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Mathematical modelling and improvement of ion exchange water treatment energy-saving technologies in power engineering

A A Chichirov[1*], N D Chichirova[1], A A Filimonova[1] and O E Babikov[1]

[1] Kazan state power engineering university, 51 Krasnoselskaya Street, Kazan 420066, Russian Federation

[*]corresponding author: pinpin3@yandex.ru

Abstract. A mathematical model of the ion-exchange filter regeneration process of a wastewater treatment plant is presented in this paper. In the model the ionite filter is considered as a chemical through-passage reactor with bulk material, final length, periodical action in a stationary mode. The one-parameter diffusion model used for the description with the Dankwerts boundary conditions makes it possible to calculate with sufficient accuracy the output concentration curves of the reagent and products.

1. Introduction

In thermal and electric energy production systems (primarily at heat and power plants), wastewater treatment plants (WTP) are the main source of wastewater, which are highly mineralized, energy- and resource-consuming (reagents). Various technologies are proposed and implemented at many heat and power plants, which allow to reduce reagents unit cost and wastewater volumes. First of all, this refers to the most widespread ionite methods. Such technologies as block arrangement of multistage wastewater treatment plants filters, block-counter-current regeneration, counter-current regeneration, treated regeneration solution reuse are introduced. At the same time, regime characteristics and constructive features were chosen empirically, which doesn't guarantee optimal solutions.

The purpose of the work is mathematical modeling of the ionite filters regeneration process based on the of fundamental laws of physics, chemistry, hydrodynamics.

2. Theory

The ionite filter is similar to a cylinder loaded with a fixed solid ionite, in which the flow of water and reagent solution transfers along one axis (z) and the exchange chemical reaction of the reagent for chemo-sorbed ions (product) proceeds. Therefore, it is logical to consider it as a flow chemical reactor, and use the one-parameter diffusion model to describe it [1,2].

The equation of the component mass conservation according to convective and diffusion flows and chemical reactions in the flow reactor (Figure 1) has the form:
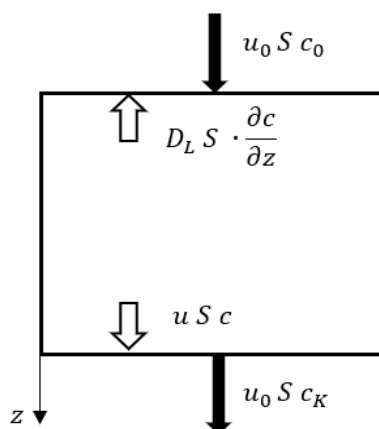
$$\frac{\partial c}{\partial \tau} = D_L \cdot \frac{\partial^2 c}{\partial z^2} - u_0 \frac{\partial c}{\partial z} - w_r \,, \tag{1}$$

where D_L – longitudinal diffusion coefficient or longitudinal mixing coefficient,

w_r – the rate of heterogeneous ion exchange chemical reaction,

u_0 – linear flow rate through the filter.

Figure 1. Flow diagram at boundaries and within the filter. S – the filter area, c_0 and c_K – the initial and final concentrations.

To solve the diffusion model equation (1), it is necessary to make reasonable assumptions and simplifications. Direct reagent exchange chemical reaction to the product should formally be recorded as:

$$w_r = \frac{dc}{d\tau} = k \, c_R \tilde{c}_P \ , \tag{2}$$

where $\tilde{c}_P$ – concentration (content, fraction) of the product in the solid phase of ionite. According to the laws of chemical thermodynamics, in the case when a solid is involved in the reaction, its concentration is taken equal to one. Therefore, it is possible to record:

$$w_r = \frac{dc}{d\tau} = Kc_R , \tag{3}$$

where the constant K has a more complex meaning than the homogeneous reaction speed constant.

In practice [3], we should return to the dimensionless form of the basic equation record (1), using new variables for coordinates $L = \frac{z}{l_0}$, for time $\theta = \frac{\tau}{\bar{\tau}}$, and for the concentration $C = \frac{c}{c_0}$. Where the characteristic time is $\bar{\tau} = \frac{l_0}{u_0}$. We should multiply all parts of the equation (1) by l_0 and divide by u_0.

As a result, we have:

$$\frac{\partial C}{\partial \theta} = \frac{D_L}{u_0 l_0} \cdot \frac{\partial^2 C}{\partial L^2} - \frac{\partial C}{\partial L} - K\bar{\tau}C . \tag{4}$$

It is accepted that the multiplier $\frac{u_0 \cdot l_0}{D_L}$ is the dimensionless Peclet (Pe) criterion of similarity.

The equation (4) will be written as:

$$\frac{1}{Pe} \cdot \frac{\partial^2 C}{\partial L^2} - \frac{\partial C}{\partial L} - K\bar{\tau}C = \frac{\partial C}{\partial \theta} . \tag{5}$$

For the product (P) there must be a similar equation. To simplify the problem, we accept that the chemical reaction is the equivalent product substitution for the reagent in the ionite solid phase and there is no specific reagent accumulation (sorption). Then the sum of reagent substance (the number of

equivalents moles (N_R) and product (N_P) in the liquid phase will be equal to the quantity of reagent entered: $N_{R,0} = N_R + N_P$.

Using the number of equivalents moles as the substance quantity and the concentration of equivalents moles as the substance concentration – it is possible to get rid of the reagent ions charges and product and to simplify writing of equation

To solve the equation (4) we should formulate restrictions. We consider that ion exchange filter in the regeneration stage is:

1) Liquid phase filled with solid grains

2) In stationary mode is flow-through ($u_0 = const$)

3) Chemical reactor of the final length

4) Periodic action (consecutive end-time actions)

5) With the first-order irreversible heterogeneous chemical reaction

6) Isothermic

7) With ideal flow structure ($D_L = const$)

The boundary conditions for this case are set from the mass balance condition at the filter boundaries (Danckwerts conditions). At the filter entrance, the flows sum of the substance coming to the boundary ($L = 0$) must be equal to the flow of the substance coming from the boundary ($L = 0 + 0$). In the dimensionless form of the record we have:

$$c_0 - c_{0+0} + \left(\frac{1}{Pe} \cdot \frac{dc}{dL} \right)_{0+0} = 0 , \text{L=0} \tag{6}$$

At the final length filter outlet, it is assumed that the reaction flow is interrupted with a reaction stop (loading the ionite only inside the filter):

$$\left(\frac{dc}{dL} \right)_{1-0} = 0 , \text{L=1} \tag{7}$$

To solve the obtaining problem of the response function (output concentration curves $c(\theta)$) at the outlet of the filter in the original equation (5), the coordinate is fixed at $L = 1$ and the only variable remains time (θ).

In addition, since the case of the periodic action reactor with an obvious sharp change in conditions at the borders, it is advisable to zoning or, in terms of time, splitting the backwashing process into stages.

Two stages are visible for the regeneration process:

1 – regeneration is the income of a permanent concentration $C_{R,0} = 1$ reagent solution ($C_R = 0$) to the filter, in a dimensionless form, at a constant speed u_0 at time θ_R .

2 – reaction mass is pushed out by water with concentration ($C_R = 0$), at a constant speed (u_0) for a period of time $\theta > \theta_R$.

For all the assumptions and limitations made, equation (5) can be solved. As a result of analytical integration, the solution of equation (5) is obtained in the form of the equations system, including model parameters taking into account the exponential dependence of the response function on time. The equations system $C = \exp(\theta, \theta_R, \theta_P, Pe, K, \overline{\tau})$ is a mathematical model of the whole process: regeneration - displacement (washing) of the filter:

θ_0 – zero point of time, corresponds to the start of reagent solution passing through filter,

θ_L – the time when the product and/or reagent is released from the filter ($L = 1$). Defined by the criterion Pe : $\theta_L = \dfrac{\tau_L}{\overline{\tau}} = \dfrac{Pe}{(Pe+1)}$,

θ_R – reagent solution skip time,

θ_P – the form of expression of the number of product equivalents in the ion filter. Determined from the ratio: $\dfrac{N_P}{N_R} = \dfrac{\theta_P}{\theta_R}$,

$\theta_{\max R}$ – the time the reagent concentration at the output of the maximum value has been reached,

$\theta_{\max R} = \dfrac{Pe}{Pe+1} + \theta_R$. Indicates the transition from regeneration to the wipe phase (washing),

$C(\theta_{\max R})$ – maximum reagent output concentration, $C(\theta_{\max R}) = 1 - \exp(-(Pe+1)\cdot(\theta_R - \theta_P))$,

$\theta_{\max P}$ – the time when the product concentration reaches the maximum value at the filter outlet,

$\theta_{\max P} = \dfrac{\theta_P \cdot (Pe+1)}{\langle k\,\overline{\tau}\rangle + Pe}$,

$\langle k\,\overline{\tau}\rangle$ – normalized indicator of heterogeneous reaction rate, $\langle k\,\overline{\tau}\rangle = \dfrac{k\,\overline{\tau}}{k\,\overline{\tau}+1}$,

$C_{\max P}$ – maximum output product concentration, $C_{\max P} = 1 - \exp\left(-\langle k\,\overline{\tau}\rangle \cdot (Pe+1)\cdot \theta_{\max P}\right)$.

In Figure 2 the calculated concentration curves of the reagent and product at different criteria Pe are presented, allowing to visualize the characteristics of the model.
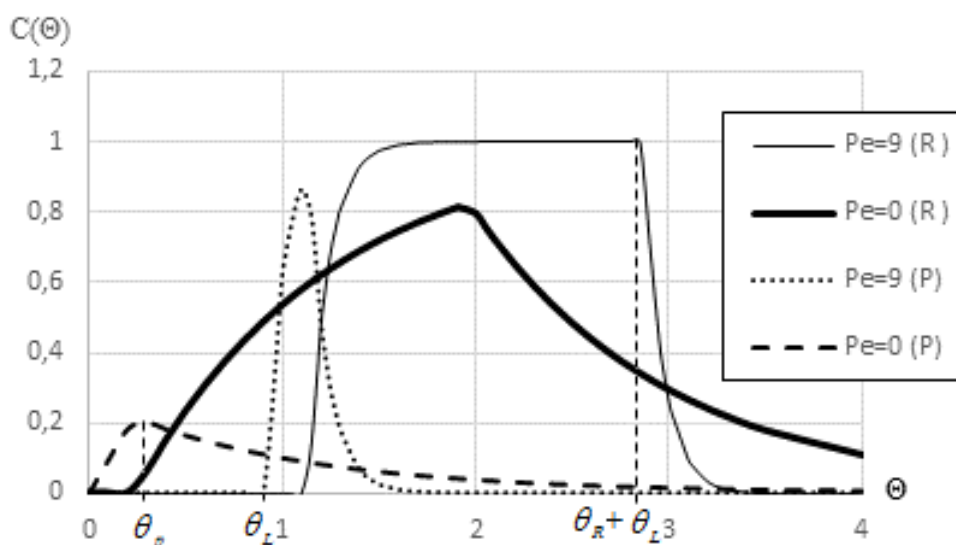
**Figure 2.** Reagent (Re) and Product (P) concentration output curves for different Pe numbers, under the condition that $k\,\overline{\tau} \to \infty, \dfrac{\theta_P}{\theta_R} = 0.1$.

3. Comparison of theoretical (calculated) values with experimental data

Comparison of theoretical (calculated) output concentrations values with experimental data obtained during regeneration of industrial ion filter shows good accordance. In Figure 3 the output concentration curves of alkali, silicon dioxide (product 1), organic substances (product 2) at regeneration of the second stage anionite filter of chemical water purification-2 on the Nizhnekamsk HPP-1 by 2.6% alkaline regeneration solution with flow rate $u_0 = 7.8$ m/h, feed time (τ_R) 60 min. Filter diameter $(D_F = 3m)$, filter path length ($l_0 = 3m$). Download – high-base anionite. Relative equivalents amount of desorbiated silicon dioxide $\dfrac{N_{SiO_2}}{N_{NaOH}} = 0.04$, organic substances – 0.004.

The parameters of the real process were calculated according to the diffusion model. The value of the criterion Pe = 1.5. This means that in a filter with structural characteristics (D_F, l_0), the volume of ionite loading, the diameter of the ionite grain) and the regime characteristics (u_0, c_{NaOH}, τ_R) the implemented hydrodynamic mode is between ideal displacement and ideal mixing. In almost the midpoint. Apparent rate constant desorption SiO_2 18000 sec^{-1}. Half-reaction time (desorption time of half sorbed SiO_2) 8.5 min. Therefore, the reaction proceeds at an average speed, but sufficient to separate and backwash most (but not 100%) of the filter. For organic substances K = 0.22, half-reaction time 3.5 hours. That is, during the regeneration, only a part of the organic substances is removed, which explains the ionite "poisoning".
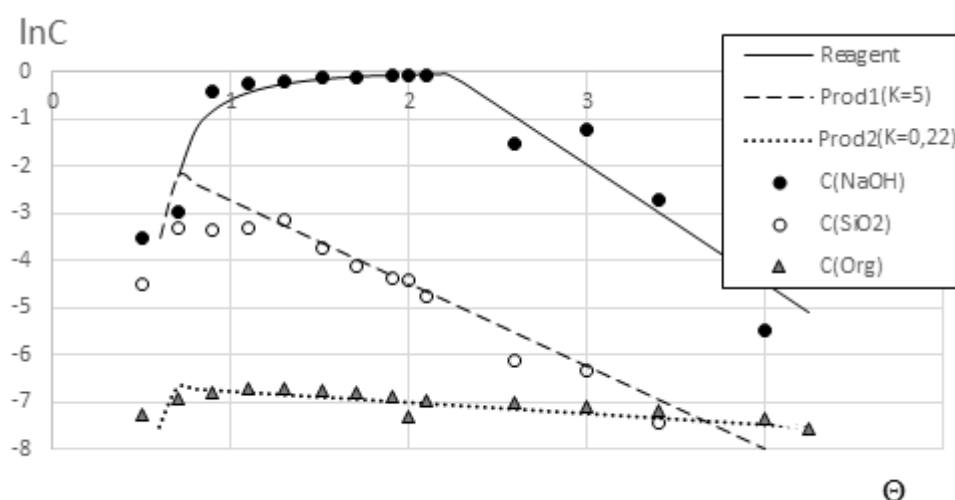
Figure 3. Output concentrations of reagent $(NaOH)$, product 1 (SiO_2), product 2 (organic substances) at regeneration of the second stage anionite filter of chemical water purification-2 on the Nizhnekamsk HPP-1. Solid lines – the diffusion model calculation.

4. Conclusions

The obtained data indicates that the implemented regeneration mode and the filter design do not achieve the ideal displacement mode, at which the theoretically possible minimum reagent flow, minimum wastewater volume and maximum product output are possible. Consequently, it is possible to carry out scientific research to improve both the design and the technology of regeneration.

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