Interpolation of Boundary Condition at Time-Interval of Unknown Lenghth for the Problem of Convective Diffusion in a Three-Layered Water Filter

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Abstract— **On the basis of mathematical model of convective diffusion in a three-layered filter it is formulated a contact-initial-boundary value problem for description of mass transfer of pollution accompanying the sorption processes. It is proposed the algorithm for establishing the estimation of values of sought function (concentration of pollution) at the lower boundary of the filter on the basis of the interpolation of experimental data. It is taken into account that the right end of the interpolation segment is unknown. It is determined the exact solutions of contact-initial-boundary value problems of mass transfer with provision for both diffusive and convective mechanisms of transfer as well as sorption processes, which is based on integral transformations over space variables in the contacting regions. Is it designed software and established regularities of convective diffusion process in the three-layered filter.**

Keywords— mathematical modelling; simulation; convective diffusion; three-layered water filter; integral transformation; interpolation; boundary condition

I. INTRODUCTION

At present, the problem of water purification to the state of drinking water, as well as the purification of domestic and industrial sewage for secondary use, occupies an important place. One of the varieties of such filters is the bulk filters [6, 7], consisting of granular congestion of various filtration properties.

We have proposed an approach to the mathematical description of the processes of convective diffusion of impurity particles, which are accompanied by their sorption onto a skeleton, in a multi-phase multicomponent body, consisting of the steps:

- construction of the mathematical model in a linearized version; on this basis the formulation of the contact-initial-boundary value problem, taking into account the conditions of non-ideal contact for the concentration of pollution, which is carried over with a convective moving solution;
- obtaining the exact analytical solution of the formulated problem by the method of integral transformations separately in different porous layers of the filter;
- simulation of the obtained solutions which contains the following sub-steps:
    - construction of algorithms for each structural part of the solution of the contact-initial-boundary value problem for numerical analysis of
        - concentrations of pollutants in the water porous solution in both filter layers and the corresponding mass fluxes using the well-known numerical integration method, namely Newton-Kotes closed type for 7 and 10;
        - the concentration of pollution particles sorbed on the skeleton of the filter, for which we have developed the method of numerical integration of a double integral with variable upper limits;
        - finding the saturation time of the filter based on the algorithm proposed by us for solving a nonlinear functional equation on an interval of unknown length;
- develop software and use it to analyze the obtained results.

At the same the problem of imposing a boundary condition on the lower boundary of the water filter remains unresolved. In this work we propose to use the procedure of interpolation of experimental data at the lower boundary of the filter with taken into account that the right end of the interpolation segment is unknown.

II. INITIAL-BOUNDARY VALUE PROBLEM OF CONVECTIVE DIFFUSION IN A THREE-LAYERED WATER FILTER

When formulating the reference relationships of the transport model for pollution in a three-layered filter (Fig. 1), we assume that an arbitrary area of each layer consists of a skeleton and a water solution that fills the porous space. We accept that in the filtration process, the skeleton is not deformed, and the porosity remains constant (we do not take into account the changes associated with the sorption of the impurity substance). The water solution is two-component and consists of particles of both water and the polluting substance. The pollution particles are in two states, namely in the convective moving solution and on the surface of the skeleton [2,3].

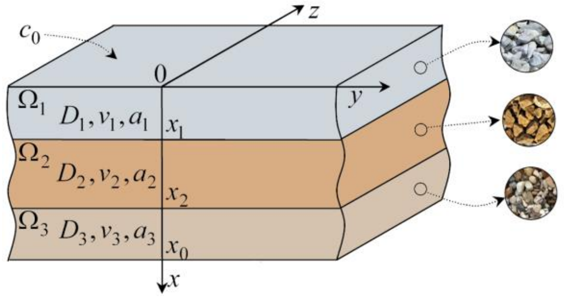

Figure 1. Three-layered filter in which particles of pollution migrate

In the case of one-dimensional (vertical) convective diffusion the mass transfer process of admixture is described by the following sets of equations:

in the domain Ω_1 ($x \in \Omega_1$), $\Omega_1 =]0; x_1[$:

$$\frac{\partial c_1^{(1)}(t,x)}{\partial t} = d_1 \frac{\partial^2 c_1^{(1)}(t,x)}{\partial x^2} - v_1 \frac{\partial c_1^{(1)}(t,x)}{\partial x} - a_1 c_1^{(1)}(t,x), \quad (1)$$

$$\frac{\partial c_2^{(1)}(t,x)}{\partial t} = a_1 c_1^{(1)}(t,x);$$

in the domain Ω_2 ($x \in \Omega_2$), $\Omega_2 =]x_1; x_2[$:

$$\frac{\partial c_1^{(2)}(t,x)}{\partial t} = d_2 \frac{\partial^2 c_1^{(2)}(t,x)}{\partial x^2} - v_2 \frac{\partial c_1^{(2)}(t,x)}{\partial x} - a_2 c_1^{(2)}(t,x), \quad (2)$$

$$\frac{\partial c_2^{(2)}(t,x)}{\partial t} = a_2 c_1^{(2)}(t,x);$$

in the domain Ω_3 ($x \in \Omega_3$), $\Omega_3 =]x_2; x_0[$:

$$\frac{\partial c_1^{(3)}(t,x)}{\partial t} = d_3 \frac{\partial^2 c_1^{(3)}(t,x)}{\partial x^2} - v_3 \frac{\partial c_1^{(3)}(t,x)}{\partial x} - a_3 c_1^{(3)}(t,x), \quad (3)$$

$$\frac{\partial c_2^{(3)}(t,x)}{\partial t} = a_3 c_1^{(3)}(t,x).$$

where $c_i^{(j)}(t,x)$ is the concentration of impurities (the lower index indicates the state of the particles so as $i = 1$ corresponds to the water solution and $i = 2$ corresponds to the surface of the skeleton; the upper index indicates the number of the sublayer of the filter; d_j and v_j ($j = \overline{1,3}$) are the coefficients of admixture diffusion and convective transport in the layer j, a_j ($j = \overline{1,3}$) are the coefficients of intensity of sorption.

At the boundary of the contact of the layers, it is satisfied the conditions of the equality of chemical potentials and total mass fluxes, which we write in the form [2]:

at the first contact boundary $x = x_1$

$$\lambda^{(1)} c_1^{(1)}(t,x)\Big|_{x=x_1} = c_1^{(2)}(t,x)\Big|_{x=x_1}, \quad (4)$$

$$d_1 \frac{\partial c_1^{(1)}}{\partial x} - v_1 c_1^{(1)}\Bigg|_{x=x_1} = d_2 \frac{\partial c_1^{(2)}}{\partial x} - v_2 c_1^{(2)}\Bigg|_{x=x_1};$$

at the second contact boundary $x = x_2$

$$\lambda^{(2)} c_1^{(2)}(t,x)\Big|_{x=x_2} = c_1^{(3)}(t,x)\Big|_{x=x_2}; \quad (5)$$

$$d_2 \frac{\partial c_1^{(2)}}{\partial x} - v_2 c_1^{(2)}\Bigg|_{x=x_2} = d_3 \frac{\partial c_1^{(3)}}{\partial x} - v_3 c_1^{(3)}\Bigg|_{x=x_2}$$

where $\lambda = \lambda_1 / \lambda_2$ is the ratio of the coefficients of concentration ratio of coefficients dependence of chemical potentials in the states 1 and 2, which determines the value of jump of concentration function at the contact boundary.

We accept that in the initial moment the particles of pollution are absent in the filter:

$$c_1^{(j)}(t,x)\Big|_{t=0} = c_2^{(j)}(t,x)\Big|_{t=0} = 0 \qquad j = \overline{1,3} \quad (6)$$

We assume that the value of constant admixture concentration is known at the upper surface of the body:

$$c_1^{(1)}(t,x)\Big|_{x=0} = c_0 \equiv \text{const}. \quad (7)$$

At the lower surface of the body, generally speaking, the values of both the concentration of pollution and the diffusion flux of the substance are unknown. To determine the value of the sought function, we propose the following algorithm.

III. Estimation of Boundary Condition for Concentration at the Lower Surface of the Body

Note that the function of particle concentration $F(t)$ at the boundary of the water filter $x = x_0$ is a continuous or piecewise-continuous function of a time variable, that is, it belongs to space $PC[0;T]$, $t < T < \infty$. With that, for small times it equals zero (which is explained by the need for some time for the admixture to pass through the filter and the filter's effective operation). A schematic behavior of the function $F(t)$ can be shown as follows

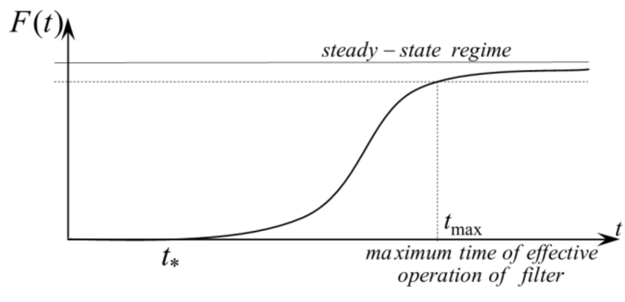

Figure 2. Schematic behavior of the function $F(t)$

Let it is known (or we can measure) the value of the concentration function at the lower boundary $x = x_0$ at certain points in time:

t	t_1	t_2	t_3	t_4	t_5	…	t_n
$F(t)$	0	0	0	$F(t_4)$	$F(t_5)$	…	$F(t_n)$

In this case $t_* = t_3$ (see Fig. 2).

Remark also, if several series of measurements were carried out at the same time moments, then the values of the function $F(t)$ at points t_j are determined as averaged values (Fig. 3):

$$F(t_j)=\frac{1}{K_j}\sum_{i=1}^{K_j}F^{(i)}(t_j), \quad j=1,...,n,$$

where i is the experiment series number, $i=1,...,K_j$, K_j is the number of measurements in the point t_j.

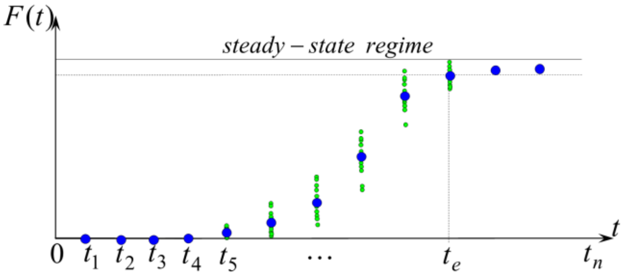

Figure 3. Schematic representation of experiment series and corresponding averaged values

Stage 1. By having a set of experimental (measured) data, we can construct an interpolation function. Here we use the Lagrange form to interpolate to a segment $[0,t_e]$ in the form of a polynomial [4]:

$$F(t)=\sum_{k=0}^{n}F(t_k)\frac{(t-t_0)(t-t_1)\ldots(t-t_n)}{(t_k-t_0)(t_k-t_1)\ldots(t_k-t_n)}. \quad (8)$$

Let us note that, in fact, the right end of interpolation segment (the point t_e) is unknown. Accordingly, the moment of stop of the experimental series is unknown. Considering the purpose of the investigation, i.e. establishing the parameters of the filter operation, we use the existence of a time of saturation of the filter, i.e. loss of sorption capacity. After the moment of saturation t_p, which is also unknown, only the process of convective diffusion of pollution particles occurs in the body, and the process of cleaning the contaminated solution is stopped. Accordingly, we should stop the experimental measurements and shut down the filter.

Stage 2. To determine upper-bound estimate of the admixture concentration function at the lower boundary of the body and to determine the estimation time of saturation, we solve the simplified convective diffusion problem in the three-layer body under the contact, initial and boundary conditions (4)-(7) and the boundary condition on the flux at the boundary $x=x_0$ proposed by A. Bomba and A. Safonik [1]. Namely,

in the domain $\Omega_1=]0;x_1[$

$$\frac{\partial c_{1est}^{(1)}(t,x)}{\partial t}=d_1\frac{\partial^2 c_{1est}^{(1)}(t,x)}{\partial x^2}-v_1\frac{\partial c_{1est}^{(1)}(t,x)}{\partial x}, \quad (9)$$

in the domain $\Omega_2=]x_1;x_2[$:

$$\frac{\partial c_{1est}^{(2)}(t,x)}{\partial t}=d_2\frac{\partial^2 c_{1est}^{(2)}(t,x)}{\partial x^2}-v_2\frac{\partial c_{1est}^{(2)}(t,x)}{\partial x}, \quad (10)$$

in the domain $\Omega_3=]x_2;x_0[$:

$$\frac{\partial c_{1est}^{(3)}(t,x)}{\partial t}=d_3\frac{\partial^2 c_{1est}^{(3)}(t,x)}{\partial x^2}-v_3\frac{\partial c_{1est}^{(3)}(t,x)}{\partial x} \quad (11)$$

under the contact conditions (4) and (5), the initial conditions (6) and the boundary condition (7) at the upper surface of the filter.

At the lower surfaces of the body, the constant value of the diffusion flux of pollution particles is supported

$$\left.\frac{\partial c_{1est}^{(3)}(t,x)}{\partial x}\right|_{x=x_0}=0 \quad (12)$$

Stage 3 of determination of t_p, i.e. steady-state output (determination of concentration with certain accuracy). Let the difference between concentrations at the current time t and the saturation time t_p be less than the preset number ε

$$\left|c_{1est}^{(3)}(t,x_0)-c_{1est}^{(3)}(t_p,x_0)\right|<\varepsilon.$$

Then, solving this inequality, we find the saturation time t_p.

Stage 4. Construction of the interpolation polynomial (8) on the segment $[0,t_p]$. So we obtain the approximate function $F(t,t_p)$, where $t_n=t_p$.

Then the boundary condition at the lower surface of the body takes the form

$$\left.c_1^{(3)}(t,x)\right|_{x=x_0}=F(t,t_p). \quad (13)$$

IV. Solving the formulated contact-initial-boundery value problem

Note that the function of particle concentration $F(t)$ at the boundary of the water filter $x=x_0$ is a continuous or piecewise-continuous function of a time variable, that is, it belongs to space $PC[0;T]$, $t<T<\infty$. With that, for small times it equals zero (which is explained by the need for

We redefine the sought functions at the contact boundaries

$$\lambda^{(1)}c_1^{(1)}(t,x)\Big|_{x=x_1}=c_1^{(2)}(t,x)\Big|_{x=x_1}=g_1(t,x_1)\equiv g_1(t) \quad (14)$$

$$\lambda^{(2)}c_1^{(2)}(t,x)\Big|_{x=x_2}=c_1^{(3)}(t,x)\Big|_{x=x_2}=g_2(t,x_1)\equiv g_2(t) \quad (15)$$

On the strength of (14) and (15) we write the concentrations at the contact boundaries per functions $g_1(t,x_1)$ and $g_2(t,x_2)$

$$c_1^{(1)}(t,x)\Big|_{x=x_1}=\frac{1}{\lambda^{(1)}}g_1(t);\; c_1^{(2)}(t,x)\Big|_{x=x_1}=g_1(t);$$

$$c_1^{(2)}(t,x)\Big|_{x=x_2}=\frac{1}{\lambda^{(2)}}g_2(t);\; c_1^{(3)}(t,x)\Big|_{x=x_2}=g_2(t);$$

Then we perform integral transformations over the variable x separately in the domains Ω_1, Ω_2 and Ω_3.

In the domain $\Omega_1=]0;x_1[$ we apply the following finite integral transformation [5]

$$\bar{c}_1(t,n)=\int_0^{x_1}c_1^{(1)}(t,x)\exp\left(\frac{-v_1x}{2d_1}\right)\sin(y_nx)dx,\; y_n=\frac{n\pi}{x_1}$$

with inverse transform

$$c_1^{(1)}(t,x)=\frac{2}{x_1}\exp\left(\frac{v_1 x}{2d_1}\right)\sum_{n=1}^{\infty}\bar{c}_1(t,n)\sin(y_n x)\,. \quad (16)$$

In the domain $\Omega_2=]x_1;x_2[$ we apply the finite integral transformation with shift [5]

$$\bar{c}_2(t,m)=\int_{x_1}^{x_2}c_1^{(2)}(t,x)\exp\left(\frac{-v_2(x-x_1)}{2d_2}\right)\sin(y_m(x-x_1))dx\,,$$

$$y_m=\frac{m\pi}{(x_2-x_1)}\,.$$

For this transformation we obtain the formula of inverse transformation in the form

$$c_1^{(2)}(t,x)=\frac{2}{x_2-x_1}\exp\left(\frac{v_1(x-x_1)}{2d_2}\right)\sum_{m=1}^{\infty}\bar{c}_2(t,m)\sin(y_m(x-x_1))\,. \quad (17)$$

In solving the contact-initial-boundary value problem (9)-(11) with conditions (4)-(7) and (12) in the third sublayer $\Omega_3=]x_2;x_0[$, the finite integral transformation with shift is applied [5]

$$\bar{c}_3(t,k)=\int_{x_2}^{x_0}c_1^{(3)}(t,x)\exp\left(\frac{-v_3(x-x_2)}{2d_3}\right)\sin(y_k(x-x_2))dx\,,$$

$$y_k=\sqrt{\lambda_k^2-\frac{v_3^2}{4d_3^2}}\,,\ \lambda_k^2\sim\left(\frac{\pi k}{x_0-x_2}\right)^2$$

$$c_1^{(3)}(t,x)=2\exp\left(\frac{v_3(x-x_2)}{2d_3}\right)\sum_{k=1}^{\infty}\frac{\bar{c}_3(t,k)\sin(y_k(x-x_2))}{x_0-x_2+\dfrac{v_3}{2d_3\lambda_k^2}}\,. \quad (18)$$

After performing the inverse transformations (16)-(18) of the corresponding expressions, the result written in the points $x=x_1$ and $x=x_2$ is substituted in relations (6) and (7). Then we obtain the set of two integral equations

$$d_1\frac{2}{x_1}\exp\left(\frac{v_1x_1}{2d_1}\right)\sum_{n=1}^{\infty}e^{-\left(a_1+y_n^2d_1+\frac{v_1^2}{4d_1}\right)t}\times$$

$$\int_0^t e^{-\left(a_1+y_n^2d_1+\frac{v_1^2}{4d_1}\right)t'}\left(d_1y_nc_0+\frac{d_1y_n}{\lambda^{(1)}}e^{-\left(\frac{v_1x}{2d_1}\right)}g_1(t)(-1)^{n+1}\right)dt'y_n(-1)^n=$$

$$=d_2\frac{2}{x_2-x_1}\sum_{m=1}^{\infty}e^{-\left(a_2+y_m^2d_2+\frac{v_2^2}{4d_2}\right)t}\int_0^t e^{-\left(a_2+y_m^2d_2+\frac{v_2^2}{4d_2}\right)t'}\times$$

$$\times\left(d_2y_mg_1(t')+d_2y_m\frac{(-1)^{m+1}}{\lambda^{(2)}}g_2(t')\right)dt'y_m\,;$$

$$d_2\frac{2}{x_2-x_1}\exp\left(\frac{v_2(x_2-x_1)}{2d_2}\right)\sum_{m=1}^{\infty}e^{-\left(a_2+y_m^2d_2+\frac{v_2^2}{4d_2}\right)t}\int_0^t e^{-\left(a_2+y_m^2d_2+\frac{v_2^2}{4d_2}\right)t'}\times$$

$$\times\left(d_2y_mg_1(t')+d_2y_m\frac{(-1)^{m+1}}{\lambda^{(2)}}g_2(t')\right)dt'y_m(-1)^m=$$

$$=d_3\frac{2}{x_0-x_2}\sum_{k=1}^{\infty}e^{-\left(a_3+y_k^2d_3+\frac{v_3^2}{4d_3}\right)t}\times$$

$$\times\int_0^t e^{-\left(a_3+y_k^2d_3+\frac{v_3^2}{4d_3}\right)t'}F(t',t_p)\big(d_3y_kg_1(t')\big)dt'y_k\,.$$

We solve the obtained set of equation with respect to the functions $g_1(t')$ and $g_2(t')$. In with way we obtain expressions for the concentrations of the pollution particles in water solution in three sublayers of the filter.

To find the concentration of particles sorbed on the skeleton of the filter, we use the second equations of the reference sets (1)-(3). So we have

$$c_2^{(j)}(t,x)=a_j\int_0^t c_1^{(j)}(t',x)dt'\,,\ j=\overline{1,3}\,. \quad (19)$$

For numerical analysis of (19) we work up the method of double integration with variable upper limits on the basis of the quadratures in the inner region of integration and the triangulation split along the variable limit $t''=t'$ (where t'' is the variable of inner integral).

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