

Andrzej ANISZEWSKI

PRÓBA MATEMATYCZNEGO MODELOWANIA JAKOŚCI UJMOWANEJ WODY GRUNTOWEJ

A TRIAL OF MATHEMATICAL MODELLING OF THE DRAWING GROUND WATER QUALITY

Politechnika Szczecińska, Zakład Inżynierii Wodnej
Technical University of Szczecin, Chair of Water Environment Engineering

Streszczenie

W artykule przedstawiono matematyczny model transportu stabilnych i pasywnych zanieczyszczeń w przepływie wody gruntowej, uwzględniając procesy adwekcji i adsorpcji. W oparciu o wcześniejsze badania laboratoryjne stężeń zanieczyszczeń na modelu fizycznym oraz wykorzystując rozwiązanie numeryczne prezentowanego modelu matematycznego obliczono parametry adsorpcji k_1 i n dla nieliniowej funkcji opisującej ten proces. W dalszej kolejności opracowano doświadczalne zależności parametrów adsorpcji od parametrów charakteryzujących równocześnie warstwę wodonośną oraz przepływ wody gruntowej. Zależności te pozwalają na lepszą ocenę prognozy jakości zasobów wód gruntowych dopływających do ujęć wody gruntowej.

Summary

The article presents mathematical modelling of transporting both stable and passive contaminations in ground water flow taking into consideration processes of advection and adsorption. On the grounds of the earlier laboratory investigations related to contamination concentrations on the physical model and using numerical solution of the presented mathematical model the adsorption parameters k_1 for the nonliner function describing the process were calculated. This was followed by determining experimental (empirical) dependence between the adsorption parameters and the parameters characterizing at the same time the aquiferous layer and the ground water flow. This dependence allows for a better prognosis evaluation of the resources of ground water flowing into ground water intakes.

1. INTRODUCTION AND OBJECTIVE

The paper addresses the advection and adsorption of some conservative contaminants such as chlorides, heavy metals or non-biodegradable toxic organics, which begin to appear more frequently in the ground water. The effect of the molecular diffusion was neglected as considered negligible when compared to advection and adsorption processes [Weinberger and Mandel, 1973]. The main objective of the paper was determination of the relationships between soil adsorption capacity and selected parameters characterising the aquifer layer and ground water flow. The soil particle diameter (d_{10}) was used to characterise the aquifer; the pressure (head) line slope (I) was used as the parameter characterising ground water flow. The non-linear adsorption process is represented by the two adsorption parameters k_1 and n [Barovic, 1979; Kowal, 1990]. Based on earlier laboratory experiments the empirical relationships of parameters k_1 and n , for effective grain size (d_{10}) and porosity (p) as well as pressure line slope of ground water (I) were worked out. Rhodamine as a conservative tracer was used in the laboratory experiments.

2. MODELLING CONTAMINANT TRANSPORT IN GROUND WATER

Conservative contaminant pollutant transport incorporating reversible sorption process, the well - known spatial advection - dispersion equation, resulting from the transport continuity [Ogata, 1970; Aniszewski, 1998] is:

$$\frac{\partial C}{\partial t} + v_x \frac{\partial C}{\partial x} + v_y \frac{\partial C}{\partial y} + v_z \frac{\partial C}{\partial z} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} - g_1 \quad (1)$$

where: C - pollutant concentration in ground water [$g \cdot m^{-3}$]; v_x, v_y, v_z - components of Darcy velocity [$m \cdot s^{-1}$]; D_x, D_y, D_z - components of dispersion [$m^2 \cdot s^{-1}$]; t - co-ordinate of time [s]; g_1 - term describing the reversible sorption process [$g \cdot m^{-3} \cdot s^{-1}$]; x, y, z - co-ordinates of the assumed reference system [m].

In equation (1) the mechanical dispersion constants D_x, D_y and D_z were selected on the assumption that co-ordinate axes (x, y, z) coincide with mixing axes. In further analysis for homogeneous soil medium it was assumed, that ground water flow is one-dimensional in axis x with the constant Darcy velocity in this direction v_x . Thus, in the further analysis components of Darcy velocities in the rest directions were neglected ($v_y = v_z = 0$) and at the same time the advection terms in these directions ($v_y \frac{\partial C}{\partial y} = v_z \frac{\partial C}{\partial z} = 0$). For the laboratory experiments Darcy velocities (v_x), soil characteristic diameters (d_{10}) and value of molecular diffusion coefficient (D_M), the numerical range of Peclet number ($Pe = v_x d_{10}/D_M$) was defined at $5,0 \leq Pe \leq 580,0$. Based on the calculated values of Peclet number it can be assumed, that in pollutant mass transport in ground water flow, the advection transport dominates ($v_x \frac{\partial C}{\partial x}$) [Szymkiewicz, 1995]. Based on the laboratory experiments in the soil column, the feasibility of neglecting the

longitudinal dispersion ($v_x \partial^2 C / \partial x^2$) was confirmed, when small lengths of the measured frontal zones generated by this dispersion were taken into account. The example of measured lengths of frontal zones in the particular cross - sections on the model were presented by Aniszewski (1998). Taking into account the small diameter of the soil column and at the same time quick concentration equalisation in the cross-sections on the column length, in equation (1) the transverse dispersion terms ($D_y \partial^2 C / \partial y^2 = D_z \partial^2 C / \partial z^2 = 0$) were also neglected.

Thus, the equation (1) can be written as:

$$\frac{\partial C}{\partial t} + v_x \frac{\partial C}{\partial x} = -g_1 \quad (2)$$

The term g_1 in the equation (2) describes the reversible physical sorption process, which can be expressed in the form [Barovic, 1979; Miller and Weber, 1984]:

$$g_1 = \frac{\rho(1-p)}{p} \frac{\partial S}{\partial t} \quad (3)$$

where: S - mass of sorbed pollutants on the soil particles related to the mass of the soil sample [-]; ρ - density of the soil media [$g \cdot m^{-3}$]; p - porosity coefficient of the soil [-].

The term ($\partial S / \partial t$) can be expressed as the sum of the two components [Kowal, 1990]:

$$\frac{\partial S}{\partial t} = \frac{\partial S_a}{\partial t} - \frac{\partial S_d}{\partial t} \quad (4)$$

where: $\partial S_a / \partial t$, $\partial S_d / \partial t$ - terms expressing process of pollutant adsorption on the ground grains and desorption from the ground grains, respectively [s^{-1}].

Adsorption process was described by means of a non - linear function close to empirical Freundlich isotherm widely used in literature (Kowal, 1990):

$$\frac{\partial S_a}{\partial t} = k_1 \frac{p}{\rho(1-p)} C^n \quad (5)$$

where: k_1 - rate coefficient of pollutant concentration reduction caused by adsorption [$m^{3(n-1)} \cdot g^{-(n-1)} \cdot s^{-1}$]; n - constant index exponent of non-linear adsorption [-].

In the further analysis, desorption process was neglected ($\partial S_d / \partial t = 0$) taking into account steady and continuous flow of pollutants into the ground water [Barovic, 1979; Kowal, 1990]. Taking into account the equation (5), the equation (3) can be written as:

$$g_1 = \frac{\rho(1-p)}{p} k_1 \frac{p}{\rho(1-p)} C^n = k_1 C^n \quad (6)$$

It should be noticed, that the equation (6) is related to the constant value of ground porosity (p).

Thus, taking into account the equation (6), the general equation (2) can be written as:

$$\frac{\partial C}{\partial t} + v_x \frac{\partial C}{\partial x} = -k_1 C^n \quad (7)$$

For numerical solution of the equation (7) the initial and boundary conditions were assumed, which for the soil column can be written in the form:

– boundary condition

$$C = C_0 \text{ for } x = 0 \text{ and for } 0 \leq t \leq \infty \quad (8)$$

initial condition

$$C = 0 \text{ for } t = 0 \text{ and for } 0 < x \leq \infty \quad (9)$$

The cross - section $x = 0$ was situated in distance of ca. 10 cm from the tracer outlet, where concentration equalisation in the whole cross - section of the soil column took place. To solve equation (7) implicit differential scheme, the „up - wind scheme” was used, which makes the use of the grid presented in Figure 1. In this figure $\Delta \xi = h^* = \Delta x/L$ expresses the assumed dimensionless grid step along longitudinal axis x (ξ). On the contrary $\Delta \tau = w^* = v_x \Delta t/L$ expresses calculated according to (13) dimensionless grid step along time axis t (τ).

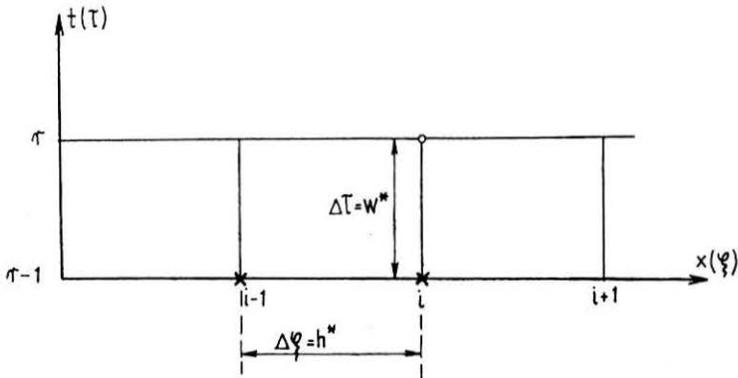


Fig. 1. Node grid for the assumed differential scheme "up - wind scheme"

The differential equation (7) can be written as:

$$b C_{i,r} + A_1 C_{i,r}^n = B C_{i,r-1} + h_1 C_{i-1,r-1} \quad (10)$$

for the auxiliary relationships:

$$\frac{1}{w^*} - \frac{1}{h^*} = B; \quad \frac{1}{w^*} = b; \quad \frac{1}{h^*} = h_1; \quad \frac{k_1 L C_o^{(n-1)}}{v_x} = A_1 \quad (11)$$

where: C_o - initial tracer concentration in the cross - section $x = 0$; L - actual length of the soil column.

Equation (10) is a non - linear algebraic equation, which was solved by means of the "regula falsi" method (consecutive secants). Time step Δt was assumed to eliminate the effect of numerical diffusion. Equation (10) generates numerical diffusion, coefficient of which v_n can be written as:

$$v_n = \frac{v_x \Delta x}{2} (1 - C_a) \quad (12)$$

the symbol of C_a expresses the Courant number which can be defined as:

$$C_a = \frac{v_x \Delta t}{\Delta x} \quad (13)$$

It follows that the eq. 10 will not produce the numerical diffusion for $C_a \leq 1$. Stability analysis of the eq. (10) proved, that it is relatively stable. Stable numerical solution is possible for $C_a = 1$ [Szymkiewicz, 1995]. The solution of the equation (7) by means of eq. (10) can be done by the computer program „SORPCJA - 1” [Aniszewski, 1998].

3. RESULTS AND DISCUSSION: LABORATORY EXPERIMENTS

Based on the colorimetrically measured concentrations of tracer solution on the physical model and utilising the numerical solution results of the equation (10), the values of adsorption parameters k_1 and n were estimated. The empirical relationships of the adsorption parameter depended on both groundwater head slope I and diameter d_{10} ; complied with the values of constant spatial ground porosity p and adsorption index exponents n .

The empirical relationship was assumed in the exponential form:

$$k_1 = a_1 \exp[-b_1 \cdot I] \quad (14)$$

where:

$$\left. \begin{aligned} a_1 &= 0,2259 \cdot 10^{-4} d_{10} + 0,4214 \cdot 10^{-6} \\ b_1 &= 3,2629 d_{10} + 20,0337 \end{aligned} \right\} \quad (15)$$

The values of (d_{10}) diameters according to (15) are in [mm] and those of (I), according to (14) in [%].

The graph of the calculated and the equalised values of (k_1) parameters in relation to (I) line slopes for the three chosen diameters (d_{10}) complied with the values of constant spatial ground porosity (p) and adsorption index exponents (n) was presented in Figure 2.

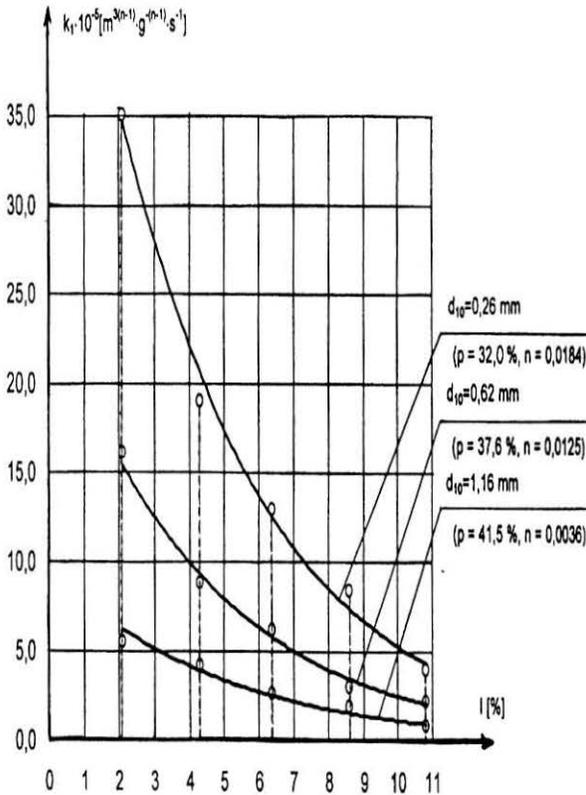


Fig. 2 Values of adsorption coefficients (k_1) in relation to pressure line slopes of ground water (I), effective grain size (d_{10}), porosity (p) and index exponents (n): \circ - the calculated values according to (10), — - the equalised values according to (14)

The empirical relationship of the adsorption index exponents n from the diameters d_{10}

in the range of spatial porosity $32,0 \leq p \leq 41,5 \%$ was also worked out.

The empirical relationship can be written as:

$$n = b_2 d_{10} + c \quad (16)$$

where :

$$\left. \begin{aligned} b_2 &= -0,1672 \cdot 10^{-1} \\ c &= 1,0230 \end{aligned} \right\} \quad (17)$$

The values of (d_{10}) diameters according to (16) are in [mm].

The graph of the relationships of the adsorption index exponents (n) from the characteristic diameters (d_{10}) was presented in Aniszewski [1998].

4. CONCLUSIONS

Experiments on the physical adsorption process, conducted on the physical soil column model confirmed the quantitative relationships between the parameters characterising the soil medium and the ground water flow in fine and coarse sands. The empirical relationships developed here, should facilitate better practical estimation of the water quality from groundwater source intakes.

5. REFERENCES

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