

A PHYSICO-MATHEMATICAL MODEL FOR SOLUTE TRANSPORT IN GROUNDWATER

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ABSTRACT. In this paper a model for solute transport in groundwater, including physico-mathematical basis, numerical method some simple example simulations is briefly presented. This model has been gradually improved in both simulation and methodology.

1. Introduction

Water quality becomes a limiting factor in the development and the use of water resources. In some regions, the quality of both surface and groundwater resources deteriorates, special attention should be devoted to the pollution of groundwater in aquifer. Serious environmental problems arise when polluted groundwater emerges at ground surface or discharges into rivers and lakes.

The objective of this study is to illustrate the laws governing the movement and accumulation of pollutant in groundwater flow, and to develop numerical scheme that can be used to simulate pollutant's distribution in aquifer. A system of computer programs, named STG version 1.0, has been developed and its results are also verified by comparing with analytical solutions.

2. Physico-Mathematical basis

2.1. The motion equation of groundwater flow

The mechanisms of density and pressure force for flow are expressed by a general form of Darcy's law to describe fluid flow in porous media [1]:

$$\mathbf{v} = -\frac{k_r}{\varepsilon s \mu} \mathbf{k} [\nabla p - \rho_1 \mathbf{g}] \quad (2.1)$$

where $\nabla = (\partial/\partial x, \partial/\partial y, \partial/\partial z)$, \mathbf{v} is the fluid flow vector, p - the pressure at point $\mathbf{r} = (x, y, z)$ in the flow domain, ε - porosity, ρ_1 - fluid density, μ - fluid viscosity, \mathbf{k} - solid matrix permeability, \mathbf{g} - the gravitational acceleration vector.

The relative permeability to fluid flow k_r and the saturations are evaluated by the Van Genuchten's formulae [5], as follows:

$$k_r = \sqrt{S} \left[1 - \left(1 - S^{\frac{n}{n-1}} \right)^{\frac{n-1}{n}} \right]^2 \quad s = s_r + (1 - s_r) \left[1 + (ap_c)^n \right]^{\frac{n}{n-1}}$$

in which $S = (s - s_r)/(1 - s_r)$, s_r is a residual saturation, below it the fluid becomes immobile, p_c - capillary pressure. a and n are parameters depending on material of the flow domain.

2.2. The fluid mass balance equation in groundwater flow

Considering a control volume having the shape of a rectangular parallel-piped box centered at (x, y, z) , and using some transformations on partial derivatives to introduce environmental parameters, rate of change of concentration, etc. the following mass balance equation is obtained:

$$\left[\rho_1 s S_{op} + \varepsilon \rho_1 \frac{\partial s}{\partial p} \right] \frac{\partial p}{\partial t} + \left[\varepsilon s \frac{\partial \rho_1}{\partial C_1} \right] \frac{\partial C_1}{\partial t} + \nabla(\varepsilon s \rho_1 \mathbf{v}) = Q_p \quad (2.2)$$

where $Q_p = Q_p(\mathbf{r}, t)$ is the fluid mass source including solute mass dissolved at an interior point \mathbf{r} in the flow domain, C_1 is the solute mass concentration in groundwater, S_{op} is specific pressure storativity which depends on the porous matrix compressibility α and the fluid compressibility β by $S_{op} = (1 - \varepsilon)\alpha + \varepsilon\beta$. The exact form of the fluid mass balance is obtained by employing Darcy's law:

$$\left[\rho_1 s S_{op} + \varepsilon \rho_1 \frac{\partial s}{\partial p} \right] \frac{\partial p}{\partial t} + \left[\varepsilon s \frac{\partial \rho_1}{\partial C_1} \right] \frac{\partial C_1}{\partial t} - \nabla \left[\frac{\rho_1 k_r}{\mu} \mathbf{k} [\nabla p - \rho_1 \mathbf{g}] \right] = Q_p \quad (2.3)$$

2.3. The solute mass balance equation in groundwater flow

The total flux of a pollutant by advection, dispersion and diffusion, is expressed by $\mathbf{J}^c = \varepsilon s [\mathbf{v} \rho_1 C_1 - \mathbf{D}_h (\nabla \rho_1 C_1)]$ in which \mathbf{D}_h is the hydrodynamic dispersion, [1]. By considering a control volume and taking into account all components in the construction of a balance equation, the solute mass balance equation in groundwater flow is:

$$\frac{\partial}{\partial t} [\varepsilon s \rho_1 C_1 + (1 - \varepsilon) \rho_s C_s] = -\nabla \mathbf{J}^c + \varepsilon s \rho_1 \Gamma_1 + (1 - \varepsilon) \rho_s \Gamma_s + Q_p C_p \quad (2.4)$$

where Γ_1 is the solute mass source in fluid per unit fluid mass due to production reactions, Γ_s adsorbate source per unit solid matrix mass due to production reactions within adsorbed material itself, C_p - solute concentration of fluid source,

ρ_s - density of solid grains in solid matrix, C_s - specific concentration of adsorbate on solid grains.

The production terms Γ_1 and Γ_s for solute and adsorbate, respectively, can be evaluated by linear models $\Gamma_1 = \gamma_0^1 + \gamma_1^1 C_1$, $\Gamma_s = \gamma_0^s + \gamma_1^s C_s$ where γ_0^1 , γ_1^1 , γ_0^s , γ_1^s are production rates.

Using the following balance equations in solid and liquid phases

$$\frac{\partial(\varepsilon s \rho_1)}{\partial t} = Q_p - \nabla(\varepsilon s \rho_1 \mathbf{v}) \quad \frac{\partial}{\partial t}[(1 - \varepsilon)\rho_s] + \nabla[(1 - \varepsilon)\rho_s \mathbf{v}_s] = 0$$

with noted that $|\mathbf{v}_s| \approx 0$ and $\partial C_s / \partial t = \lambda \cdot \partial C_1 / \partial t$, where λ is the proportional factor determined by Freundlich, Langmuir or linear model, after manipulating [8] the solute mass balance equation (4) becomes:

$$\begin{aligned} & [\varepsilon s \rho_1 + (1 - \varepsilon)\lambda \rho_s] \frac{\partial C_1}{\partial t} + \varepsilon s \rho_1 \nabla C_1 - \nabla[\varepsilon s \mathbf{D}_h \nabla(\rho_1 C_1)] = \\ & = Q_p(C_p - C_1) + \varepsilon s \rho_1 \gamma_0^1 + \varepsilon s \rho_1 \gamma_1^1 C_1 + (1 - \varepsilon)\rho_s \gamma_0^s + (1 - \varepsilon)\rho_s \gamma_1^s C_s \end{aligned} \quad (2.5)$$

SPECIFIC CASES. Let R and ζ be factors determined by

$$R = 1 + \left(\frac{1}{\varepsilon} - 1\right) \frac{\rho_s}{\rho_1} \frac{1}{s} \lambda \quad \zeta = \frac{Q_p}{\varepsilon s \rho_1 + (1 - \varepsilon)\lambda \rho_s} = \frac{1}{R} \frac{Q_p}{\varepsilon s \rho_1} \quad (2.6)$$

When ε , ρ_1 and s are constants, C_p and production rates are zero. The solute transport equation (2.5) reduces to the simple form as follows:

$$R \frac{\partial C_1}{\partial t} = \nabla(\mathbf{D}_h \nabla C_1) - \mathbf{v} \nabla C_1 - \zeta R C_1 \quad (2.7)$$

The R factor decreases the value of the right-hand term or retards the solute transport process, so called retardation factor. The ζ factor depends on Q_p without solute concentration source and dilutes the concentration of pollutant and so called decay factor.

- *One-dimensional form.* When \mathbf{D}_h is a constant, in the one dimensional case, equation (5) becomes, [1, 5]:

$$R \frac{\partial C_1}{\partial t} = \mathbf{D}_h \frac{\partial^2 C_1}{\partial x^2} - \mathbf{v} \frac{\partial C_1}{\partial x} - \zeta R C_1 \quad (2.8)$$

- *Two-dimensional form.* Similarly, (2.5) can be manipulated to the following form of the two-dimensional case, [2, 3, 4]:

$$R \frac{\partial C_1}{\partial t} = D_{xx} \frac{\partial^2 C_1}{\partial x^2} + 2D_{xy} \frac{\partial^2 C_1}{\partial x \partial y} + D_{yy} \frac{\partial^2 C_1}{\partial y^2} - v_x \frac{\partial C_1}{\partial x} - v_y \frac{\partial C_1}{\partial y} - \zeta R C_1 \quad (2.9)$$

2.4. Initial and boundary conditions

In order to yield a solution for a particular studied case, the partial equations expressing the balance of fluid mass (2.3) and of a pollutant constituent (2.5) have to be supplemented by appropriate initial and boundary conditions. These conditions should be obtained from actual observations of the considered region. Initial conditions include the specification of pressure and concentration at some initial time at all points of the flow domain. Boundary conditions, generally, are given in the form of Dirichlet, Neumann, or Cauchy type.

3. Numerical methods

The three-dimensional bounded volume of an aquifer D , in which groundwater flow and solute transport is to be simulated, is completely divided up into a single layer of contiguous blocks, called quadrilateral finite elements. All twelve edges of each block are straight and four of these edges are parallel to the z -coordinate direction.

The xy -coordinate of the midpoint of each z -edge is referred to as a nodal point and represents the entire z -edge of element. So the element has a three-dimensional shape but always has only four nodes, and a finite element mesh of the problem is created by these nodes. The domain D , thus may be defined in three space dimensions but the problem is discretized and solved numerically in two dimensional model. Such a method reduces number of hydrogeologic data need to be collected.

The numerical approximation of the equation (2.3) with its corresponding conditions can be performed by the Galerkin-Petrov technique of the finite element method and by the finite difference method.

The resulting system of linear equations to determine pressure p_i^{n+1} at node i and at time step $n + 1$ is:

$$\sum_{j=1}^{nn} \left[\frac{A_i}{\Delta t_{n+1}} \delta_{ij} + B_{ij} + \nu_i \delta_{ij} \right] p_j^{n+1} = Q_i^{n+1} + \nu_i p_{BCi}^{n+1} + D_i^{n+1} + \frac{A_i}{\Delta t_{n+1}} p_i^n + \left[\frac{dC}{dt} \right]_i^n E_i^n \quad (3.1)$$

where $i = 1, \dots, nn$, nn is the number of nodes, δ_{ij} is the Kronecker delta, ν_i - the conductance, p_{BCi}^{n+1} - the specified pressure at node i . Fluid sources, $\Delta t_{n+1} = t^{n+1} - t^n$, $p_i^n = p_i(t^n)$, and $p_i^{n+1} = p_i(t^{n+1})$. A_i , B_{ij} , E_i , D_i and V_i are determined by:

$$A_i = \left\{ \rho_1 s S_{op} + \varepsilon \rho_1 \frac{\partial s}{\partial p} \right\} V_i; \quad B_{ij} = \iint_D \left\{ \frac{\rho_1 k_r}{\mu} \mathbf{k}^e \nabla \varphi_j \right\} \nabla \omega_i B(x, y, t) dx dy$$

$$E_i = \left\{ \varepsilon s \frac{\partial \rho_1}{\partial C_1} \right\}_i V_i, \quad D_i = \iint_D \left\{ \left[\frac{\rho_1 k_r}{\mu} \mathbf{k}^e \nabla \varphi_j \right] \langle \rho_1 \mathbf{g} \rangle \right\} \nabla \omega_i B(x, y, t) dx dy$$

$$\left\{ \frac{dC}{dt} \right\}_i^n = \frac{C_i^{n+1} - C_i^n}{\Delta t_{n+1}}, \quad V_i = \iint_D B(x, y, t) \varphi_i dy dx.$$

Similarly, the form of the discretized solute mass balance equation (2.5) is also implemented and the resulting system to determine concentration C_i^{n+1} is:

$$\sum_{j=1}^{nn} \left\{ \frac{A_i^{n+1}}{\Delta t_{n+1}} \delta_{ij} + D_{ij}^{n+1} + B_{ij}^{n+1} + \left[G_i^{n+1} + G_{Li}^{n+1} + (Q_i^{n+1} + Q_{BC_i}^{n+1}) \right] \delta_{ij} \right\} C_i^{n+1} =$$

$$= Q_i^{n+1} C_{p_i}^{n+1} + Q_{BC_i}^{n+1} C_{BC_i}^{n+1} + F_{N,i}^{n+1} + E_i^{n+1} + G_{Ri}^{n+1} + \frac{A_i^{n+1}}{\Delta t_{n+1}} C_i^n, \quad i = 1, \dots, nn \quad (3.2)$$

where $A_i = \{ \varepsilon_i s \rho_1 + (1 - \varepsilon) \lambda \rho_s \}_i V_i$, $C_i^n = C_i(t^n)$, $C_i^{n+1} = C_i(t^{n+1})$, $Q_{BC_i} = V_i(p_{BC_i} - p_i)$ and:

$$B_{ij} = \iint_D \{ \varepsilon s \rho_1 \langle \mathbf{D}_h \rangle \nabla \varphi_j \} \nabla \varphi_j B dy dx, \quad D_{ij} = \iint_D \{ \varepsilon s \rho_1 \langle \mathbf{v} \rangle \nabla \varphi_j \} \omega_i B dx dy$$

$$G_i = \{ \varepsilon s \rho_i \gamma_1^1 C_1 \}_i V_i, \quad G_{Ri} = \{ (1 - \varepsilon) \rho_s \gamma_1^0 R_L \}_i V_i$$

$$E_i = \{ \varepsilon s \rho_i \gamma_0^1 + (1 - \varepsilon) \rho_s \gamma_0^0 \}_i V_i, \quad G_{Li} = \{ (1 - \varepsilon) \rho_s \gamma_1^0 R_R \}_i V_i$$

$$F_{N,i}(t) = -F_{OUT,i}(t) = - \iint_D \{ \varepsilon s \langle \mathbf{D}_h \rangle \nabla (\rho_1 C_1) \} \cdot \mathbf{n} \varphi_i d\gamma$$

in which, φ_i and ω_i are the basis and symmetric weighting function, respectively, and \mathbf{n} is the unit outward normal vector to the three-dimensional surface bounding the region to be simulated. The above double-integrals are evaluated by the method of Gaussian integration.

4. STG Simulation

The following illustration outlines a number of examples whose results serve to verify the accuracy of the first STG simulations for a range of flow and transport problems. The Student-test of significance is applied to compare STG results analytical solutions.

- *One-dimensional case.* Let us consider a shallow, homogeneous, isotropic aquifer with its vertical section presented in figure 1. A Chemical waste inflow is being continuously poured into the ditch with the rate of $0.1 \text{ m}^3/\text{day}$ per unit length of it. The concentration of a certain non-reactive constituent in this waste is $10 \text{ kg}/\text{m}^3$. Using the equation (2.8) with $R = 1$, $\zeta = 0$, $v = 1 \text{ m}/\text{day}$, the initial condition $C_1(x, 0) = 0$ and boundary conditions:

$$\text{when } x \rightarrow \infty, \partial C_1 / \partial x = 0$$

$$\text{when } x = 0, -D_h \partial C_1 / \partial x + v C_1 = v C_0 \exp(-t) \text{ if } t_0 \geq t > 0, = 0 \text{ if } t > t_0$$

where C_0 is the concentration of waste inflow. The analytical solution illustrated in [3] and sketched by solid lines in figures 3, 4. The STG numerical solution obtained with 94 nodes, 46 elements and plotted by dot-points in the corresponding figures.

- *Two-dimensional case.* Consider the equation (2.9) with: $D_{xy} = 0$, $D_{xx} = 1 \text{ m}^2/\text{day} = 10 D_{yy}$, $v_x = 1 \text{ m}/\text{day}$, $v_y = 0$, Liquid waste from a factory is being discharged into a surface impoundment $2d = 100 \text{ m}$ long and 5 m wide. Aquifer is homogeneous, isotropic, saturated with steady flow as shown in figure 2. Using the following conditions:

$$C(0, y, t) = \begin{cases} C_0 e^{-t} & \text{if } -d \leq y \leq d, \\ 0 & \text{if } y < -d \text{ or } y > d, \end{cases} \quad \lim_{x \rightarrow \infty} \frac{\partial C}{\partial x} = 0, \quad \lim_{y \rightarrow \infty} \frac{\partial C}{\partial y} = 0$$

the analytical solution is given in [4]. By partitioning the flow domain into 160 nodes, 135 elements and $C_0 = 1000 \text{ ppm}$, the STG solution obtained and plotted in figures from 5 to 8.

Using the Student-test of significance in comparison the analytical and STG solutions leads to the conclusion that the difference between these is non-significant.

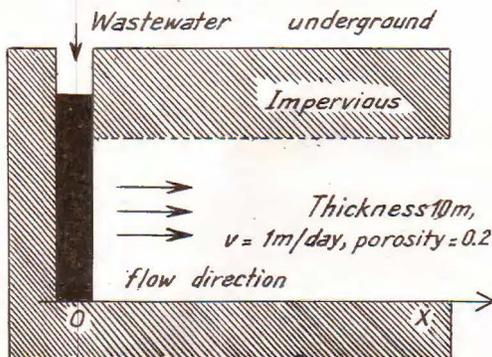


Fig. 1. Vertical section of the aquifer along the direction of flow

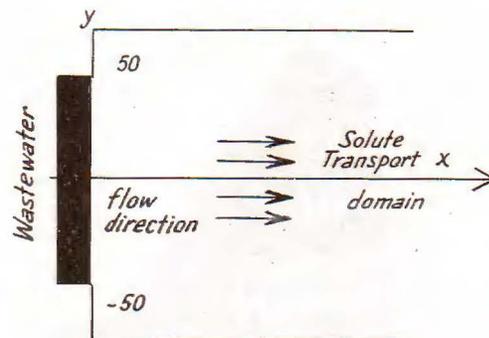


Fig. 2. Plan view of the flow and the source of contamination

COMPARISON OF STG RESULTS AND ANALYTICAL SOLUTIONS
One-dimensional solute transport case

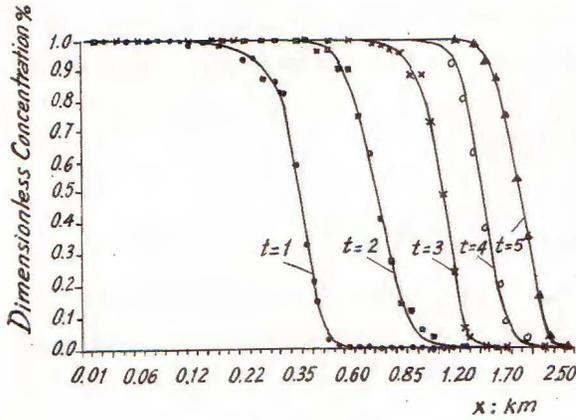


Fig. 3.

$V = 1 \text{ m/day}, D_h = 10 \text{ m}^2/\text{day}, t \text{ in years}$

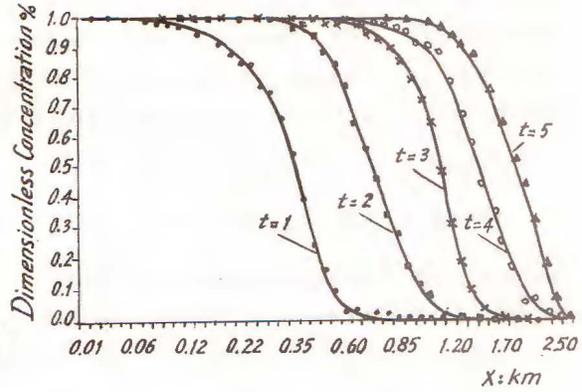


Fig. 4.

$V = 1 \text{ m/day}, D_h = 10 \text{ m}^2/\text{day}, t \text{ in years}$

Two-dimensional solute transport case

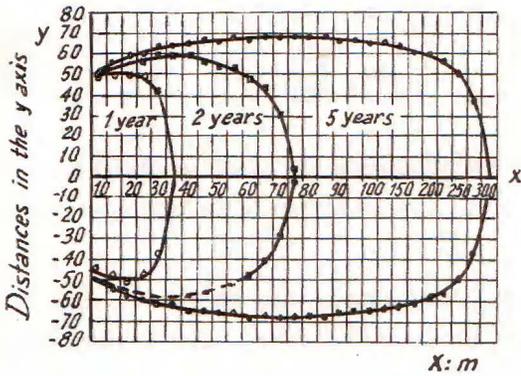


Fig. 5. Zones of concentration greater than 10%

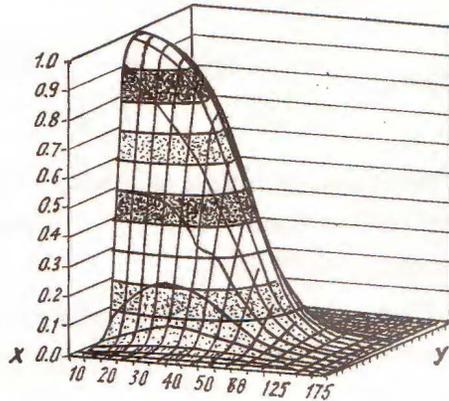


Fig. 6. Concentration surface after 1 year

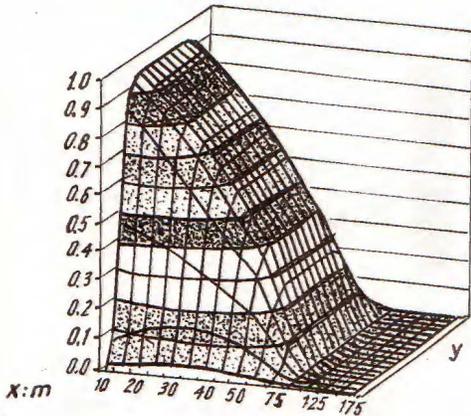


Fig. 7. Concentration surface after 3 years

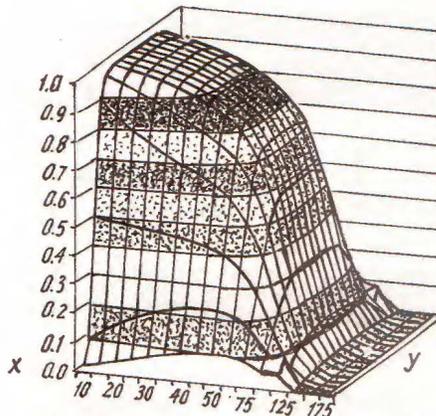


Fig. 8. Concentration surface after 5 years

Using STG model to solve a problem in a specified three dimensional region requires more data, especially hydrogeologic observation. Such as problem and some other related investigations will be represented in a next publication.

5. Conclusions

1. The equations (2.3) and (2.5) in three dimensions are obtained by taking physical properties of aquifer into account, and these partial differential equations describe the solute transport phenomenon with single-species in groundwater.

2. The specific cases of these equations are the ones introduced in the works [1]-[5].

3. Using the Galerkin-Petrov technique, the equations (2.3), (2.5) with their appropriate initial and boundary conditions are discretized and the system (3.1), (3.2) are used in solving numerically the problem of single-species solute transport in groundwater.

4. Comparison between STG solutions and analytical solutions for two special cases shows that the model results are acceptable.

5. This numerical model will be improved and tested step by step before applying it to complicated problems in reality.

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Received January 15, 1999

MÔ HÌNH TOÁN LÝ VỀ LAN TRUYỀN CHẤT TRONG NƯỚC NGẦM

Bài báo này thiết lập hệ các phương trình đạo hàm riêng (2.3), (2.5) cho bài toán ba chiều về lan truyền chất trong nước ngầm, dùng phương pháp Galerkin-Petrov và phương pháp sai phân hữu hạn để giải bài toán bằng hệ (3.1) và (3.2) sau khi đã rời rạc miền không gian của bài toán theo một lưới phẳng các phần tử hữu hạn tứ giác.

Trường hợp đặc biệt của (2.5) cũng đã được xem xét dưới dạng (2.7), (2.8), (2.9) và hoàn toàn trùng khớp với các kết quả nêu trong các công trình (2.1)-(2.5). Chương trình máy tính mang tên STG bước đầu cũng đã được thiết lập để giải bài toán.

Kiểm nghiệm qua một số trường hợp đơn giản, có nghiệm giải tích - kết quả từ phép kiểm định Student chứng tỏ những kết quả bước đầu này của STG là có thể chấp nhận được. Việc khảo sát lời giải số cho trường hợp ba chiều cùng với nhiều vấn đề khác đang được tiến hành và sẽ trình bày trong các bài báo kế tiếp.

Mô hình toán cùng với các phương pháp số và chương trình máy tính STG đang được tiếp tục nghiên cứu và cải tiến dần để có thể ứng dụng trong mô phỏng bài toán lan truyền chất trong các môi trường nước ngầm.