

A TVD METHOD FOR CONTAMINANT TRANSPORT IN POROUS MEDIA

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Abstract. *The objective of this work is to present a numerical study of contaminant migration in saturated porous media. For this purpose, the advection-diffusion equation describing the evolution of contaminant plumes in a vertical cross section of an aquifer is discretized employing a Total Variation Diminishing method (TVD), which provides an efficient way to eliminate spurious numerical oscillations. The stationary velocity field is computed using a hybridized mixed method. The initial concentration needed to determine the solution was specified using data from well samples. Numerical examples showing the implementation of the algorithm to describe groundwater contamination by cadmium in the Pampeano aquifer are presented.*

1 INTRODUCTION

Hydrology phenomena have been studied for a long time^{1,7} and many of its concepts are very well established, as well as their qualitative behaviour. Flows through porous media have been described for a long time on the basis of empirical laws, such as Darcy's, whose applicability has some limitations.

In this paper we employ a TVD numerical procedure to simulate the evolution in time of a plume of cadmium contaminant in a typical aquifer (the Pampeano aquifer) located on the northeast of the Province of Buenos Aires, Argentina.

When chemical species are dissolved in groundwater they may undergo adsorption on the surface of porous media, which can be modelled by either linear or nonlinear isotherms.

The presence of the isotherm influences the behaviour of the concentration front. In this paper adsorption reactions are modelled by means of a linear isotherm.

The pressure equation is solved using a hybridized mixed method and the flow field is assumed to be independent of the concentration of the dissolved chemicals.

2 THE DIFFERENTIAL MODEL

Let $C(x,t)$ denote the mass concentration of the contaminant and q_w the flux velocity vector. We will consider a porous domain with boundary $\Gamma = \Gamma^T \cup \Gamma^B \cup \Gamma^L \cup \Gamma^R$. If no adsorption reactions occur between the contaminant and the surrounding porous medium, then the transport is determined by convection and diffusion, and conservation of mass of the contaminant implies that

$$\frac{\partial}{\partial t} (\phi C(x,t)) + \nabla \cdot (D \nabla C(x,t)) - q_w \cdot \nabla C(x,t) = f(x,t) \quad x \quad (2.1.)$$

In (2.1.) ϕ denotes the porosity, $D = D(q_w)$ the diffusion tensor and f the external contaminant source rate of injection.

Taking adsorption into account, the mass balance equation becomes

$$\frac{\partial}{\partial t} (\phi (C(x,t) + S(x,t))) + \nabla \cdot (D \nabla C(x,t)) - q_w \cdot \nabla C(x,t) = f(x,t) \quad x \quad (2.2.)$$

In (2.2.) ρ_s denotes the bulk density of the soil and S is the adsorbed concentration. In this study we consider a linear adsorption isotherm of the form

$$S(x,t) = k_d C(x,t) \quad (2.3.)$$

where k_d is an empirical distribution coefficient.

Taking equation (2.3) into account, equation (2.2) can be written in the form

$$R \frac{\partial C(x,t)}{\partial t} + \nabla \cdot (D \nabla C(x,t)) - q_w \frac{\partial C(x,t)}{\partial x} = f(x,t) \quad (2.4.)$$

where

$$R = 1 + k_d \quad (2.5.)$$

and R is the retardation factor (dimensionless).

We used a simplification of the dispersion equation, i.e., the tracer hypothesis⁷. This hypothesis consists in uncoupling the concentration and velocity equations, so that the velocity does not depend on the concentration. Under the incompressibility assumption, we have that

$$\nabla \cdot q_w = 0 \quad (2.6.)$$

Also, satisfies Darcy's law stated in the form

$$q_w = -\frac{K}{\mu} [\nabla p_w + \rho_w g z] = -\frac{K}{\mu} \nabla \phi \quad (2.1.)$$

where K is the rock permeability, μ the water viscosity, ρ_w the water density, p_w the water pressure and g the gravity constant. Thus ϕ represents the water potential. The dispersion tensor has the form⁴

$$D = \left(d_m I + |q_w| \left(E_L(q_w) + E_T(q_w) \right) \right)$$

where $E(q_w)$ is a 2×2 matrix representing orthogonal projection along the velocity vector and $E^-(q_w) = I - E(q_w)$. Also, d_m , E_L and E_T denote the molecular, longitudinal and transversal diffusion coefficients.

To define the system, initial and boundary conditions must be specified. The initial condition is defined by specifying the concentration at the initial time. For the concentration equation, the boundary conditions were chosen to be of Neumann type with no contaminant diffusion cross the boundaries.

For the pressure equation, we choosed a combination of Dirichlet and Neumann boundary conditions to fit the flow field data.

Thus we will solve equations (2.4)--(2.7) with the boundary conditions

$$D C^? = 0 \tag{2.8.}$$

$$q^? = q_0 \quad T \quad B \tag{2.9.}$$

$$p = p_R \quad R \tag{2.10}$$

$$p = p_L \quad L \tag{2.11}$$

Adsorption-desorption processes are represented in the model as surface complexation reactions. For these reactions, equilibrium or nonequilibrium conditions may be assumed⁸.

To achieve numerical stability and control numerical, the spatial and temporal discretization should satisfy the spatial and temporal discretization should as follows:³

$$P = \frac{q \ x}{D} \leq 2$$

$$C = \frac{q \ t}{x} \leq 1$$

where t is the time step and x is the spatial discretization.

The grid Peclet criterium expresses the ratio of the spatial discretization and the dispersion length. The Courant number is physically interpreted as the ratio of the advective distance during one time step to the spatial discretization.

3 THE TVD METHOD AND THE FLUX LIMITERS.

Unfortunately, the numerical simulation of advective-diffusive-reactive transport equations is often plagued with serious difficulties. Almost all standard methods yield numerical solutions with excessive oscillations². To eliminate the numerical oscillations, the TVD scheme have been proposed^{5,6}. The TVD property guarantees then the total variation of the solution of a equation will not increase as the solution progresses in time. The discretization of the diffusive terms corresponds to a simple five--points finite difference scheme. Notice that in any standard discretization of (2.4)--(2.7) the convective term requires the values of the concentration at the mid points of the sides of each rectangle of the grid, which are obtained employing a flux limiter.

We choosed the Van Leer flux limiter, defined by

$$= \frac{r + |r|}{1 + |r|}$$

where the ratios r between the fluxes are

$$r = \frac{c_i - c_{i-1}}{c_{i+1} - c_i}$$

4 THE GEOLOGICAL SCENARIO

The Pampeano aquifer is the upper unit of the sedimentary sequence. It is a silt clay with sandy intercalations which present calcium carbonate in different shapes. It represents a homogeneous regional group, both from an hydraulic and from a chemical point of view¹⁰.

The regional groundwater flow is towards the La Plata River and the water table depth oscillates between 3 and 4 meters. The region is a industrial area where problems with groundwater pollution have been detected in several areas.

5 THE HYPOTHESIS OF THE MODEL

In the example considered here here we investigate the evolution in time of a contaminant plume of cadmium which undergoes linear adsorption while being transported within the Pampeano aquifer, which is modelled as an homogeneous saturated porous medium of 6 km in the horizontal direction and 33 m in depth. We also assume that contaminant was introduced in the domain some years ago during a short time period, and no extra sources of the same contaminant were added afterwards. This assumption was based on the fact that there are no previous available data of cadmium concentration measurements. It is at our disposal cadmium concentration measurements in two wells separated by a distance of 3.5 km. The samples were taken from the upper part of the Pampeano aquifer.

In the absence of additional field data, we used interpolation to obtain cadmium concentration in a region near the wells, assuming that concentration decreases with depth. We remark that the location of the contamination sources is subject to some uncertainty. Consequently, we assumed an initial conditions based on field data measurements at the wells and eliminated additional external sources of the contaminant. The porosity of the Pampeano aquifer is reported to be 0.10, while a hydraulic conductivity value of the 0.7 m/day was used¹⁰. Also, a longitudinal dispersivity of 0.05 m²/day and a transverse dispersivity of 0.03 m²/day were used as diffusion coefficients.

We approximated the cadmium isotherm by means of a linear function. The constant value k_d for this function was chosen¹¹ to be 0.02. We employ a bulk density of 2.67 gr/cm³.

6 SIMULATIONS RESULTS

Results of the simulations of cadmium transport with mass transfer controlled with

adsorption are shown in this section. The figures show the spatial distribution of the dissolved cadmium concentration fronts after 20, 60, 100 and 160 days, which follows the regional flow pattern. The spacing grid was chosen to be $x = 100$ m. and $z = 1$ m. All simulations were run with a time step of 20 days, with a total simulation time of 600 days. The concentration of cadmium of the two field samples were of 0.532 and 0.157 mg/l (the acceptable values are less than 0.05 mg/l). The figures demonstrate due to the combined effects of diffusion, convection and adsorption, concentration values fall below the acceptable value of 0.05 mg/l after three months aquifer of simulation.

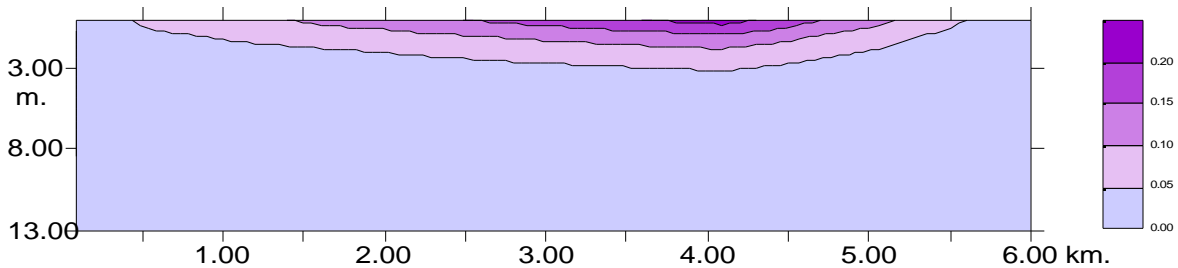


Figure Error! Unknown switch argument.: Concentration by 20 days.

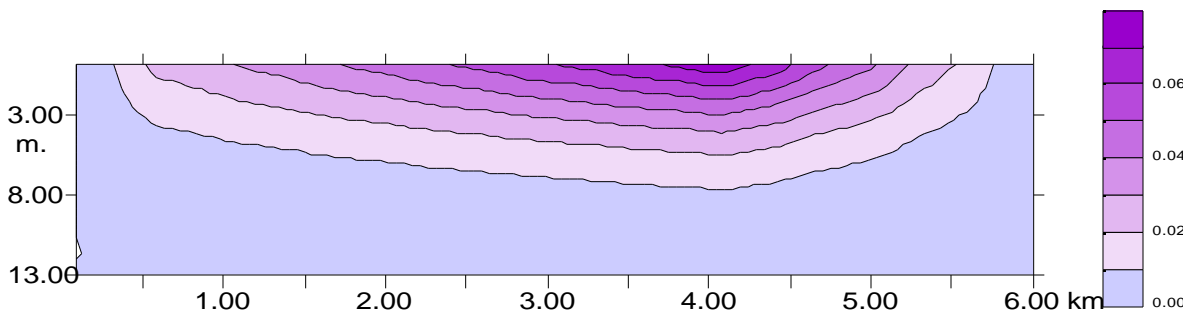


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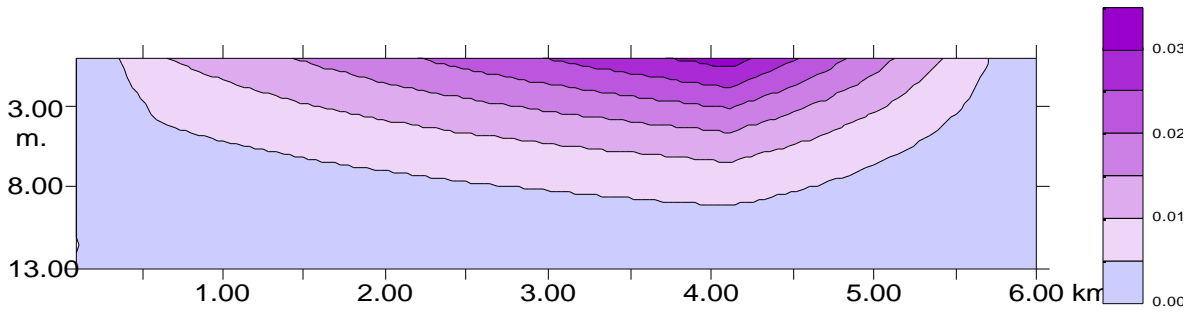


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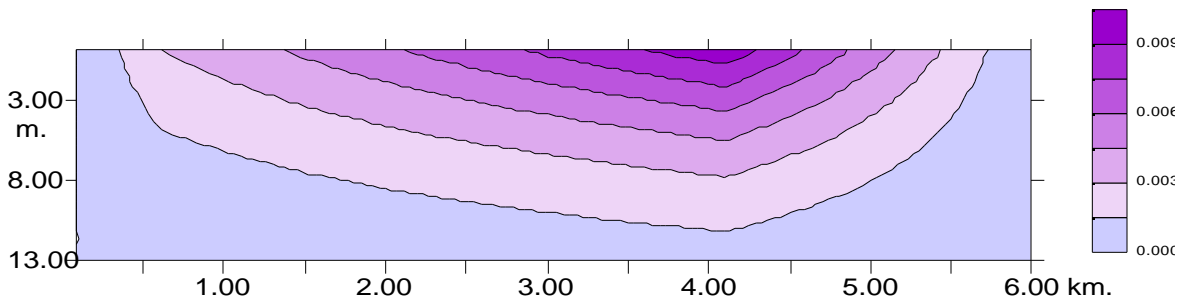


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7 CONCLUSIONS

This paper presents a numerical method for solution of reactive transport problems. The technique derives from mathematical manipulation of the convective term through the implementation of flux limiters. The transport model has been employed to simulate cadmium transport in the Pampeano aquifer, which is considered to be a single hydraulic unit with groundwater flowing eastward at a Darcy velocity of 2×10^3 m/days under steady flow conditions. The figures show that the simulation required 100 days to reach a concentration distribution below the acceptable values. The transport equation is derived by applying the law of conservation of mass to a differential volume element of a porous medium. Since the objective of the numerical simulations must allow tracking the relative importance of each ingredient to the overall group of phenomena, the space and time discretizations must be accurate and allow minimum numerical dispersion. A good approach is a finite difference schemes with mass flux controls, such as TVD schemes for conservation laws. The numerical

results presented here support the validity of the method.

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