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Задача масопереносу з частково невідомими граничними значеннями концентрації

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The problem of mass transfer with partially unknown limits values of concentration

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У статті розглядається задача масопереносу з частково невідомими граничними значеннями концентрації. Для представленої задачі, що має єдиний розв'язок, приведено сукупність оцінок різницевих аналогів операторів та умови стійкості відповідної неоднорідної різницевої схеми. Отримано, що використання регуляризуючого алгоритму на основі узагальненого принципу нев'язки дає рішення екстремальної задачі, що враховує неповну визначеність значень концентрації.
Ключові слова: різницева схема, сіткова область, параметр регуляризації, різницевий оператор, функціонал.

In this paper we consider the problem of mass transfer with partially unknown limits values of concentration. It is indicated that the presented the initial-boundary value problem has unique solution. A set of estimates for the difference approximations of operators is presented. For the scheme in the canonical form obtained estimates for its operators too. It is shown with the help of locally one-dimensional schemes the stability of the resulting inhomogeneous difference scheme and the conditions for its stability are presented. It is obtained that the using of a regularizing algorithm on the basis of the generalized discrepancy principle gives the solution of the corresponding extremum problem. The solution of this task exists and is unique. It takes into account incomplete certainty of concentration values.
Key Words: difference scheme, grid region, regularization parameter, difference operator, functional.

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Introduction

Usually getting solution of the problem of determination the distribution of the Cs^{137} radionuclide in the area of soil aeration in the system of hydro technical shafts-terraces provides for known values on the limits of area. In practice, exact values of the limit values concentration are impossible to get accurately. In addition, the initial values are measured only in limited number of points. Therefore, we can calculate the distribution of the radionuclide concentration only approximately.

Accounting for this situation when modeling the processes of mass transfer in a limited area are takes place can give the using of a regularizing algorithm on the basis of the generalized discrepancy principle.

The model of mass transfer and the existence of unique solution

Having in mind the construction of surfaces shafts-terraces we investigated two-dimensional model of mass transfer:

$$Zu \equiv \frac{\partial u}{\partial t} + Lu \equiv \frac{\partial u}{\partial t} - \sum_{i=1}^{2} \frac{\partial}{\partial x_i}\left(D(x)\frac{\partial u}{\partial x_i}\right) + \sum_{i=1}^{2} V\frac{\partial u}{\partial x_i} =$$
$$= f(x,t) \equiv -\lambda u_0 \varphi(x)\delta(t-0),$$
$$\left. \left(-\sum_{i=1}^{2} D(x)\frac{\partial u}{\partial x_i} + Vu \right)\right|_{x\in\Gamma} = k(\Gamma)c_0 q_0(x), \quad t\in[0,T]$$
$$\left. \left(-\sum_{i=1}^{2} D(x)\frac{\partial u}{\partial x_i} + Vu \right)\right|_{x\in\partial\Omega\setminus\Gamma} = 0, \quad t\in[0,T].$$
$$u(x,0)=0, \quad x\in\Omega,$$

in the bounded area $Q=\Omega\times(0\le t\le T),\ \Omega\subset R^2$ with piecewise smooth surface $\partial\Omega$, λ– half-decomposition factor, $\varphi(x_1,x_2)$ – the function describing the surface of the shaft-terrace Г, $\varphi(x_1,x_2)\in L_2(\Omega)$, u_0 – surface contamination, $u(x,t)$ – the concentration of the substance in the point $x=(x_1,x_2)$ at the moment *t*, $u(x,t)$ is twice continuously differentiated by *x* on Ω and continuously differentiated by *t* on $[0,T]$.

Let's denote

$$Au=-\sum_{i=1}^{2}\frac{\partial}{\partial x_i}\left(D(x)\frac{\partial u}{\partial x_i}\right),$$

$$Bu=\sum_{i=1}^{2}V\frac{\partial u}{\partial x_i}.$$

The operator Au is elliptical in closed area $x\in\Omega+\partial\Omega$, $D(x)$ – continuously differentiable in the closed area $\overline{Q}$, an integral and limited in the relevant area, V – positive constant, $k(\Gamma)=k\cdot\cos(\alpha(\Gamma))$, k – the coefficient of conductivity (absorption) for surface, $\alpha(\Gamma)$ – the slope of the segment of terraces, q_0 – the flow of water coming from atmospheric precipitation with a concentration of the substance c_0.

In [1, 2] shows the existence of a unique generalized solution of this problem in the space with the norm

$$\|u\|_H^2=\int_Q\left(u_t^2+\sum_{i=1}^{2}\left(\frac{\partial u}{\partial x_i}\right)^2\right)dQ.$$

Using results of these works has been obtained

$$\frac{d}{dt}\|u\|_Q\le\|f\|_Q+\delta\|u\|_H,$$

where $\|u\|_Q^2=\int_Q u^2dQ$ - the norm in $L_2(Q)$.

The difference approximations

In [3] was substantiated splitting method for difference approximations of this task of mass transfer. Used difference operators gives the opportunity to go to locally one-dimensional if necessary.

In Ω we used uniform for all variables difference grid $\omega_h=\{x\,|\,x=(x_1,x_2),\ x_1=i_1h_1,\ x_2=i_2h_2, h_1=x_{i_1+1}-x_{i_1}, h_2=x_{i_2+1}-x_{i_2}, i_1=\overline{1,N_1-1},\ i_2=\overline{1,N_2-1}\}$ in which ω - the set of internal nodes, $\partial\omega$ - the set of external nodes.

Let denote the difference solution of the problem at time *t* as $y(x,t), x\in\omega\cup\partial\omega, t>0$. For grid functions that satisfy the initial (in $D(L)$) and boundary conditions (on $\partial\omega$), we define a Hilbert space $\overline{H}$, the scalar product and the norm in which are $(y,v)=\sum_{x\in\omega}yvh_1h_2$, $\|y\|=\sqrt{(y,y)}$.

To the operator *A* on the set of functions $y\in\overline{H}$ we put in line the difference operator $Ay=-\sum_{i=1}^{2}\frac{\partial}{\partial x_i}\left(Dy_{x_i}\right)_{\bar{x}_i}$, the operator *B* - the difference operator $By=\sum_{i=1}^{2}Vy_{\hat{x}_i}$.

Under conditions of the second order of approximation we take difference operator *A* in the following form

$$Ay=-\sum_{i=1}^{2}\frac{\partial}{\partial x_i}\left(Dy_{x_i}\right)_{\bar{x}_i}=-\sum_{j=1}^{2}\frac{1}{h_j}\left(a_{i_j+1}y_{x_{i_j}}-a_{i_j}y_{x_{i_j-1}}\right),$$

where

$$\frac{a_{i_j+1}+a_{i_j}}{2}=D_{i_j}+O(h_j^2),$$

(i.e. $a_{i_j}=\frac{D_{i_j}+D_{i_j-1}}{2}$, $j=1,2,\ i_j=\overline{1,N_j}$ [4]).

Taking into account the previously obtained estimates for norms of *A* and *B* operators are obtained the following estimates:

$$(By,y)\le c_1\|y\|^2,\ \|By\|^2\le\frac{8V^2}{h^2_{\min}}\|y\|^2,$$

$$(Ay,y)\le c_2\|y\|^2,\ \|Ay\|^2\le\frac{64D_{\max}}{h^2_{\min}}\|y\|^2.$$

Difference Scheme

After space discretization an operator-difference scheme is obtained

$$\frac{dy}{dt}+Ay+By=\varphi,$$

$$y(x,0)=0,$$

$$-\sum_{i=1}^{2}Dy_{x_i}+Vy\Big|_{x\in\Gamma}=\varphi_\circ,$$

$$-\sum_{i=1}^{2}Dy_{x_i}+Vy\Big|_{x\in\partial\Omega\setminus\Gamma}=0.$$

For y^k as the difference solution at the at the moment of time $t_k=k\tau,\ \tau>0$, the two-layer difference scheme with weights has the form:

$$\frac{y^{k+1}-y^k}{\tau}+(A+B)(\sigma y^{k+1}+(1-\sigma)y^k)=\varphi^k,$$
$$x\in\omega,\ k=0,1,...$$
$$y^0(x)=0,\ x\in\omega.$$

In the canonical form, the scheme has the form

$$\underline{B}\frac{y^{k+1}-y^k}{\tau}+\underline{A}y^k=\varphi^k, x\in\omega,\ k=0,1,...,$$
$$\underline{B}=E+\sigma\tau(A+B),\ \underline{A}=A+B.$$

For operator A occurs

$$\left\|\underline{A}y\right\|^2\le 2\left(\left\|Ay\right\|^2+\left\|By\right\|^2\right)\le M_{AB}\left\|y\right\|^2,$$

where $M_{AB}=O(h_1^{-2}+h_2^{-2})$.

The operator $\underline{B}>0$ under conditions $\frac{h_1h_2}{(h_1+h_2)\tau}>\sigma V$.

To obtain numerical solutions we pass to locally one-dimensional schemes (with the same order of approximation) of the form

$$\frac{y^{k+1/2}-y^k}{\tau}=\Lambda_1(\sigma y^{k+1/2}+(1-\sigma)y^k)+\frac{1}{2}\varphi^k,$$
$$\frac{y^{k+1}-y^{k+1/2}}{\tau}=\Lambda_2(\sigma y^{k+1}+(1-\sigma)y^{k+1/2})+\frac{1}{2}\varphi^{k+1/2},$$
$$x\in\omega,\ k=0,1,...$$
$$y^0(x)=0,\ x\in\omega,$$
$$\Lambda_1=-(Dy_{x_1})_{\bar{x}_1}+Vy_{\hat{x}_1},\ \Lambda_2=-(Dy_{x_2})_{\bar{x}_2}+Vy_{\hat{x}_2}$$

($\underline{B}_j>0$ for $h_j\ge 2\frac{a_i}{V}$ for all $i,\ j=1,2$).

Moreover, under conditions $h_j\ge 2\frac{a_i}{V}$ we have that non-self-contained $\underline{A}>0$ and $\underline{B}>0$.

Therefore, as a condition of stability, may occur the condition such as $\underline{A}^{-1}\ge 0{,}5\tau\underline{B}^{-1}$ [4] or better results are obtained on the basis of the investigation of the transition operator from the time layer k to $k+1$.

Due to the use of such locally one-dimensional schemes in the future we are dealing with three-diagonal matrices.

Using of the regularizing algorithm

Consider the case where the values of concentration for certain boundary points measured with an error or missing. For the problem of describing mass transfer in a two-dimensional closed domain with linear bounded operators we construct a regularizing algorithm on the basis of the generalized discrepancy principle.

Let it is known that the error in setting the right-hand side of the equation, which includes the initial concentration values established on the basis of measurements, $\left\|\bar{f}-\varphi_\delta\right\|\le\delta$, $Z\bar{u}=\bar{f}$, $\delta>0$.

$\left\|Z-Z_h\right\|\le\varepsilon$, $\varepsilon>0$, and in grid region $\Omega_h^\tau=\{(x_{1i},x_{2j},\tau^k):\ h_1=x_{1i+1}-x_{1i},\ h_2=x_{2j+1}-x_{2j},\Delta\tau=\tau^{k+1}-\tau^k, i=\overline{0,N},\ j=\overline{0,M},\ k=\overline{0,K}\}$ constructed difference scheme for determining y_{ij}^k.

Has been introduced the functional

$$\Phi^\alpha[y]=\left\|Z_hy-\varphi_\delta\right\|^2+\alpha\left\|y\right\|^2,\alpha>0$$

and made the transition to the problem

$$\inf_{y\in D(Z_h)}\Phi^\alpha[y], \qquad (1)$$

where α – regularization parameter.

In [5] shown that this functional is strongly convex in a Hilbert space, which allows us to use gradient methods to find the solution $y_\eta^{(\alpha)}\in\overline{H}$ of the problem for fixed α.

The solution of abovementioned task exists and unique for $\alpha>0$ and linear bounded operator Z_h [5]. Moreover, the following estimate holds for it $\left\|y_\eta^{(\alpha)}\right\|^2\le\left\|\varphi_\delta\right\|/\sqrt{\alpha}$.

We assume that the of incompatibility of the equation $Zu=f$ with approximate data on a set $D(Z)\subset H$

$$\mu_\eta(\varphi_\delta,Z_h)=\inf_{y\in D(Z)}\left\|Z_hy-\varphi_\delta\right\|$$

was obtained with error $r(\eta)=\varepsilon+\delta$. Regularization parameter was elected in accordance with the principle of generalized discrepancy [5, 6]. All of this allows us the use of methods of regularization, i.e. we can numerically construct such α^* that satisfies the equation

$$\left\|Z_hy_\eta^{(\alpha)}-\varphi_\delta\right\|^2-(\delta+\varepsilon\left\|y_\eta^{(\alpha)}\right\|)^2=(\mu_\eta(\varphi_\delta,Z_h))^2 \qquad (2)$$

if $\left\|\varphi_\delta\right\|^2>\delta^2+(\mu_\eta(\varphi_\delta,Z_h))^2$ and look for such $y_\eta^{(\alpha)}$, which converge to the exact value $\bar{u}$ when tending to zero the input data error (for fixed α). If $\left\|\varphi_\delta\right\|^2\le\delta^2+(\mu_\eta(\varphi_\delta,Z_h))^2$ then approximate solution of equation $Zu=f$ we take $y_\eta=0$.

For the case $\mu_\eta(\varphi_\delta,Z_h)=0$ we can use the initial approximations for α to find the solution α^* of equation (2).

Conclusion

Using of a regularizing algorithm on the basis of the generalized discrepancy principle takes into account incomplete certainty of concentration values for the problem of describing mass transfer in a two-dimensional closed domain.

The solution of the corresponding problem exists and is unique.

The difference approximation of the problem, namely, the possibility of transition to locally one-dimensional difference schemes, gives the three-diagonal form of matrices for operators in systems of linear equations. It is very important if you need to solve these systems very many times.

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