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2-D Numerical Simulation of Transport and Bioremediation in a Saturated Porous Media

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Abstract

Through the present paper, we describe an integrated approach for modeling and simulation of the problem of transport and biodegradation in a saturated porous medium. The mathematical model is a nonlinear and coupled system of differential equations. The technique used here is based on the splitting method which consists on dividing the complete system of equations into sub-systems and solving each sub-system with the appropriate numerical method. Our system is a rectangular mesh in a two dimension space (a saturated aquifer) in which we are interested by modeling contaminant transport with aerobic biodegradation. The transport problem is approximated by a finite volumes schemes whereas the biological equations which are presented using a Monod kinetics are solved by an explicit forth Runge-Kutta method. The validation of the operator splitting implemented in this simulation is tested on a particular problem of transport and biodegradation with a first order kinetics (case of a low concentration of contaminant) which admit an analytical solution. The numerical results are in perfect harmony with the analytical one.

Keywords: Transport, Bioremediation, saturated aquifer, Finite volume scheme, splitting technique, Runge- Kutta method.

INTRODUCTION

Modeling contaminant transport and biodegradation in a saturated porous media is one of the most important problems in numerical simulation because the coupling between the advective- diffusive and reactive terms in the mathematical model and each term need a specific treatment for numerical resolution.

In this work, we are interested by modeling contaminant transport and biorestoration in a homogeneous medium (a saturated aquifer). The mathematical model is a coupled system which includes advective-reactive and biodegradation term which is presented here by a Monod kinetics [5].

A splitting technique [6] is proposed for solving this system which allows as to treat separately the different terms in the mathematical model. The approach decouples the transport portion from the reaction portion. So, the transport problem is solved first by a finite volume scheme [2]. The concentrations obtained from this step are then used as the initial concentrations to solve the reaction equations which are treated as ordinary differential equations and are solved with a forth –order, explicit Runge-Kutta method with time steps that are generally much smaller than those used for transport.

MATHEMATICAL MODEL

In this part, we describe the transport and biorestoration of a solute of concentration S and a dissolved oxygen of concentration O by microbes of concentration B. We suppose that the domain is homogenous and isotropic and the flow is one dimensional (in the x direction). The transport and the biodegradation model is given by the following equations:

A. Transport-diffusion-and reaction of substrates and oxygen

$$R\frac{\partial(\theta_w S)}{\partial t} = \nabla(\theta_w D_s \nabla S - \theta_w v S) + \mu_s(O,S,B) \qquad (1)$$

$$\frac{\partial(\theta_w O)}{\partial t} = \nabla(\theta_w D_o \nabla O - \theta_w v O) + \mu_o(O,S,B) \qquad (2)$$

B. Development of bacteria :

$$\frac{\partial B}{\partial t} = \mu_B B - K_d B \qquad (3)$$

C. Darcy's law:

For incompressible flow, we have the continuity equation:

$$\vec{V} = -\frac{K}{\mu(C)}(\nabla P - \beta(C))\vec{e_z} \qquad (4)$$

$$\nabla V = q \qquad (5)$$

Where :

S: The concentration of the substrate in the liquid phase (M T^{-3}); D_s is The dispersion tensor of substrate (L^2T^{-1}); Do is The dispersion tensor of oxygen (L^2T^{-1}); B is The concentration of bacteria (M L^{-3}); O is The Concentration of dissolved oxygen (ML^{-3}); K_d is The substrate constant of decay (T^{-1}); R is The retardation factor due to adsorption.; V is The pore water velocity (LT^{-1}); θ_w is The coefficient of porosity; P is The pressure; μ is The viscosity of the mixture; β is The fluid density; K is The permeability tensor of the porous medium; μ_s, μ_o and μ_B are the non linear terms given by Monod kinetics [5] which describe respectively the biodegradation of contaminant, oxygen and the microorganisms growth. We have so:

$$\mu_s = -\frac{\mu_0}{Y} B\left(\frac{S}{S+K_s}\right)\left(\frac{O}{O+K_o}\right) \qquad (6)$$

$$\mu_o = -\frac{\mu_0}{Y} \mathrm{f}\, B\left(\frac{S}{S+K_s}\right)\left(\frac{O}{O+K_o}\right) \qquad (7)$$

$$\mu_B = \mu_0 \left(\frac{S}{S+Ks}\right)\left(\frac{O}{O+K_o}\right) \qquad (8)$$

$$-\nabla\left(\frac{K}{\mu(C)}\left(\nabla P - \beta(C)\vec{ez}\right)\right) = q \qquad (9)$$

$$\frac{\delta x}{\delta y}(\alpha_{i+1/2,j}(P_{i+1,j} - P_{i,j}) - \alpha_{i-1/2,j}(P_{i,j} - P_{i-1,j})) + \frac{\delta x}{\delta y}(\alpha_{i,j+1/2}(P_{i,j+1} - P_{i,j}) - \alpha_{i,j-1/2}(P_{i,j} - P_{i,j-1})) = -\delta x((\alpha\beta)_{i,j+1/2} - (\alpha\beta)_{i,j-1/2}) + \overline{q_{i,j}} \qquad (10)$$

μ_0 is the maximum substrate utilization rate per unit mass of microorganisms; K_s is the substrate half saturation constant; Y is the yield coefficient (mass of microbial protein created per unit substrate consumed); K_o is the oxygen half saturation constant; f is the mass of oxygen rate consumed per unit mass of substrate consumed.

In this model, the flow is governed by the law of Darcy (4) and the continuity equation (5). The system (1)-(2) describes the convection, dispersion and biodegradation of substrate of concentration *S* (contaminant) and nutrient of concentration O. Biological equations given by the monod kinetics are then simulated by a set of coupled differential equations (6-7-8).

$$\int_{\Gamma i+1/2,j} d^{11}\frac{\partial S}{\partial y}dy = \frac{\delta y}{\delta x} d^{11}_{i+1/2,j}(S^{n+1}_{i+1,j} - S^{n+1}_{i,j}) \qquad (11)$$

NUMERICAL SIMULATION

A splitting technique [6] is proposed for solving the system of equations (1)-(5) which can be described in the following way: By combination of Darcy's law (equation (4)) and the continuity equation (5), we obtain the pressure equation (elliptic equation):

A finite volume scheme [2] is adapted to compute the pressure P on the center of cells. So, we consider a rectangular cell (control volume) Ω_{ij} of $\delta x \times \delta y$ size with $\partial\Omega_{ij}=\Gamma_{i+1/2,j}\cup\Gamma_{i-1/2,j}\cup\Gamma_{i,j+1/2}\cup\Gamma_{i,j-1/2}$("*Figure*1.").

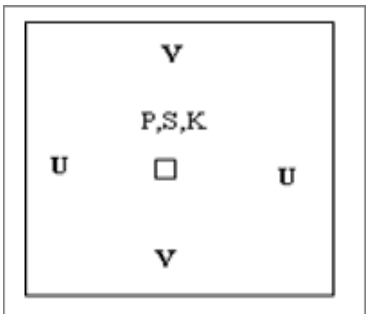

Figure 1: Representation of a control volume Ω_{ij}

The integration of equation (9) on the cell Ω_{ij} by green's formula gives the discretized equation for pressure: (we denoted $\alpha=K/\mu(C)$

By numerical solving of equation (10) with the boundary conditions as a system of equations of the form: AP=L, we get the profile of pressure at each time. In a second step, Darcy velocities are calculated on the edge of the cells by utilizing equation (4). Advection-diffusion-reaction equations (1) and (2) are decoupled by time splitting method. The integration of equation (1) without the kinetic term on the cell Ω_{ij}, by green's formula gives: (we assume that S is linear on each Γ_k)

Where d^{ij} are the coefficients of dispersion which are discretized on the control volume as it is shown in ("F*igure2.*").

$$\int_{\Gamma i+1/2,j} d^{12}\frac{\partial S}{\partial y}dy = d^{12}_{i+1/2,j+1/2}(S^{n+1}_{i+1/2,j+1/2} - S^{n+1}_{i+1/2,j+1/2}) + d^{12}_{i+1/2,j-1/2}(S^{n+1}_{i+1/2,j} - S^{n+1}_{i+1/2,j-1/2}) \quad (12)$$

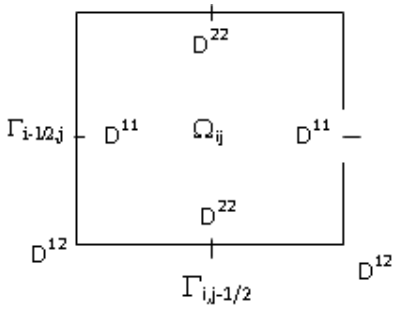

Figure 2: Discretization of dispersion coefficients

The flux $H_{i+1/2,j}$, $H_{i,j+1/2}$ and $H_{i,j-1/2}$ are obtained by the same procedure, we get so the following numerical scheme :

$$\begin{aligned} &S^{n+1}_{i,j} - \frac{\delta t}{\delta x^2}(d^{11}_{i+1/2,j}(S^{n+1}_{i+1,j} - S^{n+1}_{i,j}) - d^{11}_{i-1/2,j}(S^{n+1}_{i,j} - S^{n+1}_{i-1,j})) \\ &+ \frac{\delta t}{\delta y^2}(d^{22}_{i,j+1/2}(S^{n+1}_{i,j+1} - S^{n+1}_{i,j}) - d^{22}_{i,j-1/2}(S^{n+1}_{\mathrm{i,j}} - S^{n+1}_{i,j-1})) \\ &- \frac{\delta t}{2\,\delta x \delta y}(d^{12}_{i+1/2,j+1/2}(S^{n+1}_{i+1,j+1} - S^{n+1}_{i,j}) - d^{12}_{i-1/2,j-1/2}(S^{n+1}_{i,j} - S^{n+1}_{i-1,j-i})) \\ &+ \frac{\delta t}{2\,\delta x\,\delta y}(d^{12}_{i+1/2,j+1/2}(S^{n+1}_{i+1,j-1} - S^{n+1}_{i,j}) - d^{12}_{i-1/2,j+1/2}(S^{n+1}_{i,j} - S^{n+1}_{i-1,j+1})) + \delta t\ \mathrm{g}(\mathrm{S}^{\mathrm{n+1}}_{\mathrm{i,j}}) = S^{n+1/2}_{i,j} \end{aligned} \quad (13)$$

By numerical solving of equation (13) as a system of equation of the form: AS=B, we obtain the profile of concentration at time t+δt/2. Finally, the numerical resolution of the systems of biodegradation equations (system of equations (14)) by a forth order Runge-Kutta method using several small time steps gives the concentrations S, O, and B at time t+δt.

$$\begin{aligned} \frac{R\partial(\theta_w S)}{\partial t} &= \mu_s(\mathrm{O,S,B}) \\ \frac{\partial(\theta_w O)}{\partial t} &= \mu_0(\mathrm{O,S,B}) \\ \frac{\partial B}{\partial t} &= \mu_B B - K_d B \end{aligned} \quad (14)$$

Where μ_s,μ_0 and μ_B are given respectively by equations (6,7 and 8).

NUMERICAL TESTS:

In this part, we suppose that suppose that the domain is homogenous and isotropic, the flow is one dimensional (in x direction).

The initial conditions: S (x, y, t=0)=0 on the domain; Boundary conditions: S (0, y , t >0) = S0 if $|y| < A$; $A \in \Re$ (a localized source of injection on the y direction). The domain is semi –finite. S (x, y, t) is only defined down stern the source.

The biological and transport parameters used in the simulation are [3]: v=1m/d, R=1, Dl=40m^2/d Dt=4.5 m^2/d, K_s=0.05mg/l, K_0=1.4mg/l, μ_0=0.55(d^{-1}), Y=0.25, f=1.2, K_d=0.14 (d^{-1}).

Initially, no dissolved oxygen is present in the medium and a constant microorganism's concentration of 10^{-3}mg/l is assumed. The initial distribution of substrate concentration at time t=200 days is shown in("Figure3").

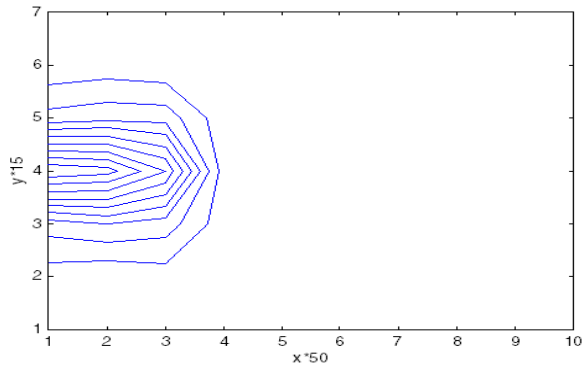

Figure 3: The profile of initial concentrations of substrate at time t=200 days

The biological processes are then simulated by injecting 10 mg/l of dissolved oxygen at the inflow boundary. In "Figure 4", we have the profile of substrate concentrations after 200 days of biorestoration.

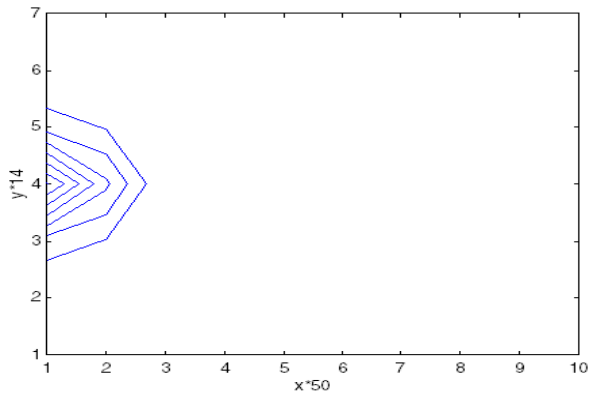

Figure 4: The profile of substrate concentrations after 200 days of biorestoration

In a second test, we simulate the microbial activities in the medium. We inject so from the inflow boundary of the domain 50 mg/l of oxygen. "Figure 5" Show the substrate concentrations after 200 days of biorestoration.

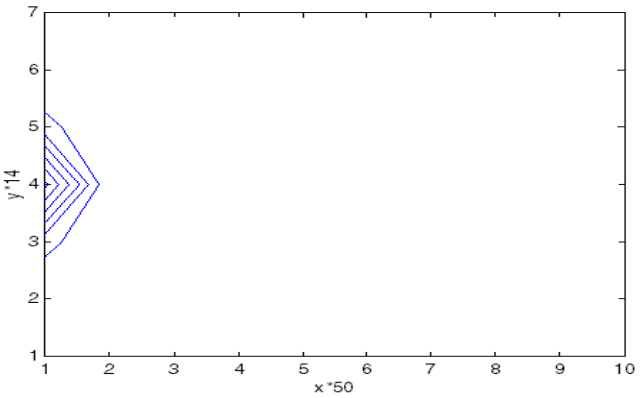

Figure 5: The profile of substrate concentrations after 200 days of biorestoration with injecting 50 mg of oxygen

Finally, the validation of the splitting technique used in this simulation was tested by comparison between numerical result and analytical solution [4] for one dimensional problem of transport and biodegradation with a first-order reaction [5]. Fig. 6 shows that the numerical result coincide with the analytical solutions.

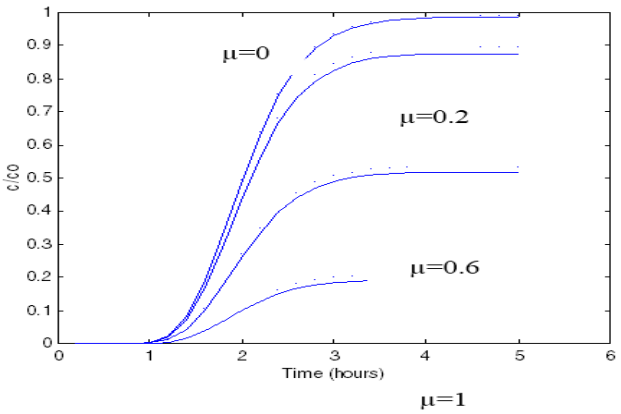

Figure 6: Analytical result (solid curve) agree with the numerical solution (curve with point) for one dimensional problem with a first order reaction

CONCLUSION

In this work, we have developed a numerical approach for solving the system of transport and biodegradation in a saturated aquifer. The method is based on a splitting technique which consists on discretizing first the convective equation with a finite volumes scheme who is very efficient for capturing the numerical instabilities as it is shown in the different tests presented. The solutions obtained from this step

are considered as intial conditions for the dispersive equation which we have treated also with a finite volumes scheme. The final solutions of this system are found by solving the biological system given by monod kinetics by a forth –runge kutta method with a time step much smaller than the transport one. In the numerical tests presented, we have shown that the augmenting in the concentration of oxygen injected from the inflow boundary enhance the rate of biodegradation of the substrate in the studied medium.

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