

MODEL BASED GROUNDWATER POLLUTION PREDICTION

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ABSTRACT

In this paper the cause of the groundwater pollution is a tank containing a liquid. In the liquid one or several pollutants are dissolved. Due to a hole/crack, which exists in the bottom of the tank the liquid filters in the soil and the pollutants migrate. A mathematical model is presented which describes the migration and reaction of a single or multiple pollutants and their interaction. This model facilitates the understanding and prediction of the groundwater pollution. Based on the model, numerical simulations are presented for groundwater pollution.

INTRODUCTION

Water pollution is a major problem in the global context. It has been suggested that it is the leading worldwide cause of deaths and diseases and it accounts for the death of more than 14000 people daily [1], [2]. The water, emerging from some deep groundwater, may have fallen as rain many thousands of years ago. Soil and rock layers are porous media, which naturally filter the groundwater to high degree of clarity. Deep groundwater is generally of very high bacteriological quality but the water typically rich in dissolved carbonates and sulphates or calcium and magnesium. Depending on the strata through which the water has found, other ions may also be present, including chloride and bicarbonate. Chlorinated organic compounds are believed to cause health risk (cancer, endocrine system disruption, birth defects, immune system disorders, reduced fertility etc.) and they have to be removed. A typical example of groundwater pollution is the following: a tank contains a liquid in which there are one or several pollutants. Due to a hole/crack which exists in the bottom of the tank, the liquid filters in the soil and the pollutants migrate. A part of them is adsorbed, a part of them react. The main questions are: which pollutants reach the groundwater, what is the period of time necessary for that and how much is the concentration? In this paper a mathematical model is presented which permits to give an answer to the above questions. It has to be noted that the model is an approximation of the reality and its applicability is limited. Calculus made in the framework of the model permits to formulate predictions, which if verified lend authenticity to the model.

A MODEL SOLUTE TRANSPORT IN SOIL

The transport of chemicals in saturated soil often requires assessing multiple interacting processes. Considered for single, multiple or reacting species in soil can be advection with moving fluids, dispersion or mechanical mixing, molecular diffusion, sorption to solids, and

chemical reactions in and between liquids and solids. Dissolved contaminants are called ‘solutes’. Advection describes the movement of a solute, such as pollutant, with the bulk fluid. Hydrodynamic dispersion describes the spreading of contaminant mass. It combines effects from local variations in pore fluid velocity “dispersion” and molecular diffusion. Sorption describes attachment of solutes to solid particles and reduces dissolved concentrations.

The reactions represent change in solute mass per unit volume soil per time. Chemical reactions of all types, biodegradation, radioactive decay, transformation of tracked products, temperature – and pressure- dependent functions, exothermic reactions, endothermic reactions and so on, influence solute transport in environment.

The governing equation [3] for saturated soil is:

$$\theta_s \frac{\partial c_i}{\partial t} + \rho_b \frac{\partial c_{p_i}}{\partial c} \cdot \frac{\partial c_i}{\partial t} + \nabla(-\theta_s \cdot D_{L_i} \cdot \nabla c_i + \bar{u} c_i) = R_{L_i} + R_{p_i} + S_{c_i} \quad (1)$$

Here c_i and c_{p_i} respectively denote the solute concentration in the liquid (mass per liquid volume), and that sorbed to solid particles (mass per dry unit weight of the solid) for species i . In the equation, θ_s (termed porosity) is the volume of fluids divided by the total fluid-solid volume; $\rho_b = (1 - \theta_s) \cdot \rho_p$ is the bulk density of the soil when ρ_p is the particle density. D_{L_i} represents the hydrodynamic dispersion tensor and \bar{u} is the vector of directional velocities, given by Darcy’s law. R_{L_i} , R_{p_i} describe reactions in the liquid and solid phase, while S_{c_i} denotes a solute source. The various equation coefficients can be arbitrary expressions that, for instance, define kinetics. When we do not employ all terms in the governing equation, then unneeded terms and coefficients we set to zero.

For the boundary conditions for solute transport see [4]. The non conservative form of Eq. (1) is:

$$\theta_s \frac{\partial c_i}{\partial t} + \rho_b \frac{\partial c_{p_i}}{\partial c} \cdot \frac{\partial c_i}{\partial t} + \nabla(-\theta_s \cdot D_{L_i} \cdot \nabla c_i) = -\bar{u} \nabla c_i + R_{L_i} + R_{p_i} + S_{c_i} \quad (2)$$

and it is valid for incompressible fluids.

RESULTS

Our computation was performed for a single pollutant migration in a cylindrical domain of radius $R = 100 \text{ m}$, assuming that the soil satisfies axial symmetry conditions in the domain and there are neither adsorption nor reaction in the domain. The groundwater level was assumed to be at -30 m underground. The hole in the tank bottom was supposed to be of radius $r = 10^{-2} \text{ m}$ and the origin of the system of coordinates is placed in the center of the hole. (Fig.1.)

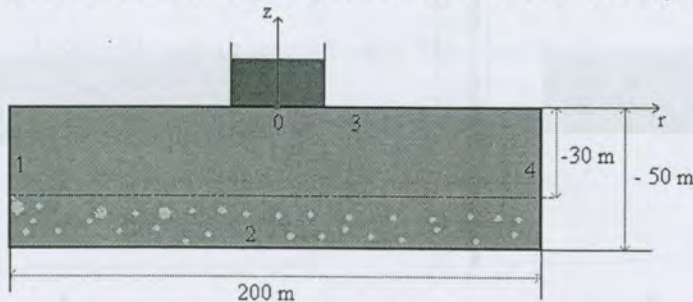


Figure 1.

From the point of view of the conditions on the boundaries 1, 2, 4 two cases were considered:

Case I. The flow conditions on 1, 2, 4 are $p = 0$ (atmosphere or gauge) and the pollutant transport conditions on 1, 2, 4 are $\vec{n} \cdot (-\theta_s \cdot D_L \cdot \nabla c + \vec{u} \cdot c) = 0$ (no flux/symmetry).

Case II. The flow conditions on 1, 2, 4 are $\frac{\delta_k \cdot K_s}{\rho_f \cdot g} \cdot \vec{n} \cdot (\nabla p + \rho_f \cdot g \cdot \nabla a) = 0$ (zero flux/symmetry)

and the pollutant transport conditions on 1, 2, 4 are $\vec{n} \cdot (-\theta_s \cdot D_L \cdot \nabla c + \vec{u} \cdot c) = 0$ (no flux / symmetry).

The condition on boundary 3 is given by the hydrostatic pressure of the liquid column in the tank. It is assumed that the liquid column height is equal to 1 m. The hydrostatic pressure acts only inside the circle of radius $r = 10^{-2}$ m.

Computation was performed in transient and steady-state regimes for different soil textures and a pollutant whose molecular diffusion coefficient $D = 8.6 \times 10^{-6} \text{ m}^2 / \text{s}$.

The results computed in *Case I*, in transient regime, for saturated sand, after 10,000 seconds is represented in Fig. 2a and in *Case II* in Fig. 2b.

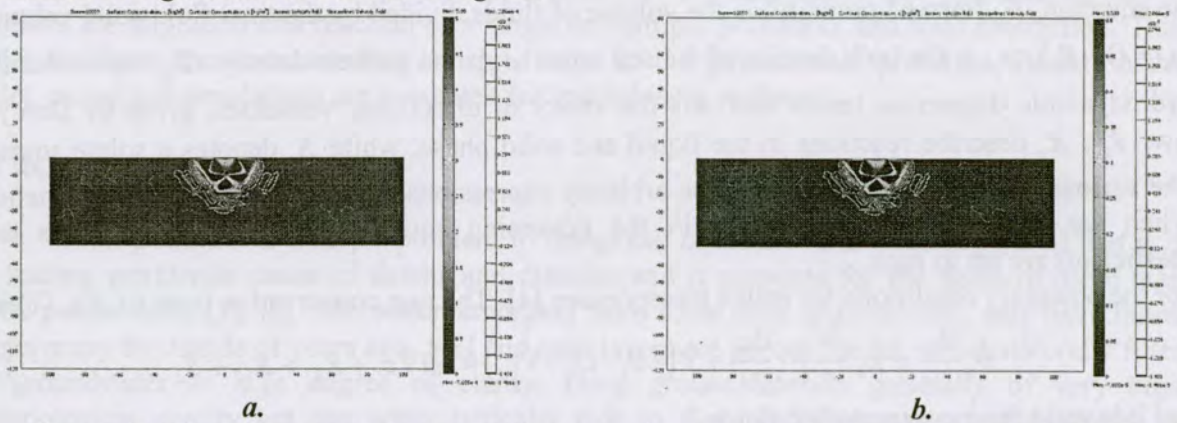


Figure 2. Pollutant transport in non stationary regime, in saturated sand, when the domain boundaries are: *a.* permeable; *b.* impermeable.

The results computed in *Case I*, in stationary regime, for saturated sand, is represented in Fig. 3a and in *Case II* in Fig. 3b.

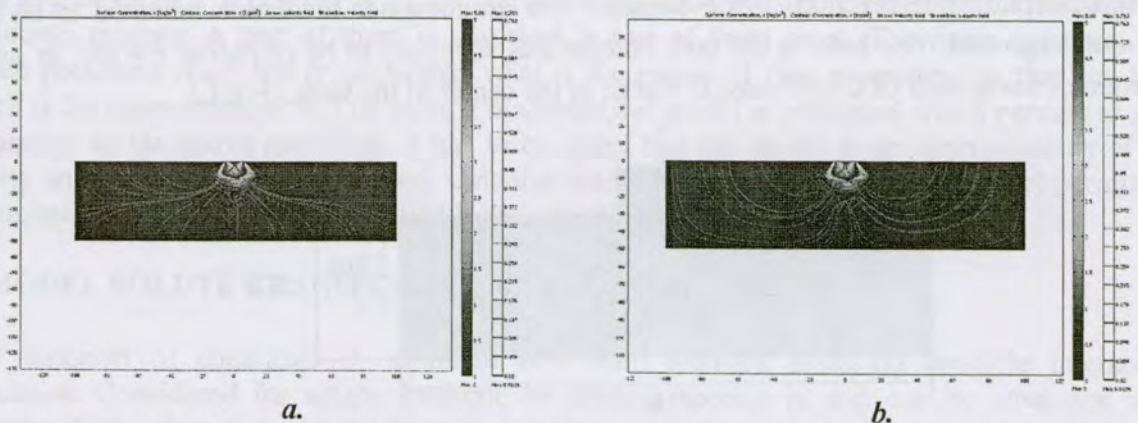


Figure 3. Pollutant transport in stationary regime, in saturated sand, when the domain boundaries are: *a.* permeable; *b.* impermeable.

Comments:

- In the first 10,000 seconds (near 3 hours) the pollutant migration in *Case I* is similar with that in *Case II* and the pollutant doesn't arrive at the groundwater level. Fig.2a, Fig.2b.
- Fig. 3a and Fig 3b represent steady state regime, reached after a certain number of days, in the *Case I* and *Case II*, respectively. According to Fig.3a, in saturated sand, the pollutant concentration in the groundwater at the level of -43 m is of $5.9521 \times 10^{-2} \text{ kg} / \text{m}^3$. Due to the impermeability conditions on the boundaries 1, 2, 4 the pollutant repartition in the considered domain, presented in Fig.3b, is different from that presented in Figs. 3a and the whole domain, including groundwater, is much more polluted.

CONCLUSIONS

- The model presented in this paper takes the form of a set of equations, boundary conditions and initial conditions.
- Computation made in the framework of the model permits the prediction of the pollutant repartition in a prior given domain at every moment.
- The model is limited in applicability because it is based on several simplifications. The idea is that if it is basically authentic (i.e. the model based prediction is in agreement with observations), then it can be made more complicated.

Acknowledgement

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LIST OF REFERENCES

- [1] Glauze W.D. (1996). Mosby Medical Encyclopedia, Revised Edition, St.Louis, MD:CV, Mosby.
- [2] Djorjevic V.H., Velicovic S.R., Cveticianiu D.M., Djushbek I.B., Veljkovic K.V., Nercovic O.M. (2008). Chlorine isotopes determination for tracking organic pollutants remediation. *Proceedings of Second-French-Serbian Summer University: Water quality control and health from concepts to action*, Editors S.Jokic, J.-M. Gustavino, L. Cot, Vinca Institute Belgrade, p. 143-145.
- [3] Bear J., Vernijt A. (1994). Modeling groundwater Flow and Pollution, D. Reidel Publishing Co.
- [4] *** Comsol Multiphysics (2008), Earth Science Module.