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Approximation of Boundary Conditions of the Second and Third Types in Convection–Diffusion Equations with Applications to Environmental Hydrophysics

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Abstract
Introduction. A finite-difference scheme approximating a boundary value problem for a parabolic-type equation in a three-dimensional setting with boundary conditions of the first-third types is considered. This paper is a continuation of the authors' previous works devoted to the numerical solution of one of the pressing problems of hydrophysics in shallow marine zones — the problem of transport, deposition, and transformation of suspended matter. The approximation of this class of problems inside the domain leads to schemes converging at a rate of $O(\tau + h^2)$, where $h^2 = h_x^2 + h_y^2 + h_z^2$, h_x, h_y, h_z and τ are the steps of the difference grid along the spatial coordinates x, y, z and time, respectively. However, the case of boundary conditions requires careful treatment, since an inaccurate approximation may reduce the overall order of accuracy of the finite-difference scheme. The methods proposed by the authors for approximating boundary conditions ensure the convergence of the finite-difference scheme at the rate of $O(\tau + h^2)$.
Materials and Methods. The authors focused on approximating third-type boundary conditions (with second-type conditions considered as a particular case). The approach is based on the central difference approximation of boundary conditions on an extended grid and the elimination of suspended matter concentration values in ghost nodes (cells).
Results. Approximations of the second- and third-type boundary conditions were constructed for a boundary value problem describing suspended matter transport. These approximations guarantee convergence of the finite-difference scheme at the rate of $O(\tau + h^2)$.
Discussion. The study may be useful in convection–diffusion problems where achieving numerical solutions with acceptable accuracy is required.
Conclusion. Future research may focus on the analysis of the constructed finite-difference schemes under physically motivated constraints on the time step τ and the grid Peclet number.

Keywords: coastal marine systems, convection–diffusion problem, finite-difference scheme, second- and third-type boundary conditions, approximation error

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Оригинальное теоретическое исследование

Аппроксимация граничных условий второго и третьего рода в краевых задачах для уравнений конвекции-диффузии с приложением к экологической гидрофизике

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Аннотация
Введение. Рассматривается разностная схема, аппроксимирующая краевую задачу для уравнения параболического типа в трехмерной постановке с условиями на границе I–III рода. Данная статья является дополнением к предыдущим работам авторов, посвященным численному решению одной из актуальных задач гидрофизики зон морского мелководья — задаче переноса, осаждения (транспорта) и трансформации взвешенного вещества. Аппроксимация указанного класса задач внутри области приводит к схемам, сходящимся со скоростью $O(\tau + h^2)$, где $h^2 = h_x^2 + h_y^2 + h_z^2$, h_x, h_y, h_z и τ — шаги разностной сетки по пространственным координатам x, y, z и времени соответственно. При этом требует аккуратного рассмотрения случай граничных условий, поскольку при неудачной их аппроксимации может понизиться порядок аппроксимации разностной схемы в целом. Предложенные авторами методы аппроксимации граничных условий обеспечивают сходимость разностной схемы со скоростью $O(\tau + h^2)$.
Материалы и методы. В своих исследованиях авторами сделан акцент на аппроксимации граничных условий третьего рода (аппроксимация граничных условий второго рода рассматривается как их частный случай). Ориентиром служит аппроксимация указанных граничных условий по формуле центральных разностей с последующим дифференцированием обеих частей уравнений диффузии-конвекции и исключением из полученных выражений функций решения в фиктивных узлах расширенной сетки.
Результаты исследования. Построены аппроксимации граничных условий II–III рода для краевой задачи, описывающей транспорт частиц взвешенного вещества, обеспечивающие сходимость разностной схемы со скоростью $O(\tau + h^2)$.
Обсуждение. Работа может быть полезна в задачах диффузии-конвекции, где необходимо добиться численного решения с приемлемой точностью.
Заключение. Дальнейшие исследования авторов могут быть направлены на исследование построенных разностных схем с учетом физически мотивированных ограничений на шаг временной сетки τ и сеточное число Пекле.

Ключевые слова: прибрежные морские системы, задача диффузии-конвекции, разностная схема, граничные условия второго и третьего рода, погрешность аппроксимации

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Introduction. We consider an initial–boundary value problem describing the transport of suspended matter of a multi-fractional composition, taking into account three spatial variables as well as the following physical parameters and processes: advective transport driven by the motion of the aquatic medium, microturbulent diffusion, and gravitational settling of suspended particles, along with the transition of particles from coarse granulometric fractions into finer ones (disintegration) and, conversely, the aggregation (coagulation) of particles of smaller fractions into larger ones [1–4].

For the continuous problem, the right-hand sides of the convection–diffusion–reaction equations governing the multi-fractional suspensions are transformed on a “lagged” time grid. Specifically, on a temporal mesh with step τ, the right-hand sides of the equations for suspended matter transport are modified as follows: for the concentration functions of fractions that enter the right-hand sides but do not belong to the fraction under consideration in the corresponding convection–diffusion–reaction equation, their values are taken from the previous time level. This approach significantly simplifies the subsequent numerical implementation of each convection–diffusion–reaction equation.

In the present study, we develop and analyze a finite-difference scheme approximating a boundary value problem for a parabolic-type equation in a three-dimensional setting with boundary conditions of the first through third types. This paper extends the authors' previous research devoted to the numerical solution of one of the pressing problems in the hydrophysics of shallow marine areas — namely, the transport, deposition (settling), and transformation of suspended matter.

As is typical, the approximation of this class of problems within the computational domain leads to schemes converging at the rate of $O(\tau + h^2)$, where $h^2 = h_x^2 + h_y^2 + h_z^2$, h_x, h_y, h_z are the spatial mesh steps and τ is the time step. At the same time, the treatment of boundary conditions requires special care, since their inaccurate approximation can reduce the overall order of accuracy of the finite-difference scheme. The boundary approximation methods proposed by the authors ensure convergence of the finite-difference scheme at the rate of $O(\tau + h^2)$.

Materials and Methods. We assume that particles of suspended matter dispersed in the water column are divided into R fractions. The problem is formulated for the domain $\bar{G}$

$$\bar{G} = \{0 \le x \le L_x, 0 \le y \le L_y, 0 \le z \le L_z\}.$$

In the rectangular Cartesian coordinate system $Oxyz$, we consider the three-dimensional convection–diffusion–reaction equation for particle settling, expressed using a skew-symmetric representation of the convective transport operator [5–10]:

$$\frac{\partial c_r}{\partial t} + C_0 c_r = Dc_r + F_r,\ r = 1,...,R,\ (x,y,z) \in \bar{G},$$

$$C_0 c_r \equiv \frac{1}{2}\left[u\frac{\partial c_r}{\partial x} + v\frac{\partial c_r}{\partial y} + \frac{\partial c_r}{\partial z} + w'\frac{\partial (uc_r)}{\partial x} + \frac{\partial (vc_r)}{\partial y} + \frac{\partial (w_r' c_r)}{\partial z}\right],$$

$$Dc_r = \frac{\partial}{\partial x}\left(\mu_{hr}\frac{\partial c_r}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu_{hr}\frac{\partial c_r}{\partial y}\right) + \frac{\partial}{\partial z}\left(\mu_{vr}\frac{\partial c_r}{\partial z}\right), \tag{1}$$

$$F_1 = (\alpha_2 c_2 - \beta_1 c_1) + \gamma_1 c_1,\ F_R = (\beta_{R-1} c_{R-1} - \alpha_R c_R) + \gamma_R c_R,$$
$$F_r = (\beta_{r-1} c_{r-1} - \alpha_r c_r) + (\alpha_{r+1} c_{r+1} - \beta_r c_r) + \gamma_r c_r,\ r = 2,...,R-1,$$

where c_r, $c_r = c_r(x, y, z, t)$ is the particle concentration at time t, $t \in [0; T]$; u, v, w — are the components of the velocity vector of the aquatic medium $\vec{U}$; w_r', $w_r' = w + w_{g,r}$, $w_{g,r}$ is the particle settling velocity determined by hydraulic size; $\mu_{h,r}$, $\mu_{v,r}$ are the horizontal and vertical diffusion coefficients; F_r is a source term; α_r, β_r are the coefficients describing the transformation rate of particles from one fraction to another, $\alpha_r \ge 0$, $\beta_r \ge 0$; γ_r is the intensity of an external particle source.

Equation (1) is supplemented with the initial condition:

$$c_r(x,y,z,0) = c_{r,0}(x,y,z),\ (x,y,z) \in \bar{G} \tag{2}$$

and boundary conditions:

– on the lateral faces of the parallelepiped G:

$$c_r = c_r',\ \text{if } u_{\vec{n}} < 0, \tag{3}$$

$$\frac{\partial c_r}{\partial \vec{n}} = 0,\ \text{if } u_{\vec{n}} \ge 0$$

($u_{\vec{n}}$ is the projection of the velocity vector onto the outward normal $\vec{n}$ at the boundary, and c' are prescribed concentration values);

– on the upper and lower boundaries of the domain G, respectively:

$$\frac{\partial c_r}{\partial z} = 0, \tag{5}$$

$$\frac{\partial c_r}{\partial z} = -\frac{w_{g,r}}{\mu_{v,r}} c_r. \tag{6}$$

In problem (1)–(6), we introduce a transformation from the z-coordinate system to the θ-coordinate system. In this framework, a Cartesian system is retained in the horizontal plane, while the vertical coordinate is replaced with a dimensionless variable θ, $\theta \in [0; 1]$.

The transformation is defined by the relation:

$$\theta = \frac{z - \eta}{h},\ x_\theta = x,\ y_\theta = y \tag{7}$$

where h is the water depth, and η is the vertical coordinate measured relative to the free surface.

Using the methods described in [11], we apply a "lagged" transformation on the temporal grid $\bar{\omega}_\tau = \{t_n = n\tau, n = 0,1,...,N_t,\ N_t\tau = T\}$. As a result, we obtain a sequence of initial–boundary value problems, linked by the initial and final data at each time level.

Equation (1) is transformed as follows:

$$\frac{\partial c_r^n}{\partial t} + C_0 c_r^n = D c_r^n + F_r^n,\ t_{n-1} < t \le t_n,\ n = 1,2,...,N_t,$$

$$C_0 c_r^n \equiv \frac{1}{2}\left[u\frac{\partial c_r^n}{\partial x} + v\frac{\partial c_r^n}{\partial y} + w_r'\frac{1}{H}\frac{\partial c_r^n}{\partial \theta} + \frac{\partial\left(u c_r^n\right)}{\partial x} + \frac{\partial\left(v c_r^n\right)}{\partial y} + \frac{1}{H}\frac{\partial\left(w_r' c_r^n\right)}{\partial \theta}\right],$$

$$D c_r^n = \frac{\partial}{\partial x}\left(\mu_{h,r}\frac{\partial c_r^n}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu_{h,r}\frac{\partial c_r^n}{\partial y}\right) + \frac{1}{H^2}\frac{\partial}{\partial \theta}\left(\mu_{v,r}\frac{\partial c_r^n}{\partial \theta}\right), \quad (8)$$

$$F_1^n = \left(\alpha_2 c_2^{n-1}(x,y,\theta,t_{n-1}) - \beta_1 c_1^n\right) + \gamma_1^n c_1^n,\ F_R^n = \left(\beta_{R-1} c_{R-1}^{n-1}(x,y,\theta,t_{n-1}) - \alpha_R c_R^n\right) + \gamma_R^n c_R^n,$$

$$F_r^n = \left(\beta_{r-1} c_{r-1}^{n-1}(x,y,\theta,t_{n-1}) - \alpha_r c_r^n\right) + \left(\alpha_{r+1} c_{r+1}^{n-1}(x,y,\theta,t_{n-1}) - \beta_r c_r^n\right) + \gamma_r^n c_r^n,\ r = 2,...,R-1.$$

with corresponding modifications of the initial and boundary conditions (2)–(6):

$$c_r^1(x,y,\theta,0) = c_{r,0},(x,y,\theta,0) \in \overline{G},$$

$$c_r^n(x,y,\theta,t_{n-1}) = c_r^{n-1}(x,y,\theta,t_{n-1}), n = 2,...,N_t,(x,y,\theta) \in G, \quad (9)$$

$$c_r^n = c',\ \text{if}\ u_{\vec{n}} < 0, \quad (10)$$

$$\frac{\partial c_r^n}{\partial \vec{n}} = 0,\ \text{if}\ u_{\vec{n}} \ge 0, \quad (11)$$

$$\frac{\partial c_r^n}{\partial \theta} = 0, \quad (12)$$

$$\frac{\partial c_r^n}{\partial \theta} = -\frac{w_{g,r}}{\mu_{v,r}} c_r^n. \quad (13)$$

It has been proved that the solutions of the transformed system converge to the solution of the original problem in the norm of the Hilbert space $L2(G)$ with accuracy $O(\tau)$ as $\tau \to 0$ [11].

To calculate the velocity field components of the aquatic medium, we employ a three-dimensional hydrodynamic model of bottom topography flow that accounts for bed friction and free-surface elevation [12–14].

Results. We assume the existence and continuity of the derivatives $\frac{\partial^2 u}{\partial x^2}, \frac{\partial^2 v}{\partial y^2}, \frac{\partial^2 w_r'}{\partial \theta^2}, \frac{\partial^2 \mu_{h,r}}{\partial x^2}, \frac{\partial^2 \mu_{h,r}}{\partial y^2}, \frac{\partial^2 \mu_{v,r}}{\partial \theta^2}$ a as well as the continuity of its second-order partial derivatives: $\frac{\partial^2 \mu_{h,r}}{\partial x^2}, \frac{\partial^2 \mu_{h,r}}{\partial y^2}, \frac{\partial^2 \mu_{v,r}}{\partial \theta^2}$. Additionally, we require that the mixed partial derivatives of c_r^n with respect to x, y, θ exist and are continuous up to the fifth order inclusively, while the mixed partial derivatives with respect to x, y, θ, t are continuous up to the second order. Furthermore, the mixed derivatives of the velocity field components u^n, v^n, ${w_r'}^n$ with respect to spatial variables x, y, θ are assumed continuous up to the second order inclusively.

To approximate problem (8)–(13), we introduce computational grids:

$$\omega = \omega_x \times \omega_y \times \omega_\theta \text{ и } \overline{\omega} = \overline{\omega}_x \times \overline{\omega}_y \times \overline{\omega}_\theta,$$

where

$$\omega_x = \left\{x : x = ih_x;\ i = 1,...,N_x - 1;\ (N_x - 1)h_x \equiv L_x - h_x\right\},\ \overline{\omega}_x = \left\{x : x = ih_x;\ i = 0,1,...,N_x;\ N_x h_x \equiv L_x\right\},$$

$$\omega_y = \left\{y : y = jh_y;\ j = 1,...,N_y - 1;\ (N_y - 1)h_y \equiv L_y - h_y\right\},\ \overline{\omega}_y = \left\{y : y = jh_y;\ j = 0,1,...,N_y;\ N_y h_y \equiv L_y\right\},$$

$$\omega_\theta = \left\{\theta : \theta = kh_\theta;\ k = 1,...,N_\theta - 1;\ (N_\theta - 1)h_\theta \equiv 1 - h_\theta\right\},\ \overline{\omega}_\theta = \left\{\theta : \theta = kh_\theta;\ k = 0,1,...,N_\theta;\ N_\theta h_\theta \equiv 1\right\}.$$

In [15], a finite-difference scheme was obtained that approximates problem (8)–(13) at the internal nodes of the grid with second-order accuracy in spatial variables and first-order accuracy in time. The finite-difference scheme approximating equation (8) can be written as:

$$\frac{\overline{c}_r^n(x_i,y_j,\theta_k) - \overline{c}_r^{n-1}(x_i,y_j,\theta_k)}{\tau} + C\overline{c}_r^n = D\overline{c}_r^n + \overline{F}_r^n,\ r = 1,2,3,\ (x_i,y_j,\theta_k) \in \omega,\ t_n \in \overline{\omega}_\tau,$$

$$C\overline{c}_r^n = \frac{1}{2h_x}\left[u^n(x_i + 0.5h_x, y_j, \theta_k)\overline{c}_r^n(x_i + h_x, y_j, \theta_k) - u^n(x_i - 0.5h_x, y_j, \theta_k)\overline{c}_r^n(x_i - h_x, y_j, \theta_k)\right] +$$

$$+\frac{1}{2h_y}\left[v^n(x_i, y_j + 0.5h_y, \theta_k)\overline{c}_r^n(x_i, y_j + h_y, \theta_k) - v^n(x_i, y_j - 0.5h_y, \theta_k)\overline{c}_r^n(x_i, y_j - h_y, \theta_k)\right] +$$

$$+\frac{1}{2H(x,y)h_\theta}\Big[w_r'^n\left(x_i,y_j,\theta_k+0.5h_\theta\right)\overline{c}_r^n\left(x_i,y_j,\theta_k+h_\theta\right)-w_r'^n\left(x_i,y_j,\theta_k-0.5h_\theta\right)\overline{c}_r^n\left(x_i,y_j,\theta_k-h_\theta\right)\Big],$$

$$D\overline{c}_r^n=\frac{1}{h_x^2}\Big[\mu_{h,r}\left(x_i+0.5h_x,y_j,\theta_k\right)\left(\overline{c}_r^n\left(x_i+h_x,y_j,\theta_k\right)-\overline{c}_r^n\left(x_i,y_j,\theta_k\right)\right)-\mu_{h,r}\left(x_i-0.5h_x,y_j,\theta_k\right)\cdot$$

$$\cdot\left(\overline{c}_r^n\left(x_i,y_j,\theta_k\right)-\overline{c}_r^n\left(x_i-h_x,y_j,\theta_k\right)\right)\Big]+\frac{1}{h_y^2}\Big[\mu_{h,r}\left(x_i,y_j+0.5h_y,\theta_k\right)\left(\overline{c}_r^n\left(x_i,y_j+h_y,\theta_k\right)-\overline{c}_r^n\left(x_i,y_j,\theta_k\right)\right)-$$

$$-\mu_{h,r}\left(x_i,y_j-0.5h_y,\theta_k\right)\left(\overline{c}_r^n\left(x_i,y_j,\theta_k\right)-\overline{c}_r^n\left(x_i,y_j-h_y,\theta_k\right)\right)\Big]+\frac{1}{H^2\left(x_i,y_j\right)h_\theta^2}\Big[\mu_{\nu,r}\left(x_i,y_j,\theta_k+0.5h_\theta\right)\cdot$$

$$\cdot\left(\overline{c}_r^n\left(x_i,y_j,\theta_k+h_\theta\right)-\overline{c}_r^n\left(x_i,y_j,\theta_k\right)\right)-\mu_{\nu,r}\left(x_i,y_j,\theta_k-0.5h_\theta\right)\left(\overline{c}_r^n\left(x_i,y_j,\theta_k\right)-\overline{c}_r^n\left(x_i,y_j,\theta_k-h_\theta\right)\right)\Big],$$

$$\overline{F}_1^n=\left(\alpha_2\overline{c}_2^{n-1}(x,y,\theta,t_{n-1})-\beta_1\overline{c}_1^n\right)+\gamma_1^n\overline{c}_1^n;\ \overline{F}_R^n=\left(\beta_{R-1}\overline{c}_{R-1}^{n-1}(x,y,\theta,t_{n-1})-\alpha_R\overline{c}_R^n\right)+\gamma_R^n\overline{c}_R^n;$$

$$\overline{F}_r^n=\left(\beta_{r-1}\overline{c}_{r-1}^{n-1}(x,y,\theta,t_{n-1})-\alpha_r\overline{c}_r^n\right)+\left(\alpha_{r+1}\overline{c}_{r+1}^{n-1}(x,y,\theta,t_{n-1})-\beta_r\overline{c}_r^n\right)+\gamma_r^n\overline{c}_r^n,\ r=2,\ldots,R-1.$$

$$\overline{F}_3^n=\left(\beta_2\overline{c}_2^{n-1}(x,y,\theta,t_{n-1})-\alpha_3\overline{c}_3^n\right)+\gamma_3^n\overline{c}_3^n,\ \left(x_i,y_j,\theta_k\right)\in\omega,\ t_n\in\overline{\omega}_\tau.$$

The overbar notation indicates that the quantities belong to the class of grid functions.

It is straightforward to verify that the approximation error $\psi^n\left(x_i,y_j,\theta_k\right)$ of the finite-difference scheme in the grid nodes $\overline{\omega}_\tau\times\omega$ satisfies the relation:

$$\psi^n\left(x_i,y_j,\theta_k\right)=O\left(\tau+h^2\right),\ n=0,1,\ldots,N_t,$$

It should also be noted that the initial condition (9) is imposed on the temporal grid $\overline{\omega}_\tau\times\omega$ exactly.

We proceed to construct a finite-difference scheme of second-order accuracy for the transport problem of suspended matter at the boundary nodes.

We assume that the following conditions are satisfied:

$$k_{11}\le\frac{h_x}{h_y}\le k_{12},\ k_{21}\le\frac{h_\theta}{h_x}\le k_{22},\ k_{31}\le\frac{h_\theta}{h_y}\le k_{32},\tag{15}$$

where k_{11}, k_{12}, k_{21}, k_{22}, k_{31}, k_{32} are some positive constants.

To approximate the boundary conditions, we introduce an extended grid:

$$\overline{\omega}^+=\Big\{\left(x_i,y_j,\theta_k\right),i=-1,0,\ldots,N_x+1,j=-1,0,\ldots,N_y+1,k=-1,0,\ldots,N_\theta+1,x_i=ih_x;y_j=jh_y;\theta_k=kh_\theta,$$

$$N_xh_x=L_x;N_yh_y=L_y;N_\theta h_\theta=1\Big\}.$$

For the nodes of the extended grid $\overline{\omega}^+\setminus\overline{\omega}$ the velocity vector components are assumed to vanish:

$$\overline{c}_r^n\left(x_i,y_j,\theta_k\right)=0,\text{ if }\left(x_i,y_j,\theta_k\right)\in\overline{\omega}^+\setminus\overline{\omega}.\tag{16}$$

In addition, we assume the components of the velocity field and the hydraulic size of the suspended particles to be known at extended grid nodes $\overline{\omega}^+\setminus\overline{\omega}$ with fractional indices, i. e. at half-grid positions: $u^n\left(-0.5h_x,y_j,\theta_k\right)$, $u^n\left(L_x+0.5h_x,y_j,\theta_k\right)$, $v^n\left(x_i,-0.5h_y,\theta_k\right)$, $v^n\left(x_i,L_y+0.5h_y,\theta_k\right)$ and $w_r'^n\left(x_i,y_j,-0.5h_\theta\right)$, $w_r'^n\left(x_i,y_j,1+0.5h_\theta\right)$.

The boundary conditions (10) are approximated as follows:

$$\begin{cases}\overline{c}_r^n\left(0,y_j,\theta_k\right)=c_r',\text{ если }u^n\left(0.5h_x,y_j,\theta_k\right)+u^n\left(-0.5h_x,y_j,\theta_k\right)>0,\\ \overline{c}_r^n\left(L_x,y_j,\theta_k\right)=c_r',\text{ если }u^n\left(L_x-0.5h_x,y_j,\theta_k\right)+u^n\left(L_x+0.5h_x,y_j,\theta_k\right)<0,\ \left(x_i,y_j,\theta_k\right)\in\overline{\omega}^+,\end{cases}\tag{17}$$

$$\begin{cases}\overline{c}_r^n\left(x_i,0,\theta_k\right)=c_r',\text{ если }v^n\left(x_i,0.5h_y,\theta_k\right)+v^n\left(x_i,-0.5h_y,\theta_k\right)>0,\\ \overline{c}_r^n\left(x_i,L_y,\theta_k\right)=c_r',\text{ если }v^n\left(x_i,L_y-0.5h_y,\theta_k\right)+v^n\left(x_i,L_y+0.5h_y,\theta_k\right)<0,\ \left(x_i,y_j,\theta_k\right)\in\overline{\omega}^+.\end{cases}\tag{18}$$

The construction of finite-difference schemes for boundary conditions (11)–(13) is demonstrated on the example of the third-type (Robin) condition — condition (13). Since boundary conditions (11) and (12) (Neumann conditions) represent particular cases of condition (13), the construction of the corresponding finite-difference approximations can be carried out by analogous reasoning.

For $\theta_k = 1$ the boundary condition (13) is equivalent to the following expression:

$$\frac{\partial c_r^n\left(x_i,y_j,1\right)}{\partial\theta}=-\frac{w_{g,r}}{\mu_{\nu,r}\left(x_i,y_j,1\right)}c_r^n\left(x_i,y_j,1\right).$$

On the grid $\overline{\omega}^+$ the nodes $(x_i, y_j, 1)$ are interior.

The finite-difference scheme at the nodes $(x_i, y_j, 1)$ of $\overline{\omega}^+$ is written as follows:

$$\frac{\overline{c}_r^n(x_i,y_j,1)-\overline{c}_r^{n-1}(x_i,y_j,1)}{\tau}+C\overline{c}_r^n(x_i,y_j,1)=D\overline{c}_r^n(x_i,y_j,1)+\overline{F}_r^n(x_i,y_j,1),\ n=1,...,N_t. \quad (20)$$

In what follows we base our reasoning on approximating the considered boundary condition by central differences on the extended grid and on eliminating from the resulting expression and from equation (20) the values of the function $\overline{c}_r^n$ in the ghost node $(x_i, y_j, 1+h_\theta)$.

In equation (20) the function $\overline{c}_r^n(x_i,y_j,1+h_\theta)$ enters the following terms:

$$\frac{1}{2H(x_i,y_j)h_\theta}\left[w_r'^n(x_i,y_j,1+0.5h_\theta)\overline{c}_r^n(x_i,y_j,1+h_\theta)-w_r'^n(x_i,y_j,1-0.5h_\theta)\overline{c}_r^n(x_i,y_j,1-h_\theta)\right],$$

$$\frac{1}{H^2(x_i,y_j)h_\theta^2}\left[\mu_{\nu,r}(x_i,y_j,1+0.5h_\theta)\left(\overline{c}_r^n(x_i,y_j,1+h_\theta)-\overline{c}_r^n(x_i,y_j,1)\right)-\mu_{\nu,r}(x_i,y_j,1-0.5h_\theta)\cdot\right.$$

$$\left.\cdot\left(\overline{c}_r^n(x_i,y_j,1)-\overline{c}_r^n(x_i,y_j,1-h_\theta)\right)\right],$$

which we denote by $C_\theta\overline{c}_r^n(x_i,y_j,1)$ and $D_\theta\overline{c}_r^n(x_i,y_j,1)$ respectively.

Since on the considered boundary $w|_{(x,y,1)}\equiv 0$, the relation for $C_\theta\overline{c}_r^n(x_i,y_j,1)$ can be brought to the form:

$$\frac{w_{g,r}}{2H(x_i,y_j)h_\theta}\left[\overline{c}_r^n(x_i,y_j,1+h_\theta)-\overline{c}_r^n(x_i,y_j,1-h_\theta)\right].$$

Rewrite condition (19) in the form:

$$\frac{\overline{c}_r^n(x_i,y_j,1+h_\theta)-\overline{c}_r^n(x_i,y_j,1-h_\theta)}{2h_\theta}=-\frac{2w_{g,r}}{\mu_{\nu,r}(x_i,y_j,1+0.5h_\theta)+\mu_{\nu,r}(x_i,y_j,1-0.5h_\theta)}\overline{c}_r^n(x_i,y_j,1) \quad (21)$$

and from it we obtain:

$$\overline{c}_r^n(x_i,y_j,1+h_\theta)=\overline{c}_r^n(x_i,y_j,1-h_\theta)-\frac{4w_{g,r}h_\theta}{\mu_{\nu,r}(x_i,y_j,1+0.5h_\theta)+\mu_{\nu,r}(x_i,y_j,1-0.5h_\theta)}\overline{c}_r^n(x_i,y_j,1).$$

For a compact presentation of the subsequent reasoning we introduce the notation:

$$\varepsilon_r=\frac{2w_{g,r}}{\mu_{\nu,r}(x_i,y_j,1+0.5h_\theta)+\mu_{\nu,r}(x_i,y_j,1-0.5h_\theta)}$$

and then

$$\overline{c}_r^n(x_i,y_j,1+h_\theta)=\overline{c}_r^n(x_i,y_j,1-h_\theta)-2h_\theta\varepsilon_r\overline{c}_r^n(x_i,y_j,1). \quad (22)$$

Substituting the value of $\overline{c}_r^n(x_i,y_j,1+h_\theta)$ obtained by formula (22) into the expression for $C_\theta\overline{c}_r^n(x_i,y_j,1)$, we obtain the approximation:

$$C_\theta\overline{c}_r^n(x_i,y_j,1)\equiv-\frac{w_{g,r}\varepsilon_r}{H(x_i,y_j)}\overline{c}_r^n(x_i,y_j,1). \quad (23)$$

As follows from equality (23), the quantity $C_\theta\overline{c}_r^n$ at the nodes of $(x_i, y_j, 1)$ is computed exactly.

Preliminary calculations show that if one uses equality (22) to approximate $D_\theta\overline{c}_r^n(x_i,y_j,1)$, then a first-order error in θ is obtained. To approximate this operator with second-order accuracy in θ the authors propose a different approach.

Expanding the functions $c_r^n(x_i,y_j,1\pm h_\theta)$ in a Taylor series in the neighbourhood of the point $(x_i, y_j, 1)$ adjacent to the boundary, we obtain an expression for the left-hand side of equality (21):

$$\frac{\overline{c}_r^n(x_i,y_j,1+h_\theta)-\overline{c}_r^n(x_i,y_j,1-h_\theta)}{2h_\theta}=\frac{\partial c_r^n(x_i,y_j,1)}{\partial\theta}+\frac{\partial^3 c_r^n(x_i,y_j,1)}{\partial\theta^3}\frac{h_\theta^2}{6}+O(h_\theta^4).$$

The last expression, taking into account condition (19), can be transformed to the form:

$$\frac{\overline{c}_r^n(x_i,y_j,1+h_\theta)-\overline{c}_r^n(x_i,y_j,1-h_\theta)}{2h_\theta}=-\frac{w_{g,r}}{\mu_{\nu,r}(x_i,y_j,1)}c_r^n(x_i,y_j,1)+\frac{h_\theta^2}{6}\frac{\partial^3 c_r^n(x_i,y_j,1)}{\partial\theta^3}+O(h_\theta^4). \quad (24)$$

Using equality (24) we find the value of the function $\overline{c}_r^n$ in the ghost node $(x_i, y_j, 1 + h_\theta)$:

$$\overline{c}_r^n\left(x_i, y_j, 1+h_\theta\right) = \overline{c}_r^n\left(x_i, y_j, 1-h_\theta\right) - 2h_\theta\,\varepsilon_r c_r^n\left(x_i, y_j, 1\right) + \frac{h_\theta^3}{3}\frac{\partial^3 c_r^n\left(x_i, y_j, 1\right)}{\partial\theta^3} + O\left(h_\theta^5\right). \tag{25}$$

Using equality (25), we compose the expression for $D_\theta \overline{c}_r^n\left(x_i, y_j, 1\right)$:

$$D_\theta \overline{c}_r^n\left(x_i, y_j, 1\right) \cong \frac{1}{H^2\left(x_i, y_j\right)h_\theta^2}\Big[\left(\mu_{v,r}\left(x_i, y_j, 1+0.5h_\theta\right) + \mu_{v,r}\left(x_i, y_j, 1-0.5h_\theta\right)\right)\left(\overline{c}_r^n\left(x_i, y_j, 1-h_\theta\right) -\right.$$

$$\left. - \overline{c}_r^n\left(x_i, y_j, 1\right)\right) - \mu_{v,r}\left(x_i, y_j, 1+0.5h_\theta\right)\left(2h_\theta\,\varepsilon_r c_r^n\left(x_i, y_j, 1\right) - \frac{h_\theta^3}{3}\frac{\partial^3 c_r^n\left(x_i, y_j, 1\right)}{\partial\theta^3}\right)\Bigg].$$

Clearly, to achieve the stated goal it is sufficient to approximate the derivative $\frac{\partial^3 c_r^n\left(x_i, y_j, 1\right)}{\partial\theta^3}$ with first-order accuracy in θ. We now construct an approximation of this derivative with the prescribed accuracy.

Differentiate both sides of equation (8) with respect to the vertical variable θ and, from the resulting equality, express the derivative $\frac{\partial^3 c_r^n}{\partial\theta^3}$. Next, pass to the limit as $\theta \to 1$ and, taking into account condition (36), we obtain:

$$\frac{\partial^3 c_r^n\left(x_i, y_j, 1\right)}{\partial\theta^3} = \frac{H^2\left(x_i, y_j\right)}{\mu_{v,r}\left(x_i, y_j, 1\right)}\left[\frac{\partial^2 c_r^n\left(x_i, y_j, 1\right)}{\partial t\partial\theta} - \mu_{h,r}\left(x_i, y_j, 1\right)\frac{\partial^3 c_r^n\left(x_i, y_j, 1\right)}{\partial x^2\partial\theta} - \mu_{h,r}\left(x_i, y_j, 1\right)\cdot\right.$$

$$\cdot\frac{\partial^3 c_r^n\left(x_i, y_j, 1\right)}{\partial y^2\partial\theta} + \left(u^n\left(x_i, y_j, 1\right) - \frac{\partial\mu_{h,r}\left(x_i, y_j, 1\right)}{\partial x}\right)\frac{\partial^2 c_r^n\left(x_i, y_j, 1\right)}{\partial x\partial\theta} + \left(v^n\left(x_i, y_j, 1\right) - \frac{\partial\mu_{h,r}\left(x_i, y_j, 1\right)}{\partial y}\right)\cdot$$

$$\cdot\frac{\partial^2 c_r^n\left(x_i, y_j, 1\right)}{\partial y\partial\theta} + \frac{1}{H\left(x_i, y_j\right)}\left(w_{g,r} - \frac{2}{H\left(x_i, y_j\right)}\frac{\partial\mu_{v,r}\left(x_i, y_j, 1\right)}{\partial\theta}\right)\frac{\partial^2 c_r^n\left(x_i, y_j, 1\right)}{\partial\theta^2} - \frac{\partial\mu_{h,r}\left(x_i, y_j, 1\right)}{\partial\theta}\cdot \tag{26}$$

$$\cdot\frac{\partial^2 c_r^n\left(x_i, y_j, 1\right)}{\partial x^2} - \frac{\partial\mu_{h,r}\left(x_i, y_j, 1\right)}{\partial\theta}\frac{\partial^2 c_r^n\left(x_i, y_j, 1\right)}{\partial y^2} + \left(\frac{\partial u^n\left(x_i, y_j, 1\right)}{\partial\theta} - \frac{\partial^2\mu_{h,r}\left(x_i, y_j, 1\right)}{\partial x\partial\theta}\right)\cdot$$

$$\cdot\frac{\partial c_r^n\left(x_i, y_j, 1\right)}{\partial x} + \left(\frac{\partial v^n\left(x_i, y_j, 1\right)}{\partial\theta} - \frac{\partial^2\mu_{h,r}\left(x_i, y_j, 1\right)}{\partial y\partial\theta}\right)\frac{\partial c_r^n\left(x_i, y_j, 1\right)}{\partial y} + \frac{1}{2}\left(\frac{\partial^2 u^n\left(x_i, y_j, 1\right)}{\partial x\partial\theta} + \frac{\partial^2 v^n\left(x_i, y_j, 1\right)}{\partial y\partial\theta} -\right.$$

$$\left.\left. - \frac{w_{g,r}}{\mu_{v,r}\left(x_i, y_j, 1\right)}\frac{\partial u^n\left(x_i, y_j, 1\right)}{\partial x} - \frac{w_{g,r}}{\mu_{v,r}\left(x_i, y_j, 1\right)}\frac{\partial v^n\left(x_i, y_j, 1\right)}{\partial y} + \frac{2w_{g,r}}{H^2\left(x_i, y_j\right)\mu_{v,r}\left(x_i, y_j, 1\right)}\frac{\partial^2\mu_{v,r}\left(x_i, y_j, 1\right)}{\partial\theta^2}\right)\cdot c_r^n\left(x_i, y_j, 1\right) - \frac{\partial F_r^n\left(x_i, y_j, 1\right)}{\partial\theta}\right].$$

It is evident that the following relations hold:

$$\frac{\partial F_1^n}{\partial\theta} = \left(-\alpha_2\frac{w_{g,2}}{\mu_{v,2}\left(x_i, y_j, 1\right)}c_2^{n-1}\left(x_i, y_j, 1, t_{n-1}\right) + \beta_1\frac{w_{g,1}}{\mu_{v,1}\left(x_i, y_j, 1\right)}c_1^n\right) + \gamma_1^n\frac{w_{g,1}}{\mu_{v,1}\left(x_i, y_j, 1\right)}c_1^n,$$

$$F_R^n = \left(-\beta_{R-1}\frac{w_{g,R-1}}{\mu_{v,R-1}\left(x_i, y_j, 1\right)}c_{R-1}^{n-1}\left(x, y, 1, t_{n-1}\right) + \alpha_R\frac{w_{g,R}}{\mu_{v,R}\left(x_i, y_j, 1\right)}c_R^n\right) - \gamma_R^n\frac{w_{g,R}}{\mu_{v,R}\left(x_i, y_j, 1\right)}c_R^n,$$

$$\frac{\partial F_r^n}{\partial\theta} = \left(-\beta_1\frac{w_{g,r-1}}{\mu_{v,r-1}\left(x_i, y_j, 1\right)}c_{r-1}^{n-1}\left(x, y, 1, t_{n-1}\right) + \alpha_r\frac{w_{g,r}}{\mu_{v,r}\left(x_i, y_j, 1\right)}c_r^n\right) +$$

$$+\left(-\alpha_{r+1}\frac{w_{g,r+1}}{\mu_{v,r+1}\left(x_i, y_j, 1\right)}c_{r+1}^{n-1}\left(x, y, 1, t_{n-1}\right) + \beta_r\frac{w_{g,r}}{\mu_{v,r}\left(x_i, y_j, 1\right)}c_r^n\right) - \gamma_r^n\frac{w_{g,r}}{\mu_{v,r}\left(x_i, y_j, 1\right)}c_r^n.$$

For reader convenience, we approximate the expression in the square brackets on the right-hand side of (26) term by term. First, note that for the coefficient $\frac{H^2\left(x_i, y_j\right)}{\mu_{v,r}\left(x_i, y_j, 1\right)}$ placed before this bracket we use the representation:

$$\frac{H^2\left(x_i, y_j\right)}{\mu_{v,r}\left(x_i, y_j, 1\right)} = \frac{2H^2\left(x_i, y_j\right)}{\mu_{v,r}\left(x_i, y_j, 1+0.5h_\theta\right) + \mu_{v,r}\left(x_i, y_j, 1-0.5h_\theta\right)}. \tag{27}$$

Consider the derivative $\frac{\partial^2 c_r^n\left(x_i, y_j, 1\right)}{\partial t\partial\theta}$. For this derivative we have:

$$\frac{\partial^2 c_r^n(x_i,y_j,1)}{\partial t\partial\theta}=\frac{1}{2h_\theta}\left(\frac{\overline{c}_r^n(x_i,y_j,1+h_\theta,t_n+\tau)-\overline{c}_r^n(x_i,y_j,1+h_\theta,t_n-\tau)}{2\tau}-\right.$$
$$\left.-\frac{\overline{c}_r^n(x_i,y_j,1-h_\theta,t_n+\tau)-\overline{c}_r^n(x_i,y_j,1-h_\theta,t_n-\tau)}{2\tau}+O(\tau^2)\right)+O(h_\theta^2)=$$
$$=\frac{1}{2\tau}\left(\frac{\overline{c}_r^n(x_i,y_j,1+h_\theta,t_n+\tau)-\overline{c}_r^n(x_i,y_j,1-h_\theta,t_n+\tau)}{2h_\theta}-\right. \tag{28}$$
$$\left.-\frac{\overline{c}_r^n(x_i,y_j,1+h_\theta,t_n-\tau)-\overline{c}_r^n(x_i,y_j,1-h_\theta,t_n-\tau)}{2h_\theta}\right)+\frac{1}{2h_\theta}O(\tau^2)+O(h_\theta^2).$$

Using equality (28), the following relations can be written:

$$\frac{\overline{c}_r^n(x_i,y_j,1+h_\theta,t_n\pm\tau)-\overline{c}_r^n(x_i,y_j,1-h_\theta,t_n\pm\tau)}{2h_\theta}=$$
$$=-\frac{w_{g,r}}{\mu_{v,r}(x_i,y_j,1)}c_r^n(x_i,y_j,1,t_n\pm\tau)+\frac{h_\theta^2}{6}\frac{\partial^3 c_r^n(x_i,y_j,1,t_n\pm\tau)}{\partial\theta^3}+O(h_\theta^4). \tag{29}$$

By means of (29) we transform equality (28) into the form

$$\frac{\partial^2 c_r^n}{\partial t\partial\theta}=-\frac{w_{g,r}}{2\tau\mu_{v,r}(x_i,y_j,1)}\left(c_r^n(x_i,y_j,1,t_n+\tau)-c_r^n(x_i,y_j,1,t_n-\tau)\right)+$$
$$+\frac{h_\theta^2}{12\tau}\left(\frac{\partial^3 c_r^n(x_i,y_j,1,t_n+\tau)}{\partial\theta^3}-\frac{\partial^3 c_r^n(x_i,y_j,1,t_n-\tau)}{\partial\theta^3}\right)+\frac{1}{2h_\theta}O(\tau^2)+O(h_\theta^2). \tag{30}$$

For the expression $\frac{w_{g,r}}{2\tau\mu_{v,r}(x_i,y_j,1)}\left(c_r^n(x_i,y_j,1,t_n+\tau)-c_r^n(x_i,y_j,1,t_n-\tau)\right)$ we have:

$$\frac{w_{g,r}}{2\tau\mu_{v,r}(x_i,y_j,1)}\left(c_r^n(x_i,y_j,1,t_n+\tau)-c_r^n(x_i,y_j,1,t_n-\tau)\right)=\frac{w_{g,r}}{2\tau\mu_{v,r}(x_i,y_j,1)}\frac{\partial c_r^n(x_i,y_j,1,t_n)}{\partial t}+O(\tau^2). \tag{31}$$

Taking into account relation (31), we transform expression (30). We obtain:

$$\frac{\partial^2 c_r^n}{\partial t\partial\theta}=-\varepsilon_r\frac{\partial c_r^n(x_i,y_j,1,t_n)}{\partial t}+\frac{1}{2\tau}\frac{h_\theta^2}{6}\left(\frac{\partial^3 c_r^n(x_i,y_j,1,t_n+\tau)}{\partial\theta^3}-\frac{\partial^3 c_r^n(x_i,y_j,1,t_n-\tau)}{\partial\theta^3}\right)+\frac{1}{2h_\theta}O(\tau^2)+O(h_\theta^2+\tau^2).$$

Introducing the notation $\varphi(x_i,y_j,1,t_n\pm\tau)=\frac{\partial^3 c_r^n(x_i,y_j,1,t_n\pm\tau)}{\partial\theta^3}$, the last equality can be written in the form:

$$\frac{\partial^2 c_r^n}{\partial t\partial\theta}=-\varepsilon_r\frac{\partial c_r^n(x_i,y_j,1,t_n)}{\partial t}+\frac{h_\theta^2}{6}\left(\frac{\varphi(x_i,y_j,1,t_n+\tau)-\varphi(x_i,y_j,1,t_n-\tau)}{2\tau}\right)+\frac{1}{2h_\theta}O(\tau^2)+O(h_\theta^2+\tau^2).$$

From this it follows that

$$\frac{\partial^2 c_r^n}{\partial t\partial\theta}=-\varepsilon_r\frac{\partial c_r^n(x_i,y_j,1,t_n)}{\partial t}+\frac{h_\theta^2}{6}\left(\frac{\partial\varphi(x_i,y_j,1,t_n)}{\partial t}+O(\tau^2)\right)+\frac{1}{2h_\theta}O(\tau^2)+O(h_\theta^2+\tau^2).$$

In accordance with the Courant condition, the quantity τ is bounded, and thus the equality $\frac{1}{2h_\theta}O(\tau^2)=O(h_\theta)$ can be considered valid. Taking this into account, we have:

$$\frac{\partial^2 c_r^n}{\partial t\partial\theta}=-\varepsilon_r\frac{\partial c_r^n(x_i,y_j,1,t_n)}{\partial t}+\frac{h_\theta^2}{6}\frac{\partial\varphi(x_i,y_j,1,t_n)}{\partial t}+O(h_\theta+\tau^2).$$

Taking into account the last relation, and assuming boundedness of the derivative $\frac{\partial\varphi(x_i,y_j,1,t_n\pm\tau)}{\partial t}=$ $=\frac{\partial^4 c_r^n(x_i,y_j,1,t_n\pm\tau)}{\partial t\partial x^3}$, we can write:

$$\frac{\partial^2 c_r^n}{\partial t\partial\theta}=-\varepsilon_r\frac{\partial c_r^n(x_i,y_j,1,t_n)}{\partial t}+O(h_\theta+\tau^2). \tag{32}$$

Next, consider the derivative $\frac{\partial^3 c_r^n(x_i, y_j, 1)}{\partial x^2 \partial \theta}$.

Taking into account inequality $k_{21} \le \frac{h_\theta}{h_x} \le k_{22}$ from (16), we have:

$$
\begin{aligned}
&\frac{\partial^3 c_r^n(x_i, y_j, 1)}{\partial x^2 \partial\theta} = \frac{1}{2h_\theta}\left(\frac{\partial^2 \overline{c}_r^n(x_i, y_j, 1+h_\theta)}{\partial x^2} - \frac{\partial^2 \overline{c}_r^n(x_i, y_j, 1-h_\theta)}{\partial x^2}\right) + O(h_\theta^2) = \\
&= \frac{1}{2h_\theta}\left(\frac{\overline{c}_r^n(x_i+h_x, y_j, 1+h_\theta) - 2\overline{c}_r^n(x_i, y_j, 1+h_\theta) + \overline{c}_r^n(x_i-h_x, y_j, 1+h_\theta)}{h_x^2} - \right. \\
&\left. - \frac{\overline{c}_r^n(x_i+h_x, y_j, 1-h_\theta) - 2\overline{c}_r^n(x_i, y_j, 1-h_\theta) + \overline{c}_r^n(x_i-h_x, y_j, 1-h_\theta)}{h_x^2} + O(h_x^2)\right) + O(h_\theta^2) = \\
&= \frac{1}{h_x^2}\left(\frac{\overline{c}_r^n(x_i+h_x, y_j, 1+h_\theta) - \overline{c}_r^n(x_i+h_x, y_j, 1-h_\theta)}{2h_\theta} - 2\frac{\overline{c}_r^n(x_i, y_j, 1+h_\theta) - \overline{c}_r^n(x_i, y_j, 1-h_\theta)}{2h_\theta} + \right. \\
&\left. + \frac{\overline{c}_r^n(x_i-h_x, y_j, 1+h_\theta) - \overline{c}_r^n(x_i-h_x, y_j, 1-h_\theta)}{2h_\theta}\right) + \frac{1}{2h_\theta} O(h_x^2) + O(h_\theta^2) = \\
&= \frac{1}{h_x^2}\left(\frac{\overline{c}_r^n(x_i+h_x, y_j, 1+h_\theta) - \overline{c}_r^n(x_i+h_x, y_j, 1-h_\theta)}{2h_\theta} - 2\frac{\overline{c}_r^n(x_i, y_j, 1+h_\theta) - \overline{c}_r^n(x_i, y_j, 1-h_\theta)}{2h_\theta} + \right. \\
&\left. + \frac{\overline{c}_r^n(x_i-h_x, y_j, 1+h_\theta) - \overline{c}_r^n(x_i-h_x, y_j, 1-h_\theta)}{2h_\theta}\right) + O(h_\theta^2 + h_x).
\end{aligned} \tag{33}
$$

Based on equality (24), the following relation can be written:

$$
\frac{\overline{c}_r^n(x_i \pm h_x, y_j, 1+h_\theta) - \overline{c}_r^n(x_i \pm h_x, y_j, 1-h_\theta)}{2h_\theta} = -\varepsilon_r c_r^n(x_i \pm h_x, y_j, 1) + \frac{h_\theta^2}{6}\frac{\partial^3 c_r^n(x_i \pm h_x, y_j, 1)}{\partial\theta^3} + O(h_\theta^4). \tag{34}
$$

Using (34), we transform relation (33) into the form:

$$
\begin{aligned}
&\frac{\partial^3 c_r^n(x_i, y_j, 1)}{\partial x^2 \partial\theta} = -\frac{\varepsilon_r}{h_x^2}\left(c_r^n(x_i+h_x, y_j, 1) - 2c_r^n(x_i, y_j, 1) + c_r^n(x_i-h_x, y_j, 1)\right) + \\
&+ \frac{h_\theta^2}{6h_x^2}\left(\frac{\partial^3 c_r^n(x_i+h_x, y_j, 1)}{\partial\theta^3} - 2\frac{\partial^3 c_r^n(x_i, y_j, 1)}{\partial\theta^3} + \frac{\partial^3 c_r^n(x_i-h_x, y_j, 1)}{\partial\theta^3}\right) + O(h_\theta^2 + h_x).
\end{aligned} \tag{35}
$$

Applying the equality:

$$
\frac{1}{h_x^2}\left(c_r^n(x_i+h_x, y_j, 1) - 2c_r^n(x_i, y_j, 1) + c_r^n(x_i-h_x, y_j, 1)\right) = \frac{\partial^2 c_r^n(x_i, y_j, 1)}{\partial x^2} + O(h_x^2),
$$

expression (35) can be rewritten as:

$$
\frac{\partial^3 c_r^n(x_i, y_j, 1)}{\partial x^2 \partial\theta} = -\varepsilon_r \frac{\partial^2 c_r^n(x_i, y_j, 1)}{\partial x^2} + \frac{h_\theta^2}{6h_x^2}\left(\frac{\partial^3 c_r^n(x_i+h_x, y_j, 1)}{\partial\theta^3} - 2\frac{\partial^3 c_r^n(x_i, y_j, 1)}{\partial\theta^3} + \frac{\partial^3 c_r^n(x_i-h_x, y_j, 1)}{\partial\theta^3}\right) + O(h_\theta^2 + h_x).
$$

Let $\varphi(x_i \pm h_x, y_j, 1) = \frac{\partial^3 c_r^n(x_i \pm h_x, y_j, 1)}{\partial\theta^3}$, $\varphi(x_i, y_j, 1) = \frac{\partial^3 c_r^n(x_i, y_j, 1)}{\partial\theta^3}$. Then the last equality can be written in the form:

$$
\frac{\partial^3 c_r^n(x_i, y_j, 1)}{\partial x^2 \partial\theta} = -\varepsilon_r \frac{\partial^2 c_r^n(x_i, y_j, 1)}{\partial x^2} + \frac{h_\theta^2}{6}\left(\frac{\varphi(x_i+h_x, y_j, 1) - 2\varphi(x_i, y_j, 1) + \varphi(x_i-h_x, y_j, 1)}{h_x^2}\right) + O(h_\theta^2 + h_x). \tag{36}
$$

This equality can be transformed into the form:

$$
\frac{\partial^3 c_r^n(x_i, y_j, 1)}{\partial x^2 \partial\theta} = -\varepsilon_r \frac{\partial^2 c_r^n(x_i, y_j, 1)}{\partial x^2} + \frac{h_\theta^2}{6}\left(\frac{\partial^2 \varphi(x_i, y_j, 1)}{\partial x^2} + O(h_x^2)\right) + O(h_\theta^2 + h_x).
$$

Taking into account the last relation and assuming the boundedness of the derivative $\frac{\partial^2 \varphi(x_i, y_j, 1)}{\partial x^2} = \frac{\partial^5 c_r^n(x_i, y_j, 1)}{\partial x^2 \partial \theta^3}$, for the term $\mu_{h,r}(x_i, y_j, 1)\frac{\partial^3 c_r^n(x_i, y_j, 1)}{\partial x^2 \partial \theta}$ on the right-hand side of equality (26), we can write:

$$\mu_{h,r}(x_i, y_j, 1)\frac{\partial^3 c_r^n(x_i, y_j, 1)}{\partial x^2 \partial \theta} = -\varepsilon_r \mu_{h,r}(x_i, y_j, 1)\frac{\partial^2 c_r^n(x_i, y_j, 1)}{\partial x^2} + O(h_\theta). \quad (37)$$

By carrying out similar reasoning for the derivative $\frac{\partial^3 c_r^n(x_i, y_j, 1)}{\partial x \partial \theta^2}$, we obtain:

$$\mu_{h,r}(x_i, y_j, 1)\frac{\partial^3 c_r^n(x_i, y_j, 1)}{\partial y^2 \partial \theta} = -\varepsilon_r \mu_{h,r}(x_i, y_j, 1)\frac{\partial^2 c_r^n(x_i, y_j, 1)}{\partial y^2} + O(h_\theta). \quad (38)$$

Let us turn to the mixed derivative $\frac{\partial^2 c_r^n(x_i, y_j, 1)}{\partial x \partial \theta}$. Following the reasoning presented earlier, we have:

$$\begin{gathered}\frac{\partial^2 c_r^n(x_i, y_j, 1)}{\partial x \partial \theta} = \frac{1}{2h_\theta}\left(\frac{\partial \overline{c}_r^n(x_i, y_j, 1+h_\theta)}{\partial x} - \frac{\partial \overline{c}_r^n(x_i, y_j, 1-h_\theta)}{\partial x}\right) + O(h_\theta^2) = \frac{1}{2h_\theta}\cdot \\ \cdot\left(\frac{\overline{c}_r^n(x_i+h_x, y_j, 1+h_\theta) - \overline{c}_r^n(x_i-h_x, y_j, 1+h_\theta)}{2h_x} - \frac{\overline{c}_r^n(x_i+h_x, y_j, 1-h_\theta) - \overline{c}_r^n(x_i-h_x, y_j, 1-h_\theta)}{2h_x} + \right. \\ \left. + O(h_x^2)\right) + O(h_\theta^2) = \frac{1}{2h_x}\left(\frac{\overline{c}_r^n(x_i+h_x, y_j, 1+h_\theta) - \overline{c}_r^n(x_i+h_x, y_j, 1-h_\theta)}{2h_\theta} - \right. \\ \left. - \frac{\overline{c}_r^n(x_i-h_x, y_j, 1+h_\theta) - \overline{c}_r^n(x_i-h_x, y_j, 1-h_\theta)}{2h_\theta}\right) + \frac{1}{2h_\theta}O(h_x^2) + O(h_\theta^2).\end{gathered} \quad (39)$$

Based on equality (39), the following relation can be written:

$$\frac{\overline{c}_r^n(x_i \pm h_x, y_j, 1+h_\theta) - \overline{c}_r^n(x_i \pm h_x, y_j, 1-h_\theta)}{2h_\theta} = -\varepsilon_r c_r^n(x_i \pm h_x, y_j, 1) + \frac{h_\theta^2}{6}\frac{\partial^3 c_r^n(x_i \pm h_x, y_j, 1)}{\partial \theta^3} + O(h_\theta^4). \quad (40)$$

Using (40), we transform relation (39) into the form:

$$\frac{\partial^2 c_r^n(x_i, y_j, 1)}{\partial x \partial \theta} = -\frac{\varepsilon_r}{2h_x}\left(c_r^n(x_i+h_x, y_j, 1) - c_r^n(x_i-h_x, y_j, 1)\right) + \frac{h_\theta^2}{12h_x}\left(\frac{\partial^3 c_r^n(x_i+h_x, y_j, 1)}{\partial \theta^3} - \frac{\partial^3 c_r^n(x_i-h_x, y_j, 1)}{\partial \theta^3}\right) + O(h_\theta^2 + h_x). \quad (41)$$

Since the following equality holds:

$$\frac{1}{2h_x}\left(c_r^n(x_i+h_x, y_j, 1) - c_r^n(x_i-h_x, y_j, 1)\right) = \frac{\partial c_r^n(x_i, y_j, 1)}{\partial x} + O(h_x^2),$$

expression (41) can be rewritten as:

$$\frac{\partial^2 c_r^n(x_i, y_j, 1)}{\partial x \partial \theta} = -\varepsilon_r \frac{\partial c_r^n(x_i, y_j, 1)}{\partial x} + \frac{h_\theta^2}{12h_x}\left(\frac{\partial^3 c_r^n(x_i+h_x, y_j, 1)}{\partial \theta^3} - \frac{\partial^3 c_r^n(x_i-h_x, y_j, 1)}{\partial \theta^3}\right) + O(h_\theta^2 + h_x).$$

Let $\varphi(x_i \pm h_x, y_j, 1) = \frac{\partial^3 c_r^n(x_i \pm h_x, y_j, 1)}{\partial \theta^3}$, $\varphi(x_i, y_j, 1) = \frac{\partial^3 c_r^n(x_i, y_j, 1)}{\partial \theta^3}$. Then the last equality can be written as:

$$\frac{\partial^2 c_r^n(x_i, y_j, 1)}{\partial x \partial \theta} = -\varepsilon_r \frac{\partial c_r^n(x_i, y_j, 1)}{\partial x} + \frac{h_\theta^2}{6}\left(\frac{\varphi(x_i+h_x, y_j, 1) - \varphi(x_i-h_x, y_j, 1)}{2h_x}\right) + O(h_\theta^2 + h_x). \quad (42)$$

This expression can be further transformed into the form:

$$\frac{\partial^2 c_r^n(x_i, y_j, 1)}{\partial x \partial \theta} = -\varepsilon_r \frac{\partial c_r^n(x_i, y_j, 1)}{\partial x} + \frac{h_\theta^2}{6}\left(\frac{\partial \varphi(x_i, y_j, 1)}{\partial x} + O(h_x^2)\right) + O(h_\theta^2 + h_x).$$

Taking into account the last relation and assuming the boundedness of the derivative $\frac{\partial \varphi(x_i, y_j, 1)}{\partial x} = \frac{\partial^4 c_r^n(x_i, y_j, 1)}{\partial x \partial \theta^3}$, for the term $\left(u^n(x_i, y_j, 1) - \frac{\partial \mu_{h,r}(x_i, y_j, 1)}{\partial x}\right)\frac{\partial^2 c_r^n(x_i, y_j, 1)}{\partial x \partial \theta}$ on the right-hand side of equality (26), we can write:

$$\left(u^n\left(x_i,y_j,1\right)-\frac{\partial\mu_{h,r}\left(x_i,y_j,1\right)}{\partial x}\right)\frac{\partial^2 c_r^n\left(x_i,y_j,1\right)}{\partial x\partial\theta}=-\varepsilon_r\left(u^n\left(x_i,y_j,1\right)-\frac{\partial\mu_{h,r}\left(x_i,y_j,1\right)}{\partial x}\right)\frac{\partial c_r^n\left(x_i,y_j,1\right)}{\partial x}+O\left(h_\theta\right). \tag{43}$$

By applying similar reasoning to the derivative $\frac{\partial^2 c_r^n\left(x_i,y_j,1\right)}{\partial y\partial\theta}$ with respect to the term $\left(u^n\left(x_i,y_j,1\right)-\frac{\partial\mu_{h,r}\left(x_i,y_j,1\right)}{\partial x}\right)\frac{\partial^2 c_r^n\left(x_i,y_j,1\right)}{\partial x\partial\theta}$ from the right-hand side of equality (26), we obtain the relation:

$$\left(v^n\left(x_i,y_j,1\right)-\frac{\partial\mu_{h,r}\left(x_i,y_j,1\right)}{\partial y}\right)\frac{\partial^2 c_r^n\left(x_i,y_j,1\right)}{\partial y\partial\theta}=-\varepsilon_r\left(v^n\left(x_i,y_j,1\right)-\frac{\partial\mu_{h,r}\left(x_i,y_j,1\right)}{\partial y}\right)\frac{\partial c_r^n\left(x_i,y_j,1\right)}{\partial y}+O\left(h_\theta\right). \tag{44}$$

Now let us turn to the derivative $\frac{\partial^2 c_r^n\left(x_i,y_j,1\right)}{\partial\theta^2}$. We have:

$$\frac{\partial^2 c_r^n\left(x_i,y_j,1\right)}{\partial\theta^2}=\frac{1}{2h_\theta}\left(\frac{\partial\overline{c}_r^n\left(x_i,y_j,1+h_\theta\right)}{\partial\theta}-\frac{\partial\overline{c}_r^n\left(x_i,y_j,1-h_\theta\right)}{\partial\theta}\right)+O\left(h_\theta^2\right). \tag{45}$$

Using expression (25), which defines the value of the function $\overline{c}_r^n$ at the fictitious node (x_i, y_j, $1+h_\theta$), we obtain:

$$\frac{\partial\overline{c}_r^n\left(x_i,y_j,1+h_\theta\right)}{\partial\theta}=\frac{\partial}{\partial\theta}\left(\overline{c}_r^n\left(x_i,y_j,1-h_\theta\right)+2h_\theta\varepsilon_r c_r^n\left(x_i,y_j,1\right)-\frac{h_\theta^3}{3}\frac{\partial^3 c_r^n\left(x_i,y_j,1\right)}{\partial\theta^3}+O\left(h_\theta^5\right)\right)=$$

$$=\frac{\partial\overline{c}_r^n\left(x_i,y_j,1-h_\theta\right)}{\partial\theta}+2h_\theta\varepsilon_r\frac{\partial\overline{c}_r^n\left(x_i,y_j,1\right)}{\partial\theta}-\frac{h_\theta^3}{3}\frac{\partial^4 c_r^n\left(x_i,y_j,1\right)}{\partial\theta^4}+O\left(h_\theta^4\right).$$

Taking the last equality into account, we rewrite equality (45) in the form:

$$\frac{\partial^2 c_r^n\left(x_i,y_j,1\right)}{\partial\theta^2}=-\varepsilon_r\frac{\partial\overline{c}_r^n\left(x_i,y_j,1\right)}{\partial\theta}+O\left(h_\theta\right). \tag{46}$$

It is straightforward to derive the following approximations with accuracy $O(h_x)$ and $O(h_y)$:

$$\frac{\partial\mu_{h,r}\left(x_i,y_j,1\right)}{\partial\theta}\cdot\frac{\partial^2 c_r^n\left(x_i,y_j,1\right)}{\partial x^2}\cong\frac{1}{h_\theta h_x^2}\left(\mu_{h,r}\left(x_i,y_j,0.5h_\theta\right)-\mu_{v,r}\left(x_i,y_j,-0.5h_\theta\right)\right)\cdot$$
$$\cdot\left(\overline{c}_r^n\left(x_i+h_x,y_j,1\right)-2\overline{c}_r^n\left(x_i,y_j,1\right)+\overline{c}_r^n\left(x_i-h_x,y_j,1\right)\right), \tag{47}$$

$$\frac{\partial\mu_{h,r}\left(x_i,y_j,1\right)}{\partial\theta}\frac{\partial^2 c_r^n\left(x_i,y_j,1\right)}{\partial y^2}\cong\frac{1}{h_\theta h_y^2}\left(\mu_{h,r}\left(x_i,y_j,0.5h_\theta\right)-\mu_{v,r}\left(x_i,y_j,-0.5h_\theta\right)\right)\cdot$$
$$\cdot\left(\overline{c}_r^n\left(x_i,y_j+h_y,1\right)-2\overline{c}_r^n\left(x_i,y_j,1\right)+\overline{c}_r^n\left(x_i,y_j-h_y,1\right)\right), \tag{48}$$

$$\left(\frac{\partial u^n\left(x_i,y_j,1\right)}{\partial\theta}-\frac{\partial^2\mu_{h,r}\left(x_i,y_j,1\right)}{\partial x\partial\theta}\right)\frac{\partial c_r^n\left(x_i,y_j,1\right)}{\partial x}\cong\frac{1}{2h_x}\left[\frac{1}{h_\theta}\left(u^n\left(x_i,y_j,1+0.5h_\theta\right)-u^n\left(x_i,y_j,1-0.5h_\theta\right)\right)-\right.$$
$$-\frac{1}{h_x h_\theta}\left(\mu_{v,r}\left(x_i+0.5h_x,y_j,1+0.5h_\theta\right)-\mu_{v,r}\left(x_i-0.5h_x,y_j,1+0.5h_\theta\right)-\right.$$
$$\left.\left.-\mu_{v,r}\left(x_i+0.5h_x,y_j,1-0.5h_\theta\right)+\mu_{v,r}\left(x_i-0.5h_x,y_j,1-0.5h_\theta\right)\right)\right]\left(\overline{c}_r^n\left(x_i+h_x,y_j,1\right)-\overline{c}_r^n\left(x_i-h_x,y_j,1\right)\right), \tag{49}$$

$$-\frac{1}{h_y h_\theta}\left(\mu_{v,r}\left(x_i,y_j+0.5h_y,1+0.5h_\theta\right)-\mu_{v,r}\left(x_i,y_j-0.5h_y,1+0.5h_\theta\right)-\right.$$
$$\left.\left.-\mu_{v,r}\left(x_i,y_j+0.5h_y,1-0.5h_\theta\right)+\mu_{v,r}\left(x_i,y_j-0.5h_y,1-0.5h_\theta\right)\right)\right]\left(\overline{c}_r^n\left(x_i,y_j+h_y,1\right)-\overline{c}_r^n\left(x_i,y_j-h_y,1\right)\right). \tag{50}$$

When approximating $c_r^n\left(x_i,y_j,1\right)$ we replace it with its discrete analogue $\overline{c}_r^n\left(x_i,y_j,1\right)$.
Then

$$\frac{\partial^2 u^n\left(x_i,y_j,1\right)}{\partial x\partial\theta}c_r^n\left(x_i,y_j,1\right)\cong\frac{1}{h_\theta}\left(\frac{u^n\left(x_i+0.5h_x,y_j,1+0.5h_\theta\right)-u^n\left(x_i-0.5h_x,y_j,1+0.5h_\theta\right)}{h_x}-\right.$$
$$\left.-\frac{u^n\left(x_i+0.5h_x,y_j,1-0.5h_\theta\right)-u^n\left(x_i-0.5h_x,y_j,1-0.5h_\theta\right)}{h_x}\right)c_r^n\left(x_i,y_j,1\right), \tag{51}$$

$$\frac{\partial^2 v^n(x_i,y_j,1)}{\partial y\partial\theta}c_r^n(x_i,y_j,1) \cong \frac{1}{h_\theta}\left(\frac{v^n(x_i,y_j+0.5h_y,1+0.5h_\theta)-v^n(x_i,y_j-0.5h_y,1+0.5h_\theta)}{h_y}-\right.$$
$$\left.-\frac{v^n(x_i,y_j+0.5h_y,1-0.5h_\theta)-v^n(x_i,y_j-0.5h_y,1-0.5h_\theta)}{h_y}\right)c_r^n(x_i,y_j,1), \quad (52)$$

$$\frac{w_{g,r}}{\mu_{v,r}(x_i,y_j,1)}\frac{\partial u^n(x_i,y_j,1)}{\partial x}c_r^n(x_i,y_j,1) \cong \frac{2w_{g,r}}{\mu_{v,r}(x_i,y_j,1+0.5h_\theta)+\mu_{v,r}(x_i,y_j,1-0.5h_\theta)}\cdot$$
$$\cdot\left(\frac{u^n(x_i+0.5h_x,y_j,1)-u^n(x_i-0.5h_x,y_j,1)}{h_x}\right)c_r^n(x_i,y_j,1), \quad (53)$$

$$\frac{w_{g,r}}{\mu_{v,r}(x_i,y_j,1)}\frac{\partial v^n(x_i,y_j,1)}{\partial y}c_r^n(x_i,y_j,1) \cong \frac{2w_{g,r}}{\mu_{v,r}(x_i,y_j,1+0.5h_\theta)+\mu_{v,r}(x_i,y_j,1-0.5h_\theta)}\cdot$$
$$\cdot\left(\frac{v^n(x_i,y_j+0.5h_y,1)-v^n(x_i,y_j-0.5h_y,1)}{h_y}\right)c_r^n(x_i,y_j,1), \quad (54)$$

$$\frac{2w_{g,r}}{H^2(x_i,y_j)\mu_{v,r}(x_i,y_j,1)}\frac{\partial^2\mu_{v,r}(x_i,y_j,1)}{\partial\theta^2}c_r^n(x_i,y_j,1) \cong \frac{2w_{g,r}}{H^2(x_i,y_j)\left(\mu_{v,r}(x_i,y_j,1+0.5h_\theta)+\mu_{v,r}(x_i,y_j,1-0.5h_\theta)\right)}\cdot$$
$$\cdot\frac{1}{h_\theta^2}\left(\mu_{v,r}(x_i,y_j,1+0.5h_\theta)-2\mu_{v,r}(x_i,y_j,1)+\mu_{v,r}(x_i,y_j,1-0.5h_\theta)\right)c_r^n(x_i,y_j,1). \quad (55)$$

As a result of substituting approximations (32), (37), (38), (43)–(55) into equality (26), with accuracy $O(h_\theta)$ (or higher), and rearranging the terms, we obtain:

$$\frac{\partial^3\overline{c}_r^n(x_i,y_j,1)}{\partial\theta^3} = \vartheta_1 + O(h_\theta), \quad (56)$$

where

$$\vartheta_1 = \vartheta_{10}\left(\vartheta_{11}\overline{c}_r^n(x_i,y_j,1-h_\theta)+\vartheta_{12}\overline{c}_r^n(x_i,y_j+h_y,1)+\vartheta_{13}\overline{c}_r^n(x_i,y_j-h_y,1)+\vartheta_{14}\overline{c}_r^n(x_i,y_j,1+h_\theta)+\right.$$
$$\left.+\vartheta_{15}\overline{c}(x_i,y_j,1-h_\theta)+\vartheta_{16}\overline{c}(x_i,y_j,1)\right).$$

After substituting the derived representations for the coefficients ϑ_{1i}, $i = 1..., 6$ into the approximation formula given above, one can obtain the final approximation of the third-kind boundary condition, which is not presented here due to its cumbersomeness.

Using equality (56) for $D_\theta\overline{c}_r^n(x_i,y_j,1)$, we can write:

$$D_\theta\overline{c}_r^n(x_i,y_j,1) \cong \frac{1}{H^2(x_i,y_j)h_\theta^2}\left[\left(\mu_{v,r}(x_i,y_j,1+0.5h_\theta)+\mu_{v,r}(x_i,y_j,1-0.5h_\theta)\right)\cdot\right.$$
$$\left.\cdot\left(\overline{c}_r^n(x_i,y_j,1-h_\theta)-\overline{c}_r^n(x_i,y_j,1)\right)-\mu_{v,r}(x_i,y_j,1+0.5h_\theta)\left(2h_\theta\,\varepsilon_r c_r^n(x_i,y_j,1)-\frac{h_\theta^3}{3}\vartheta_1\right)\right]. \quad (57)$$

The approximation error of scheme (57) at the boundary nodes of grid $\overline{\omega}^+$ for $\theta_k = 1$ is $O(\tau + h_\theta^2)$.

Discussion. The paper addresses issues related to the finite-difference approximation of a spatially three-dimensional problem of multifractional suspended matter transport. Certain difficulties arise in approximating this problem due to the necessity of ensuring the required order of approximation up to the boundary. Methods are proposed for approximating the problem with second-order accuracy in spatial variables and first-order accuracy in the temporal variable. Special attention should be given to studies related to the approximation of boundary conditions of the second and third kind. For this purpose, the authors propose methods based on approximations of boundary conditions using central difference formulas, followed by differentiation of both sides of the diffusion–convection equations and the elimination of solution functions at fictitious nodes of the extended grid.

Conclusion. Further research by the authors may focus on the analysis of the constructed difference schemes, taking into account physically motivated constraints on the time step size τ and the grid Peclet number.

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