the conditions of filtration of the solution through the ionite loading layer, the duration of filtration is determined before the first "slip" of ions into the filtrate, depends on the exchange capacity (free energy). In this case, the calculation of the exchange capacity is carried out through the maximum number of mg – eq ions absorbed by the unit mass of the ionite in equilibrium with the electrolyte solution.

The exchange capacity of ionites ranges from 600 to 5000 g – eq/m$^3$. There are static and dynamic exchange capacity, and the first is always greater than the second [11]. Application of ion exchange method of water purification. When desalting and water softening is widely used in various ion exchangers. Demineralized water is produced on ionite filters in the power industry for steam power plants. Desalination of sea or ground water with a high salt content is carried out on ionite filters in combination with electrodialysis plants. In the metallurgical industry for the extraction of noble metals from solutions using specially synthesized ion exchangers. The ion exchange method is a priority for radioactive waste treatment and removal of hazardous impurities from wastewater. In the radio engineering industry, special ionites are used to produce water with the required properties. In the chemical industry, ionites are used as catalysts in chemical processes and a means of analytical control, as well as for purification and separation of organic and inorganic synthesis products. In the food and medical industries, ionites are used to refine sugar, to improve the quality of wines and juices, to obtain drugs and vitamins [12].

**Relevance of the work**

Сорбционный (ионный) обмен является частью физико-химических методов очистки природных и сточных вод. Разработка теоретических предпосылок метода сорбционного обмена применительно к растворённым диссоциированным веществам в гидродинамических условиях является актуальной задачей [13].

**Purpose of work**

The aim of the work is to develop a theoretical model of the ion exchange process in hydrodynamic conditions.

**The task of the paper**

The problem is to obtain an equation for reducing the concentration of dissociated compounds by ion exchange in hydrodynamic filtration conditions.

**Results**

When the liquid containing dissociated ions moves through the loading layer (ion exchange resin), the extracted ions are delayed, and the loading ions enter the filtrate in an equivalent ratio. At the same time, a mass of recoverable ions accumulates in the loading column. The accumulated mass of the extracted ions depends on the exchange capacity of the charge [14,15,16,17]. Consider the process of filtering water through the ion exchange loading layer to extract dissociated compounds [16,18]. We present a diagram of the fluid motion through the loading layer for the purpose of mathematical description of the process, as shown in figure 1.
Figure 1. Scheme of the studied process.

1 – ion exchange loading;
2 – cylindrical vessel;
3 – input of source water;
4 – output of source water;
1 – 1 and 2 – 2 – design sections.

Loading 1 is placed in a vertical cylindrical vessel 2. We introduce a condition - the area of the horizontal section of the vessel is one (where D is the diameter of the vessel). Source water 3 moves from top to bottom by gravity. For mathematical calculation, we allocate an elementary layer of loading, of infinitesimal magnitude between two sections 1 – 1 and 2 – 2 thick Δx at a distance x from its surface. The cross section 1 – 1 receives water with a weight concentration of $C_1$, and passing through the elementary loading layer, the concentration decreases to $C_2$. Then, the reduction of ion concentrations in the elementary layer will be:

$$\Delta C = -(C_2 - C_1) = -\frac{\partial C}{\partial x},$$  

(3)

where $\Delta C$ – the change in the concentration of substances in the elementary layer;  
$\frac{\partial C}{\partial x}$ – concentration gradient, that is, its change by the unit height of the loading layer $\Delta x$.

The concentration gradient is expressed as a partial derivative because the concentration of ions in each section depends on two variables: the distance from the loading surface, $x$; the exchange capacity of the loading $E$ and the duration of filtration.

The minus sign in equation (3) shows that the ion concentration decreases with increasing distance $x$ from the loading surface.
Ion exchange can be considered as the interaction process of exchanging the active group of loading anions ($OH^-$, $Cl^-$, $SO_4^{2-}$) for anions in the source water.

The source water is filtered through the anionite (loading) layer, the components are removed from the source water, and replaced active groups from the loading appear in the filtrate.

Suppose that the decrease in the concentration of dissociated compounds in the elementary loading layer is $\Delta C_1$, and the increase in dissociated compounds is due to hydrodynamic conditions (speed mode) $\Delta C_2$.

Ion concentration balance at the site $\Delta x$ can be represented by the expression

$$\Delta C = \Delta C_1 - \Delta C_2,$$

where $\Delta C_1$ can be described by a dependency

$$\Delta C_1 = f(E).$$

The process of removing nitrogen-containing compounds from the source water, in addition to the exchange capacity of loading $E$, is affected by the ratio of chlorides ($Cl^-$) and sulfates ($SO_4^{2-}$). Denote this ratio by $a$, then in an elementary layer with thickness $\Delta x$, the decrease in concentration $\Delta C_1$ will be equal to

$$\Delta C_1 = a \cdot E \cdot \Delta x.$$

We consider the second term of expression (2), where $\Delta C_2$ is a function of the filtering rate [15,19,20].

$$\Delta C_2 = f(\nu).$$

Ion exchange loading is a set of spherical shapes of the same diameter. Figure 2 shows the flow diagram of the ball loading fluid flow.

![Figure 2](image_url)

**Figure 2.** Scheme of flow around the ball with a fluid flow at a speed $\nu$.
1 – the upper point of the ball; 2 – the side of the ball; 3 – the lower point of the ball.
When the liquid moves through the loading, the water flows around the particle in the form of a ball. In this case, two forces act simultaneously - the drag of pressure and the drag of friction. Approaching the ball, the flow deflects and flows around it. Then begins to move rapidly, there is an embarrassing effect. Increasing the velocity in the flow leads to a decrease in the pressure in the boundary layer of the load in the direction from point 1 to point 2. When moving to the stern of the ball, the flow expands and there is a diffusor effect, the speed decreases and the pressure increases. In the boundary layer, the pressure increases in the direction of flow from point 2 to point 3. In the boundary layer, the movement is laminar, the liquid particles are inhibited, do not overcome the increasing pressure from point 2 to point 3. Inside the boundary layer, under the influence of pressure, the particles will begin to move in the opposite direction. The return flow in the boundary layer leads to the appearance of vortices, which reduce the pressure in this area and the drag force increases.

The nature of the flow around the ball fluid flow depends on the Reynolds number, which is determined by the following relation

\[ \text{Re} = \frac{\nu \cdot d}{\nu}, \]  

where \( \nu \) – rate of undisturbed flow;  
\( d \) – the diameter of the ball download;  
\( \nu \) – the kinematic viscosity.

Based on the above, we can write \( \Delta C_2 \) as

\[ \Delta C_2 = \text{Re} \cdot \rho \cdot \Delta x. \]  

where \( \text{Re} \) – is the Reynolds number (10 to 30);  
\( \rho \) – the density of the source water;  
\( \Delta x \) – is the thickness of the elementary layer.

The obtained dependencies are substituted into the expression (4)

\[ \Delta C = \Delta C_1 - \Delta C_2 = a \cdot E \cdot \Delta x - \text{Re} \cdot \rho \cdot \Delta x = \Delta x (a \cdot E - \text{Re} \cdot \rho). \]  

In the final form the equation can be written as follows

\[ - \frac{\partial C}{\partial x} = (a \cdot E - \text{Re} \cdot \rho). \]  

where \( \frac{\partial C}{\partial x} \) – is the decrease in the concentration of compounds in the elementary layer;  
\( a \) – coefficient depending on the ratio of chlorides and sulfates in the source water;  
\( E \) – exchange capacity of ionites.

The obtained theoretical dependence relates the initial concentration of the studied substances in water, the exchange capacity of ionites, hydrodynamic and physical parameters of the flow. The presented model is based on the following prerequisites:

– the studied substances are in dissociated form;
– recoverable substances (nitrogen-containing) have a negative charge;
– the ratio of chlorides and sulfates in the source water has an effect on the purification effect;
– hydrodynamic conditions in the flow (Reynolds number from 10 to 30) are necessary;
– loading form spherical;
– the direction of the fluid flow when filtering from top to bottom.

**Conclusion**

1. As a result of the literature review, it is shown that it is possible to use the ion exchange process to
extract nitrogen-containing compounds from water.
2. The paper adopts a theoretical scheme of the filtration process with an increment of the extracted substances in the elementary layer.
3. Ball-shaped ionite is considered as a loading.
4. The limiting case of fluid flow around a sphere in the conditions of drag in the boundary layer is considered.
5. Obstacles created by the flow of liquid lead to a decrease in the effect of water purification.
6. The value of Reynolds number optimal for ion exchange is chosen.
7. The equation of reduction of concentrations of nitrogen-containing compounds by ion exchange is obtained

$$-rac{\partial C}{\partial x} = (a \cdot E - \text{Re} \cdot \rho).$$

8. This model makes it possible to predict the efficiency of the process of application of the ion exchange process for the removal of nitrogen-containing compounds in hydrodynamic conditions.

Conclusion
1. The obtained theoretical equation reflects the relationship of the initial water quality in the form of dissociated molecules, the exchange capacity of the load and the fluid flow hydrodynamics during filtration.
2. This model makes it possible to predict the effect of water purification by ion exchange in hydrodynamic conditions of fluid motion.
3. The obtained model makes it possible to obtain the basic laws of ion exchange for the study of the process under experimental conditions.

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