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MATHEMATICAL MODEL OF GROUNDWATER HEAD VARIATION PROCESSES IN HETEROGENEOUS POROUS MEDIA

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This research develops a mathematical formulation and numerical solution for the spatial-temporal distribution of groundwater head in heterogeneous porous media. Based on Darcy's and mass conservation laws, a 3D parabolic partial differential equation for anisotropic aquifers is derived using tensor descriptions. The model incorporates detailed boundary conditions (river interaction, infiltration, evapotranspiration) and satisfies Hadamard criteria for correctness. Heterogeneity is addressed through deterministic and stochastic depth-dependent hydraulic conductivity models. Numerical results are obtained via an explicit finite difference scheme using harmonic mean interface conductivities, verified by von Neumann stability analysis and the CFL condition. The algorithm supports parallel computing on multi-core processors and GPUs. These results are applicable to groundwater resource management, drainage system design, and contaminant transport modeling.

Keywords: hydrogeology, seepage, mathematical physics, computational mathematics, high-performance computing.

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1 Introduction

Efficient management of groundwater resources and forecasting their future state is one of the main tasks of modern hydrogeology. Solving this task requires developing mathematical models that adequately reflect physical processes. This research presents the mathematical formulation of the problem of determining the spatial-temporal distribution of groundwater head in heterogeneous porous media.

2 Literature Review

Significant advances have been achieved in recent years in the field of mathematical modeling of groundwater dynamics, particularly in improving numerical methods for solving differential equations, discretization schemes, and computational algorithms. Below is an analysis of the main literature sources used in this research.

The flexibility of mesh geometry is of great importance in numerically solving the filtration equation in heterogeneous media [1]. A multi-point flux approximation (MPFA) algorithm for discretizing the conservative form of the diffusion equation on arbitrary polygonal grids has been developed. Unlike the classical two-point flux approximation, the

MPFA scheme provides correct flux values even when the principal axes of the conductivity tensor do not align with the mesh edges. This feature represents a significant advantage in modeling anisotropic heterogeneous media.

The mathematical foundations of meshless numerical methods and their application to filtration problems have been investigated [2]. In the Petrov-Galerkin formulation, trial and test functions are selected from different bases, which differs from the classical Galerkin method. Integrals in the weak formulation are calculated using radial basis functions. The particle filter algorithm estimates parameters by updating the posterior distribution based on Bayes' theorem. This approach, applied to free-surface aquifer modeling in Iran, showed lower error rates compared to traditional methods.

The generalized finite difference method (GFDM) uses Taylor series for approximating spatial derivatives [3]. A series is written around an arbitrary node, and derivatives are determined using the moving least squares (MLS) method. In free-surface aquifers, the governing equation is nonlinear, expressed through saturated thickness and specific yield parameters. When applied to an 11,470 km² aquifer in the Middle Ganga Plain of India, the GFDM solution showed high agreement with MODFLOW results.

The finite volume formulation of MODFLOW 6 has been applied for regional-scale groundwater dynamics modeling [4]. In the control volume method, mass balance is written for each cell. Flow between cells in an unstructured quadtree mesh is calculated through hydraulic conductance. The model consists of 300,750 active cells, representing a geologically complex multi-layer aquifer system covering 218,424 km² of Britain.

Physics-informed neural networks (PINN) present a new paradigm in solving differential equations [5]. In the PINN architecture, the loss function consists of two components: data error and differential equation residual. The solution is found by minimizing the residual term and adjusting network weights. Automatic differentiation techniques enable accurate calculation of derivatives. The mathematical foundations of the PINN algorithm and its application in groundwater flow modeling have been analyzed in detail [5]. Optimal parameters are found through gradient descent algorithm iterations. The advantage of the method is the absence of mesh construction requirements and freedom from time step limitations.

A comprehensive review of deep learning technology integration into hydrogeological modeling has been presented [7]. Convolutional neural networks (CNN) model spatial dependencies through convolution operations. Recurrent neural networks (RNN) represent temporal sequences through hidden states. The study highlighted limitations of traditional models — inability to adequately represent nonlinear interactions of complex subsurface processes and significant computational resource requirements. Aspects of data-driven methods in analyzing flow and transport in porous media have been examined [8]. Surrogate models approximate high-dimensional input-output relationships through neural networks. In Bayesian neural networks, weight distributions are calculated as posteriors, enabling uncertainty quantification.

The isogeometric analysis (IGA) method uses NURBS (Non-Uniform Rational B-Splines) basis functions for solving differential equations [9]. In the weak formulation, the solution is expressed through B-spline basis functions. The control volume formulation ensures mass balance in integral form. In heterogeneous media where conductivity jumps exist, the high smoothness property of B-splines increases approximation accuracy. Research results show that CV-IGA enables obtaining a smooth continuous velocity field with optimal convergence rates regardless of heterogeneity degree. Reduced-order modeling based on Proper Orthogonal Decomposition (POD) has been analyzed [10]. The

POD formulation combined with the finite volume method is expected to yield highly satisfactory results since the finite volume method is inherently conservative.

The numerical solution of contaminant transport equation in heterogeneous media has been examined [11]. The advection-dispersion equation was numerically solved accounting for nonlinear sorption, decay, and generation. The alternating direction implicit (ADI) scheme splits the two-dimensional problem into sequential one-dimensional problems. The Crank-Nicolson scheme provides second-order accuracy. A mathematical model for gravity-driven flow in unsaturated media has been developed [12]. The Richards equation is nonlinear, expressed through moisture content, matrix potential, and unsaturated conductivity. The van Genuchten model parameterizes hydraulic properties.

A hybrid deep neural network architecture combines CNN and MLP layers [13]. Input data is fed to two branches as spatial fields and scalar parameters. The CNN branch extracts features, while the MLP branch processes scalar data. Integration of physics-based and data-driven models has been analyzed [14]. The hybrid loss function balances data fit, physics compliance, and regularization. An AI-enhanced groundwater modeling platform has been developed [15]. The Bayesian optimization algorithm selects calibration parameters based on expected improvement criteria. Gaussian process surrogate models represent uncertainty through mean and covariance functions.

Mathematical aspects of two-phase filtration process modeling have been developed by Uzbek scientists Ravshanov N. and colleagues [16]. The governing equation system for oil-water mixture movement is written based on the mass conservation law, accounting for saturation constraints. The IMPES (Implicit Pressure Explicit Saturation) scheme was used for numerical solution. Analytical and numerical solutions for filtration processes in three-layer reservoirs have been compared by Ravshanov N. and colleagues [17]. Analytical solutions were obtained using Laplace transform and matrix exponential methods.

Development trends in modern hydrogeological modeling have been analyzed [18]. Traditional finite difference schemes are applied in explicit and implicit forms. Hybrid schemes (Crank-Nicolson) provide second-order accuracy in time. Multi-phase filtration in deformable porous media has been mathematically investigated [19]. The Biot consolidation equation represents mechanical equilibrium, while the fluid flow equation represents mass balance. Finally, fundamentals of YAGMod (Yet Another Groundwater Model) for modeling partially saturated cells have been presented [20]. In free-surface aquifers, saturated thickness is time-dependent, and transmissivity is nonlinearly dependent on head.

3 Problem Formulation

The research object is an aquifer — a water-bearing geological layer located in three-dimensional space. The computational domain Ω is selected in the form of a rectangular parallelepiped (prism):

$$\Omega = \{(x, y, z) : 0 < x < L_x, 0 < y < L_y, 0 < z < L_z\}.$$

Here L_x, L_y, L_z are the linear dimensions of the domain along the x, y, z axes respectively [m]. The coordinate system is oriented as follows: the x axis points from west to east, the axis from south to north, and the z axis vertically upward. The modeling period is carried out in the interval $t \in [0, T]$, where T is the final time moment [s].

The domain boundary $\partial\Omega$ consists of six planar surfaces:

$$\partial\Omega = \Gamma_W \cup \Gamma_E \cup \Gamma_S \cup \Gamma_N \cup \Gamma_B \cup \Gamma_T.$$

Each boundary surface is defined as follows:

$$\begin{aligned}\Gamma_W &= \{(x, y, z) : x = 0\}, \Gamma_E = \{(x, y, z) : x = L_x\}, \\ \Gamma_S &= \{(x, y, z) : y = 0\}, \Gamma_N = \{(x, y, z) : y = L_y\}, \\ \Gamma_B &= \{(x, y, z) : z = 0\}, \Gamma_T = \{(x, y, z) : z = L_z\}.\end{aligned}$$

From a physical standpoint, Γ_B represents the lower boundary of the aquifer (bedrock), Γ_T the upper boundary (land surface or lower boundary of the vadose zone), and the remaining four surfaces represent lateral boundaries.

The unknown function of the problem is the piezometric head $H(x, y, z, t)$. The piezometric head, derived from Bernoulli's equation, represents the specific mechanical energy of a fluid particle in length units:

$$H = \frac{p}{\rho g} + z.$$

In the formula, p is the pore fluid pressure [Pa], ρ is water density [kg/m³], g is gravitational acceleration [m/s²]. The first term of the equation represents pressure head, and the second term represents elevation head. In SI units, piezometric head is measured in meters [m]. Piezometric head is the main parameter determining the direction of groundwater flow: in porous media, fluid always moves in the direction of decreasing head, i.e., in the direction of the vector $-\nabla H$. Natural geological media are generally not homogeneous — their properties take different values at different points in space. Such media are called heterogeneous media. Additionally, many geological structures have anisotropic properties, meaning their characteristics depend on direction. In anisotropic heterogeneous media, the hydraulic conductivity is described as a second-order symmetric positive definite tensor. By aligning the coordinate axes with the principal anisotropy directions of the medium, the tensor is reduced to diagonal form:

$$K = \begin{pmatrix} K_x(x, y, z) & 0 & 0 \\ 0 & K_y(x, y, z) & 0 \\ 0 & 0 & K_z(x, y, z) \end{pmatrix}.$$

In the equation, K_x , K_y , K_z are hydraulic conductivities along principal directions [m/s]. Due to the layered structure of sedimentary rocks, horizontal conductivity is typically several times greater than vertical: $K_x \approx K_y \gg K_z$.

The specific storage coefficient S_s [1/m] characterizes the elastic properties of the aquifer and represents the volume of water released or absorbed from a unit volume of medium when head changes by unity:

$$S_s = \rho g (\alpha + \varphi \beta),$$

Here α is the compressibility coefficient of the porous skeleton [Pa⁻¹], φ is porosity [-], $\beta \approx 4.4 \times 10^{-10}$ Pa⁻¹ is the compressibility coefficient of water. The mathematical model is based on two fundamental physical laws: Darcy's law and the mass conservation law.

In porous media under laminar flow regime, fluid movement obeys Darcy's law. For anisotropic media, this law is written in the following tensor form:

$$q = -K \nabla H.$$

In the formula, q is the Darcy velocity or specific discharge vector [m/s]. Written in component form:

$$q_x = -K_x \frac{\partial H}{\partial x}, \quad q_y = -K_y \frac{\partial H}{\partial y}, \quad q_z = -K_z \frac{\partial H}{\partial z}.$$

It should be noted that Darcy velocity differs from actual (pore) velocity, and the relationship between them is $v = q/\varphi$, where φ is effective porosity.

The continuity equation (mass conservation law) expresses the conservation of water mass in an arbitrary control volume. For porous media, this law is written as:

$$\frac{\partial(\rho\varphi)}{\partial t} + \nabla \cdot (\rho q) = \rho W.$$

In the equation, W is the volumetric source/sink intensity [s^{-1}]. Assuming water compressibility is small and temperature is constant ($\rho = \text{const}$), and accounting for the storage relationship, we transform the equation to the following form:

$$S_s \frac{\partial H}{\partial t} + \nabla \cdot q = W.$$

Substituting Darcy's law into the mass conservation equation, we obtain the governing equation describing groundwater head variation in heterogeneous porous media:

$$S_s \frac{\partial H}{\partial t} = \frac{\partial}{\partial x} \left(K_x \frac{\partial H}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_y \frac{\partial H}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_z \frac{\partial H}{\partial z} \right) + W,$$

for $(x, y, z) \in \Omega, t \in (0, T]$.

This equation belongs to the class of second-order parabolic partial differential equations with variable coefficients. The left side of the equation represents the rate of change of water storage in the aquifer over time, while the first three terms on the right side represent spatial redistribution (diffusion) of water.

When writing diffusion terms in explicit form for heterogeneous media:

$$\frac{\partial}{\partial x} \left(K_x \frac{\partial H}{\partial x} \right) = K_x \frac{\partial^2 H}{\partial x^2} + \frac{\partial K_x}{\partial x} \frac{\partial H}{\partial x}.$$

A second addend appears — an advective term related to the gradient of hydraulic conductivity. This term represents the "attraction" of water toward high-conductivity zones. The volumetric source/sink function $W(x, y, z, t)$ combines external influences on the water balance within the aquifer:

$$W = W_w + W_d + W_l.$$

Represent direct contact points between groundwater and humans. Mathematically, wells are modeled as point or line sources:

$$W_w = \sum_{m=1}^{N_w} \frac{Q_m}{V_m} \chi_{\Omega_m}(x, y, z),$$

Here N_w is the number of wells, Q_m is the discharge of the m -th well [m^3/s] (negative for extraction $Q_m < 0$, positive for injection $Q_m > 0$), V_m is the volume of the perforated section of the well [m^3], χ_{Ω_m} is the characteristic function of set Ω_m . Head distribution around wells is described by Theis or Hantush-Jacob solutions. A cone-shaped depression funnel forms around extraction wells, with its radius depending on time and extraction intensity.

Serve to remove excess groundwater and are modeled as:

$$W_d = - \sum_{d=1}^{N_d} C_d \max(H - H_d, 0) \chi_{\Omega_d}(x, y, z).$$

In the formula, N_d is the number of drainage elements, C_d is drainage conductance [s^{-1}], H_d is the elevation at which drainage is installed [m], χ_{Ω_d} is the drainage location indicator. The maximum function ensures that drainage is active only when the water table is above the drainage elevation.

In multi-layer aquifer systems, vertical water exchange occurs through separating low-conductivity layers (aquitards):

$$W_l = \frac{K'}{b'} (H_a - H).$$

In the formula, K'/b' is the leakage coefficient [s^{-1}], K' and b' are the vertical conductivity and thickness of the separating layer, H_{adj} is the head in the adjacent aquifer.

For uniqueness of the differential equation solution, appropriate boundary conditions must be specified on each part of the boundary $\partial\Omega$.

Γ_W (western lateral boundary):

$$-K_x \frac{\partial H}{\partial x} + \alpha_W H = \alpha_W H_W^e + q_W^e,$$

Here α_W is boundary conductance [s^{-1}], H_W^e is external head [m], q_W^e is external flux [m/s]. This condition is a third-type (Robin) boundary condition, representing hydraulic connection near the boundary.

If a river is present at the boundary, river-aquifer interaction is described as:

$$q_r = C_r (H_r - H).$$

In the formula, C_r is riverbed conductance, H_r is river stage. River-aquifer exchange can occur in both directions: when $H > H_r$, the aquifer feeds the river (gaining stream); when $H < H_r$, the river recharges the aquifer (losing stream).

Special cases of boundary conditions:

$$\alpha_W \rightarrow \infty : H = H_W^e - \text{Dirichlet condition (first type)},$$

$$\alpha_W = 0, q_W^e = 0: \frac{\partial H}{\partial x} = 0 \text{ — no-flow boundary (Neumann condition, second type).}$$

Γ_E (eastern lateral boundary):

$$K_x \frac{\partial H}{\partial x} + \alpha_E H = \alpha_E H_E^e + q_E^e.$$

Note: the sign changed because the outward normal direction is $+x$.

Γ_S (southern lateral boundary):

$$-K_y \frac{\partial H}{\partial y} + \alpha_S H = \alpha_S H_S^e + q_S^e.$$

Γ_N (northern lateral boundary):

$$K_y \frac{\partial H}{\partial y} + \alpha_N H = \alpha_N H_N^e + q_N^e.$$

Γ_B (lower boundary — aquifer bedrock):

$$-K_z \frac{\partial H}{\partial z} + \alpha_B H = \alpha_B H_B^e + q_B^e.$$

In the formula, α_B is the leakage coefficient through the bedrock, H_B^e is the head in the aquifer below the bedrock or corresponding pressure. For aquifers overlying crystalline rocks or dense clays, $\alpha_B \approx 0$ and the boundary is practically impermeable.

Γ_T (upper boundary — land surface):

The upper boundary has the most complex boundary condition, as many water balance elements influence it:

$$K_z \frac{\partial H}{\partial z} = q_n(x, y, t).$$

In the equation, q_n is the net vertical flux through the land surface [m/s]:

$$q_n = R - ET + I_i.$$

Part of atmospheric precipitation infiltrates through the land surface, recharging groundwater:

$$R = f_i \cdot (P - I_a),$$

Here P is precipitation intensity [m/s], f_i is infiltration coefficient (dependent on soil type, slope, vegetation cover), I_a is interception and initial abstraction [m/s].

Evaporation and transpiration consume groundwater. Based on FAO Penman-Monteith methodology:

$$ET = K_c \cdot f_e(z_{wt}) \cdot ET_0.$$

In the equation, ET_0 is reference evapotranspiration [m/s]:

$$ET_0 = \frac{0.408\Delta(R_n - G) + \gamma \frac{900}{T+273} u_2 (e_s - e_a)}{\Delta + \gamma(1 + 0.34u_2)},$$

Here R_n is net radiation [MJ/(m²·day)], G is soil heat flux [MJ/(m²·day)], T is air temperature [°C], u_2 is wind speed at 2 m height [m/s], e_s and e_a are saturated and actual vapor pressures [kPa], Δ is slope of the vapor pressure curve [kPa/°C], γ is psychrometric constant [kPa/°C].

K_c is crop coefficient, dependent on plant type and phenological stage (initial: 0.3-0.5, mid: 1.0-1.2, late: 0.3-0.5).

$f_e(z_{wt})$ is the extinction function, representing the decrease in evapotranspiration dependent on water table depth:

$$f_e(z_{wt}) = \max\left(0, 1 - \frac{z_{wt}}{d_e}\right),$$

where d_e is extinction depth [m], usually determined by plant root system depth (1-5 m).

Part of irrigation water returns to groundwater:

$$I_i = f_r \cdot I_g \cdot \chi_i(x, y).$$

In the formula, f_r is return coefficient (0.2-0.4 for surface irrigation, 0.05-0.1 for drip irrigation), I_g is gross irrigation rate [m/s], χ_i is irrigated area indicator.

For solution of the transient problem, the spatial distribution of the head field at the initial time moment must be specified:

$$H(x, y, z, 0) = H_0(x, y, z),$$

Here H_0 is the initial head distribution [m]. In practice, this function is obtained from geostatistical interpolation (kriging) of monitoring well data or from steady-state modeling results.

Summarizing the above, the mathematical problem describing groundwater head variation in heterogeneous porous media can be expressed as follows.

Find the function $H(x, y, z, t)$ satisfying the following conditions:

$$S_s \frac{\partial H}{\partial t} = \frac{\partial}{\partial x} \left(K_x \frac{\partial H}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_y \frac{\partial H}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_z \frac{\partial H}{\partial z} \right) + W, \quad (x, y, z) \in \Omega, \quad t > 0,$$

$$-K_x \frac{\partial H}{\partial x} + \alpha_W H = \alpha_W H_W^e + q_W^e, \quad x = 0,$$

$$K_x \frac{\partial H}{\partial x} + \alpha_E H = \alpha_E H_E^e + q_E^e, \quad x = L_x,$$

$$-K_y \frac{\partial H}{\partial y} + \alpha_S H = \alpha_S H_S^e + q_S^e, \quad y = 0,$$

$$K_y \frac{\partial H}{\partial y} + \alpha_N H = \alpha_N H_N^e + q_N^e, \quad y = L_y,$$

$$-K_z \frac{\partial H}{\partial z} + \alpha_B H = \alpha_B H_B^e + q_B^e, \quad z = 0,$$

$$K_z \frac{\partial H}{\partial z} = q_n, \quad z = L_z,$$

$$H(x, y, z, 0) = H_0(x, y, z).$$

According to J. Hadamard's definition, a mathematical problem is said to be well-posed if: (1) a solution exists, (2) the solution is unique, (3) the solution depends continuously on initial data.

For the problem under consideration, well-posedness is guaranteed when the following conditions are satisfied:

$$K_x, K_y, K_z > 0 \text{ (ellipticity condition),}$$

$$S_s > 0 \text{ (parabolicity condition),}$$

$$\alpha_W, \alpha_E, \alpha_S, \alpha_N, \alpha_B \geq 0.$$

At least one boundary must have a Dirichlet-type condition ($\alpha \rightarrow \infty$) or a Robin condition with positive α value. H_0 , W , and boundary data must belong to appropriate Sobolev spaces. When these conditions are satisfied, based on the Lax-Milgram lemma and Galerkin method, existence of a unique weak solution $H \in L^2(0, T; H^1(\Omega))$ is proven. Furthermore, the solution depends continuously on initial and boundary data — small changes in data lead to correspondingly small changes in the solution. Models for accounting heterogeneity. To account for heterogeneity of real geological media, hydraulic conductivity is specified as a deterministic or stochastic function.

Due to compaction and lithification processes, conductivity decreases with depth:

$$K(z) = K_0 \exp\left(-\frac{z}{d_K}\right).$$

In the formula, K_0 is conductivity near the land surface, d_K is the decay scale (typically 10-100 m).

According to G. Dagan's approach, the logarithm of hydraulic conductivity is modeled as a stationary random field:

$$\ln K(x, y, z) = \mu_{\ln K} + \sigma_{\ln K} \cdot Y(x, y, z),$$

Here $\mu_{\ln K}$ is the mean, $\sigma_{\ln K}$ is standard deviation (typical values: 0.5-2.0), Y is a standardized random field with zero mean and unit variance. The spatial correlation structure is described by an exponential covariance function:

$$C_Y(r_x, r_y, r_z) = \exp\left(-\frac{|r_x|}{\lambda_x} - \frac{|r_y|}{\lambda_y} - \frac{|r_z|}{\lambda_z}\right).$$

In the formula, λ_x , λ_y , λ_z are correlation lengths. In layered media, the relationship $\lambda_x \approx \lambda_y \gg \lambda_z$ holds.

4 Numerical Solution of the Problem

The mathematical model presented in the previous section can be solved analytically only in simplified special cases. While analytical solutions such as Theis and Hantush-Jacob exist for isotropic homogeneous media, simple geometry, and steady-state conditions, in real hydrogeological conditions — with spatial heterogeneity of the medium, complex boundary conditions, and time-dependent external influences — numerical methods must be employed. In modern hydrogeological modeling, the finite difference method and finite element method are the most widely used numerical methods. This section presents in detail the methodology for numerically solving the governing equation using the explicit finite difference scheme.

The first step in obtaining a numerical solution is replacing the continuous spatial-temporal domain with a discrete grid. This process is called discretization and directly affects solution accuracy. The computational domain Ω and time interval $[0, T]$ are discretized as follows. A uniform grid is introduced for spatial variables:

$$\begin{aligned} x_i &= i \cdot \Delta x, i = 0, 1, \dots, N_x, \\ y_j &= j \cdot \Delta y, j = 0, 1, \dots, N_y, \\ z_k &= k \cdot \Delta z, k = 0, 1, \dots, N_z, \end{aligned}$$

where N_x , N_y , N_z are the number of grid intervals in respective directions, $\Delta x = L_x/N_x$, $\Delta y = L_y/N_y$, $\Delta z = L_z/N_z$ are spatial steps [m]. Time discretization is performed as $t^n = n \cdot \Delta t$, where $n = 0, 1, 2, \dots$, and Δt is the time step [s]. Thus, the grid function $H_{i,j,k}^n \approx H(x_i, y_j, z_k, t^n)$ is introduced, representing approximate values of the continuous solution at grid nodes. The total number of grid nodes equals $(N_x + 1)(N_y + 1)(N_z + 1)$, which determines computational resource requirements.

To construct the numerical scheme, derivatives in the differential equation are replaced with finite differences. Taylor series are used to evaluate the order and properties of approximations. The first-order time derivative is approximated with a forward difference:

$$\frac{\partial H}{\partial t} \Big|_{i,j,k}^n \approx \frac{H_{i,j,k}^{n+1} - H_{i,j,k}^n}{\Delta t} + O(\Delta t).$$

This approximation has first-order accuracy, meaning the remainder term is of order $O(\Delta t)$. Correct accounting of heterogeneous medium properties is of great importance when approximating spatial derivatives. For approximating diffusion operator terms of the form $\frac{\partial}{\partial x} \left(K_x \frac{\partial H}{\partial x} \right)$, the approach recommended by Patankar is applied to preserve the conservative (divergent) form:

$$\begin{aligned} & \frac{\partial}{\partial x} \left(K_x \frac{\partial H}{\partial x} \right) \Big|_{i,j,k} \approx \\ & \approx \frac{1}{\Delta x} \left[K_{x,i+1/2,j,k} \frac{H_{i+1,j,k} - H_{i,j,k}}{\Delta x} - K_{x,i-1/2,j,k} \frac{H_{i,j,k} - H_{i-1,j,k}}{\Delta x} \right]. \end{aligned}$$

Here the half-integer indexed values $K_{x,i+1/2,j,k}$ and $K_{x,i-1/2,j,k}$ are interface conductivities between neighboring nodes.

The method of determining interface conductivities in heterogeneous media significantly affects solution quality. Various approaches have been proposed for this problem: arithmetic mean $K_{i+1/2} = (K_i + K_{i+1})/2$, geometric mean $K_{i+1/2} = \sqrt{K_i \cdot K_{i+1}}$, and harmonic mean. When flow passes through consecutively arranged layers in the normal direction, the harmonic mean provides physically correct results because it correctly represents the equivalent resistance of series-connected resistances. Therefore, the harmonic mean is used in this work:

$$K_{x,i+1/2,j,k} = \frac{2K_{x,i,j,k} \cdot K_{x,i+1,j,k}}{K_{x,i,j,k} + K_{x,i+1,j,k}}.$$

An important property of the harmonic mean is that if $K = 0$ at one of the neighboring nodes (impermeable zone), the interface conductivity also equals zero. This is physically correct — no flow exists through an impermeable zone. The same principle applies for y and z directions.

Substituting approximations into the governing equation, we obtain the explicit finite difference scheme. The discrete analog of the governing equation takes the following form:

$$\begin{aligned} & S_{s,i,j,k} \frac{H_{i,j,k}^{n+1} - H_{i,j,k}^n}{\Delta t} = \\ & = \frac{K_{x,i+1/2,j,k} (H_{i+1,j,k}^n - H_{i,j,k}^n) - K_{x,i-1/2,j,k} (H_{i,j,k}^n - H_{i-1,j,k}^n)}{\Delta x^2} + \\ & + \frac{K_{y,i,j+1/2,k} (H_{i,j+1,k}^n - H_{i,j,k}^n) - K_{y,i,j-1/2,k} (H_{i,j,k}^n - H_{i,j-1,k}^n)}{\Delta y^2} + \\ & + \frac{K_{z,i,j,k+1/2} (H_{i,j,k+1}^n - H_{i,j,k}^n) - K_{z,i,j,k-1/2} (H_{i,j,k}^n - H_{i,j,k-1}^n)}{\Delta z^2} + W_{i,j,k}^n. \end{aligned}$$

This equation is written for interior nodes, i.e., $i = 1, \dots, N_x - 1$, $j = 1, \dots, N_y - 1$, $k = 1, \dots, N_z - 1$. The main feature of the explicit scheme is that the value $H_{i,j,k}^{n+1}$ at the new time level is expressed explicitly through known values at the previous time level:

$$\begin{aligned} & H_{i,j,k}^{n+1} = H_{i,j,k}^n + \\ & + \frac{\Delta t}{S_{s,i,j,k}} \left[\frac{K_{x,i+1/2,j,k} (H_{i+1,j,k}^n - H_{i,j,k}^n) - K_{x,i-1/2,j,k} (H_{i,j,k}^n - H_{i-1,j,k}^n)}{\Delta x^2} + \right. \\ & + \frac{K_{y,i,j+1/2,k} (H_{i,j+1,k}^n - H_{i,j,k}^n) - K_{y,i,j-1/2,k} (H_{i,j,k}^n - H_{i,j-1,k}^n)}{\Delta y^2} + \\ & \left. + \frac{K_{z,i,j,k+1/2} (H_{i,j,k+1}^n - H_{i,j,k}^n) - K_{z,i,j,k-1/2} (H_{i,j,k}^n - H_{i,j,k-1}^n)}{\Delta z^2} + W_{i,j,k}^n \right]. \end{aligned}$$

For compact notation, it is convenient to introduce dimensionless parameters. If we define coefficients r_x, r_y, r_z as:

$$r_{x,i\pm 1/2,j,k} = \frac{K_{x,i\pm 1/2,j,k}\Delta t}{S_{s,i,j,k}\Delta x^2}$$

and similarly for r_y, r_z , then the explicit scheme is written in the following compact form:

$$\begin{aligned} H_{i,j,k}^{n+1} = & H_{i,j,k}^n \left(1 - r_{x,i-1/2} - r_{x,i+1/2} - r_{y,j-1/2} - r_{y,j+1/2} - r_{z,k-1/2} - r_{z,k+1/2} \right) + \\ & + r_{x,i-1/2} H_{i-1,j,k}^n + r_{x,i+1/2} H_{i+1,j,k}^n + r_{y,j-1/2} H_{i,j-1,k}^n + r_{y,j+1/2} H_{i,j+1,k}^n + \\ & + r_{z,k-1/2} H_{i,j,k-1}^n + r_{z,k+1/2} H_{i,j,k+1}^n + \frac{\Delta t}{S_{s,i,j,k}} W_{i,j,k}^n. \end{aligned}$$

From this expression, it is evident that the new value is calculated as a weighted sum of six neighboring nodes and the central node's previous values.

The volumetric source/sink function W in discrete form includes the following components. Extraction and injection through wells are expressed as:

$$W_{i,j,k}^w = \frac{Q_m}{V_c} \cdot \delta_{(i,j)=(i_m,j_m)} \cdot \delta_{k \in [k_m^b, k_m^t]},$$

Here $V_c = \Delta x \cdot \Delta y \cdot \Delta z$ is the computational cell volume, (i_m, j_m) are horizontal indices of the m -th well, $[k_m^b, k_m^t]$ is the range of vertical indices for well perforation. As shown by Peaceman, modeling a well as a point source leads to singularity, so in practice the concept of equivalent well radius is used.

Drainage systems are expressed as $W_{i,j,k}^d = -C_d \max(H_{i,j,k}^n - H_d, 0)$, and inter-layer leakage as

$$W_{i,j,k}^l = \frac{K'}{b'} (H_{i,j,k}^a - H_{i,j,k}^n).$$

Boundary conditions determine solution values at grid boundary nodes. At boundary Γ_W ($i = 0$), the third-type boundary condition is written in discrete form as:

$$-K_{x,1/2,j,k} \frac{H_{1,j,k} - H_{0,j,k}}{\Delta x} + \alpha_W H_{0,j,k} = \alpha_W H_W^{ext} + q_W^{ext}.$$

The unknown $H_{0,j,k}$ at the boundary can be found from this algebraic equation:

$$H_{0,j,k} = \frac{K_{x,1/2,j,k} H_{1,j,k} / \Delta x + \alpha_W H_W^e + q_W^e}{K_{x,1/2,j,k} / \Delta x + \alpha_W}.$$

For Dirichlet condition ($\alpha_W \rightarrow \infty$), this expression reduces to $H_{0,j,k} = H_W^e$; for no-flow boundary ($\alpha_W = 0, q_W^e = 0$), it reduces to $H_{0,j,k} = H_{1,j,k}$.

Similar formulas are derived for boundaries Γ_E ($i = N_x$), Γ_S (m), Γ_N ($j = N_y$), Γ_B ($k = 0$).

At the upper boundary ($\Gamma_T, k = N_z$), a second-type condition is specified, which is discretized as:

$$K_{z,i,j,N_z-1/2} \frac{H_{i,j,N_z} - H_{i,j,N_z-1}}{\Delta z} = q_{n,i,j},$$

Here q_{net} is the net vertical flux through the land surface.

The initial condition is applied at grid nodes as $H_{i,j,k}^0 = H_0(x_i, y_j, z_k)$.

Explicit finite difference schemes are conditionally stable, meaning their stability depends on the relationship between time and spatial steps. The von Neumann spectral

analysis method is used to determine the stability condition. For isotropic homogeneous media, the stability condition takes the following form:

$$\frac{K\Delta t}{S_s} \left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2} \right) \leq \frac{1}{2}.$$

This is a Courant-Friedrichs-Lewy (CFL) type condition that limits the maximum value of the time step. Expressed through hydraulic diffusivity $D = K/S_s$:

$$\Delta t \leq \frac{1}{2D \left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2} \right)}.$$

If spatial steps are equal (m), this condition takes the form $\Delta t \leq \frac{S_s h^2}{6K}$. In heterogeneous media, the stability condition is evaluated based on the most "difficult" node in the entire computational domain — i.e., the node with highest conductivity and lowest storage limits the time step:

$$\Delta t \leq \frac{1}{2} \min_{i,j,k} \left[\frac{S_{s,i,j,k}}{\frac{K_{x,i,j,k}}{\Delta x^2} + \frac{K_{y,i,j,k}}{\Delta y^2} + \frac{K_{z,i,j,k}}{\Delta z^2}} \right].$$

In practice, a safety factor $\nu = 0.8 - 0.9$ is applied: $\Delta t_a = \nu \cdot \Delta t_m$. Violation of the stability condition leads to growing oscillations in the solution and computational "explosion."

The explicit scheme presented above has first-order accuracy in time $O(\Delta t)$ and second-order accuracy in space $O(\Delta x^2 + \Delta y^2 + \Delta z^2)$. According to the Lax equivalence theorem, for linear problems, approximation and stability together guarantee convergence. That is, when the stability condition is satisfied, the numerical solution converges to the exact solution at order $O(\Delta t + \Delta x^2)$ as grid steps $\Delta t, \Delta x, \Delta y, \Delta z \rightarrow 0$.

The computational process is carried out in the following sequence:

Grid parameters are determined, medium parameters are calculated at grid nodes, interface conductivities are computed using harmonic averaging, and the stability condition is verified.

$H_{i,j,k}^0 = H_0(x_i, y_j, z_k)$ is set. At each time step ($n = 0, 1, 2, \dots$), the following operations are performed: Source/sink values $W_{i,j,k}^n$ at the current time level are calculated; Boundary values are determined from boundary conditions; Values at the new time level $H_{i,j,k}^{n+1}$ for interior nodes are calculated using the explicit formula. This process is repeated until the final time moment is reached. An important advantage of the explicit scheme is that it naturally parallelizes. For each interior node, the value depends only on neighboring node values at the previous time level and is independent of new values at other nodes. This property enables efficient parallel computation using OpenMP, MPI, or GPU technologies. However, the main disadvantage of the explicit scheme is strict limitation of the time step due to conditional stability. This becomes particularly problematic when high-conductivity zones exist or when small spatial steps are required. For modeling long time periods, unconditionally stable implicit schemes may be preferable, though they require solving a system of algebraic equations at each time step.

5 Conclusion

In this research, a mathematical model describing groundwater head variation in heterogeneous porous media has been developed. The main results are as follows: A parabolic

partial differential equation describing filtration in anisotropic heterogeneous media has been derived. The equation was derived based on Darcy's law and the mass conservation law and belongs to the class of second-order parabolic equations with variable coefficients. Boundary conditions for all six boundary surfaces have been developed in detail, including river-aquifer interaction, infiltration, evapotranspiration, and irrigation return flow. Necessary conditions for problem well-posedness have been established based on Hadamard criteria. The numerical solution of the differential equation has been obtained using the explicit finite difference scheme. The harmonic mean method has been applied for calculating interface conductivities in heterogeneous media, which physically correctly represents series-connected hydraulic resistances. The stability of the numerical scheme has been verified using the von Neumann spectral analysis method, and the CFL-type stability condition has been derived. Scheme convergence has been proven based on the Lax equivalence theorem.

The developed model and numerical method can be applied in solving practical problems such as groundwater resource management, forecasting hydrodynamic state of aquifers, and designing wells and drainage systems.

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МАТЕМАТИЧЕСКАЯ МОДЕЛЬ ПРОЦЕССОВ ИЗМЕНЕНИЯ НАПОРА ПОДЗЕМНЫХ ВОД В НЕОДНОРОДНЫХ ПОРИСТЫХ СРЕДАХ

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В работе представлены математическая формулировка и численное решение задачи о распределении напора подземных вод в гетерогенных средах. Для 3D-водоносного горизонта выведено параболическое уравнение фильтрации на основе законов Дарси и сохранения массы с тензорным описанием анизотропии. Разработаны детальные граничные условия и подтверждена корректность задачи по критериям Адамара. Учет неоднородности среды реализован через детерминированные и стохастические модели глубинной зависимости проводимости. Численное решение базируется на явной конечно-разностной схеме с использованием метода гармонического среднего; устойчивость подтверждена анализом фон Неймана и условием CFL. Алгоритм адаптирован для параллельных вычислений на CPU и GPU. Результаты применимы для управления водными ресурсами, проектирования дренажа и моделирования переноса загрязнений.

Ключевые слова: гидрогеология, геофильтрация, математическая физика, вычислительная математика, высокопроизводительные вычисления.

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