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MATHEMATICAL MODELLING OF CONTAMINANT FLOW AND TRANSPORT IN GROUND WATERS

Effective action intended to counter deterioration of ground water resources quality makes it necessary to identify the processes which have a bearing on contaminant infiltration into subterranean waters and design appropriate tools with a view to quantifying the processes in question. In view of the complexity of these issues, the most suitable method for resolving them is by mathematical modelling. The present paper discusses two related mathematical models designed to model flow and transport in a three-dimensional porous variably saturated medium in unsteady conditions.

1. INTRODUCTION

Ground water resources in Poland are an important source of water supply for the national economy. The role played by this resource in supplying drinking water makes it necessary to place special focus on the quality of subterranean waters.

In order to design effective action to counter the steady deterioration of ground water resources, it is necessary to identify properly the processes affecting contaminant migration into subterranean waters and to develop methods to quantify these processes. Given the complexity of these issues the most appropriate solution is to apply mathematical modelling.

The present paper presents two related mathematical models designed to model the flow and transport in a 3-dimensional porous variably saturated medium, in unsteady conditions.

The 3-dimensional model of the element of finite water flow through a variably saturated medium (the flow model) can be applied in the study of sub-surface flow either as an independent model or to furnish variable parameters of hydrological flow for the transport model. The flow model has been designed so as to:

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• apply to a heterogeneic and anisotropic medium composed of a required number of geological formations;

• accept predetermined initial conditions or generate them by simulating the predetermined conditions of the studied system;

• account for boundary conditions.

The 3-dimensional model of the finite element describing contaminant transport through a variably saturated medium (the transport model) has been designed so as to:

• apply to heterogeneic and anisotropic medium; account for area and point sources of pollution;

• accept predetermined initial conditions or generate them by simulating predetermined conditions of the studied system;

• account for predetermined boundary conditions;

• simulate the break up of contaminant substances or rank one;

• include three adsorption models (the linear, Freundlich and Langmuir isotherms).

The flow model and the transport model described in the coming section were developed as a part of Research Project No. PB 0437/T09/98/15 financed from the resources of the Committee for Scientific Research.

2. THE FLOW MODEL

The model for simulating ground water flow was constructed for the purpose of simulating water movement in a porous, variably saturated medium. Its most typical application is to simulate the impact of factors associated with human economy (e.g. water intake or diverse way of land use) and natural factors (e.g. the quantity of precipitation and evapotranspiration) on the volume of ground water resources.

In the flow model, the flow of water through a porous variably saturated medium is described by the primary equation (1), based on the law of mass conservation and the law of momentum conservation; its form is as follows:

$$F(h)\frac{\partial h}{\partial t} = \nabla \cdot \left[K(h)(\nabla h + \nabla z)\right] + q\,, \tag{1}$$

where:

h – pressure of the water head (L),
z – height above the reference level (L),
$K(h)$ – effective hydraulic conductivity (L/T),
$F(h)$ – volume of water capacity ($1/L$),
Q – source term ($L^3/T/L^3$),
t – time (T),

∇ – gradient,

$\nabla.$ – divergence.

Throughout the article the following notations are consistently used for the elements appearing in equation (1): L – length, T – time, M – mass. Equation (1), usually known as the Richards equation, is different from the basic equation used to calculate saturated flow in a porous medium by the non-linearity of hydraulic conductivity and conditions of water capacity. The formula is solved numerically using the technique of Galerkin's finite element.

The questions of flow in a variably saturated medium may be solved using equation (1) in association with a set of boundary conditions which are defined at the physical boundaries of the modelled system. In the flow model, the following boundary conditions may be applied: constant pressure (Dirichlet), defined flow (Cauchy), defined pressure gradient (Neumann) and variable conditions (the relationship between the flow and the pressure head).

An important element of equation (1) is the expression of the source. Similarly as in the case of the boundary conditions, the expression of the source may be constant or may vary in time. In the flow model, two options of the source are available: the source may be treated either as dispersed or as a point source. The dispersed source option is characterised by the magnitude of its output integrated from the capacity of the element. This option allows one to model large areas by making it possible to approximate the impact of large wells within a single element. The point source option generally is useful in modelling the impact of individual wells. The wells are characterised alternately by the magnitude of water flux at nodal points, for an improved presentation, by the range of impact of the well in the column of nodal points.

Numerically, the flow model is realised with the help of the calculation program PRZEPLYW (FLOW) written in FORTRAN 90. The program includes the main module and 22 procedures and may be run under DOS.

3. THE TRANSPORT MODEL

The model of contaminant transport in ground water was constructed for the purpose of simulating the movement of solutes through a porous, variably saturated medium. Typical applications of the model include: study of contaminant migration from dispersed and point sources, impact of pesticides and fertiliser on water quality and on the environment of leaky storage reservoirs (underground and surface units). Velocity fields needed to define advection of water fluxes transporting the solutes are determined with the help of the flow model described in the preceding section.

In the transport model, advection–dispersion transport of solutes in a porous, variably saturated medium is described by the primary equation (2) derived from the law of mass conservation and flux conservation; its form is as follows:

$$\Theta \frac{\partial C}{\partial t} + \rho_b \frac{\partial S}{\partial t} = \nabla \cdot (\Theta D \nabla C) - V \nabla C - \lambda (\Theta C + \rho_b S) + QC_{in} - QC \,, \tag{2}$$

where:

Θ – humidity content (L^3/L^3),
ρ_b – bulk density of the porous medium (M/L^3),
C – solute concentration (M/L^3),
S – concentration of substances in the adsorbed phase (M/M),
t – time (T),
V – Darcy's velocity (L/T),
$\nabla\cdot$ – operator indicating divergence,
∇ – operator indicating gradient,
D – tensor of the dispersion coefficient (L^2/T),
λ – material decomposition constant (T),
Q – volume of water outflow (percolation) (M/T),
C_{in} – concentration of outflowing (percolating) solutes (M/L^3).

In order to solve the transport equation (2) for an individual dependent variable, it is necessary to define the basic relationship between the concentration of a given substance in dissolved and adsorbed phases. In the transport model, one of the three relationships may be selected: the linear, Freundlich or Langmuir isotherm. Explicit solutions of the problems of advection–dispersion transport of solutes are generated by solving equation (2) using Galerkin's technique of the finite element in association with a set of boundary conditions defined at the physical boundaries of the system and, where necessary, expressions defining the source. Boundary conditions applicable in the transport model are as follows: conditions of constant concentration (Dirichlet), conditions of defined flow (Cauchy), conditions of the defined dispersion current (Neumann) and variable conditions.

Similar to boundary conditions, expressions of the source, which in equation (2) are described by the element QC_{in} may either be constant or vary in time. Also variable may be the volume of the current Q and solute concentration C_{in}. The transport model accounts for two types of sources: point and dispersed sources.

Numerically, the transport model is realised using the calculation program TRANSPO written in FORTRAN 90; the program consists of the main module and 30 procedures, which may be run under DOS.

4. EXAMPLE

To check the model application in real conditions, the study site was chosen and both numerical programs were used.

An on-site study was conducted on the infiltration basin with a total area of 2.6 ha. This area is divided into five sections with the surface from 0.42 ha to 0.63 ha. Each day the infiltration basin is flooded with 60–70 m^3 of municipal wastewater. The surface formation of the basement complex has the depth of 6–10 m and consists of dusty sands, fine and vari-size grain sands. Below there is the firm ground in the form of clay and sandy clay. Thickness of these layers is 50 m. Then, tertiary Pliocene clay is found.

The observation network (five piezometers) was installed for the ground water table observations and the pollution distribution in the surroundings of the chosen area.

For the modelling purpose the chosen area was divided into the calculation elements. This was done based on the water table map, topographic features, localization of infiltration area, way of flooded area operation and the calculation requirements. The division of modelling area was done by means of 3-dimensional grid with 2717 nodal points and 2160 calculation elements.

The calculations allowed defining the pressure, field of velocity and humidity in the unstable conditions in all 2717 nodal points for each of 73 five day time step. From the calculation the concentration of the chosen substance in the nodal points was defined as well as the components of transported materials flux for each of 10 annual time step.

The results illustrate that the contamination range depends on the substance and is about 170 m from the boundary of the flooded area (the shorter the distance, the higher the pollution concentration). The significant contamination range is 60 m from the boundary of flooded area. The shape of concentration distribution, in accordance with theoretical, corroborates undertaken assumptions and results achieved. The calculation results corroborate analytical determinations.

5. SUMMARY

The present paper presents a description of two related mathematical models – the flow and the transport model – and two numerical programs by means of which they may be realised. The models in question may be used to simulate water flow and contaminant transport through a three-dimensional porous, variably saturated medium in steady and unsteady conditions.

The models were developed in such a way that they did not require digitization of the flow field in the form of regularly formed prismatic blocs (prisms having a triangular or a rectangular base). Consequently, investigation of the heterogeneic nature of the modelled system was restricted first of all by the accessibility of data or data availability, or calculation potential of the hardware used.

A detailed simulation of the unsaturated zone makes it possible to verify the impact of variable saturation on contaminant mobility. Also vertical infiltration through the unsaturated zone with its attendant horizontal diffusion of contaminants may be included. A detailed simulation of the unsaturated zone also makes it possible to account directly for its contaminant storage capacity. Availability of various adsorption models facilitates the selection of contaminant storage capacity suited to the modelled type of contaminant.

The transport model affords a relatively accurate representation of contaminant sources thanks to using several time-dependent boundary condition types. Contaminants may be represented not only as point sources or sources with a simple geometry as is assumed in analytical solutions, but also as sources having a variable geometry. The use of the infiltration or ground water feeding, available due to the model, allows an effective simulation of flow of such water-soluble contaminants as fertilizers or pesticides whose concentrations vary in time and space.

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MATEMATYCZNE MODELOWANIE PRZEPŁYWU I TRANSPORTU ZANIECZYSZCZEŃ W WODACH PODZIEMNYCH

Efektywne przeciwdziałanie postępującemu pogarszaniu się jakości zasobów wód podziemnych wymaga rozpoznania procesów wpływających na przedostawanie się zanieczyszczeń do tych wód oraz opracowania narzędzi umożliwiających ich kwantyfikację. Ponieważ zagadnienia te są złożone, więc aby je rozwiązać, najlepiej jest zastosować metody modelowania matematycznego. Przedstawiono dwa powiązane ze sobą modele matematyczne przeznaczone do modelowania przepływu i transportu w trójwymiarowym ośrodku porowatym o zmiennym nasycaniu, w warunkach nieustalonych.

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