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BIOREMEDIATION IN A POROUS MEDIUM WITH SMALL BIO-CLOGGING

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Abstract. We investigate flow problems of relevance in bioremediation and develop a mathematical model for ground water transport of contamination (e.g. biological or chemical waste), and its remediation. Particular emphasis is placed on the study of processes involving the full coupling of reaction, transport and mechanical effects. Dimensionless analysis and asymptotic simplification are used to simplify the governing equations, which are then solved numerically. In addition we use matched asymptotic techniques to test the accuracy of the numerical simulations in the limit of large P*éc* let number.

Key words: porous flow, asymptotic analysis, numerical solution

1. Introduction

When a contaminant is released into the subsurface environment, it percolates downwards and horizontally into aquifers due to gravity forces and dispersion [1]. In this paper we consider an in-situ remediation strategy applied to a one dimensional transport of contaminant in a phreatic aquifer with varying groundwater velocity. We assume only one microbial population is involved in the biodegradation process and we ignore the effects of intermediate products.

First we consider groundwater flow where the flow rate is proportional to the pressure gradient as given by Darcy's law. Dimensional analysis and asymptotic simplification are used to simplify the governing equations, which are then solved numerically. Secondly, we incorporate the flow velocity into the biodegradation equations. Small pore clogging effects are included by expressing the volumetric liquid fraction θ_ℓ as a linear function of biomass concentration m^* but the full effects of coupling with the flow problem are neglected. In all the computations, the accuracy of the numerical simulations is tested by obtaining approximate solutions in the limit of large P*é*clet number. We use experimental parameter values from MacQuarrie et al. [3].

2. Governing Flow Model

The aquifer is assumed to be very long compared to its initial height h_0, i.e. $h_0 \ll \ell$, [2]. ℓ is the horizontal length scale of the aquifer. The phreatic aquifer has the water table as its upper boundary and from a mathematical point of view, this is a free boundary (see Fig.1).

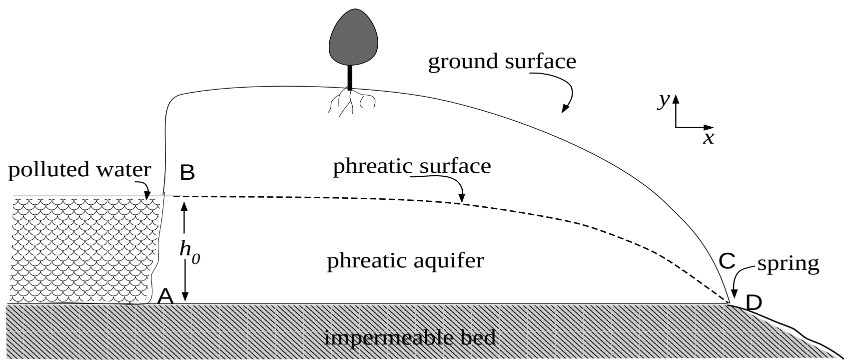

Figure 1. Porous medium boundaries and the free surface of the model problem

In the porous medium we apply Darcy's law which relates the flow velocity $\mathbf{u}^* = (u^*, v^*)$ to the applied pressure gradient. Assuming an incompressible flow through a rigid porous medium, we have a pressure distribution governed by the Laplace's equation: $\nabla^{*2} p^* = 0$ where the asterisk indicates a dimensional variable.

2.1. Dimensionless Model

The dimensionless problem is governed by:

$$u = -p_x, \quad v = -p_y - 1, \quad p_{yy} + \delta^2 p_{xx} = 0, \tag{2.1}$$

where the boundary conditions are given by the following expressions:

$$\begin{aligned} &p_y = -1 \quad \text{on } y = 0, \\ &p = 0, \quad \delta^2 h_t = -p_y - 1 + \delta^2 p_x h_x \quad \text{on } y = h, \\ &p = (1 - y) \quad \text{on } x = 0, \\ &p = 0 \quad \text{on } x = 1. \end{aligned} \tag{2.2}$$

where $\delta = h_0/\ell$. If $\delta \ll 1$, then we find the solution to (2.1) as an expansion of the form $p = p_0 + \delta^2 p_1 + \delta^4 p_2 + \dots$. The leading order approximation for p is found to be $p \approx h - y$ which fails to satisfy condition at $x = 1$, unless there is no seepage face. Thus we will also seek a solution for h as an expansion of the form: $h = h_1 + \delta^2 h_2 + \dots$.

In the case of phreatic flow, the phreatic surface always terminates at a point below the water table of the body of open water present outside the flow domain. This region (D in Fig.1), is known as the seepage face. The Dupuit approximation cannot be applied to regions where vertical flow cannot be neglected such as at the seepage face. Using the Dupuit approximation the free surface can be found to be $h = (1-x)^{1/2}$. In fact the flux will be found to be infinite at $x = 1$, this is corrected by insertion of a boundary layer.

2.1.1. Numerical Strategy

The numerical strategy involves finding an expression for the free surface $y = h_1(x)$. We choose an initial guess for the free surface. At the free boundary we use $\mathbf{u} \cdot \hat{\mathbf{n}} = 0$. If the free surface boundary condition does not satisfy $p = 0$, we shift the surface to a new position and solve the problem with a new free surface. The procedure is terminated if the conditions, $\mathbf{u} \cdot \hat{\mathbf{n}} = 0$ and $p = 0$ are both satisfied simultaneously.

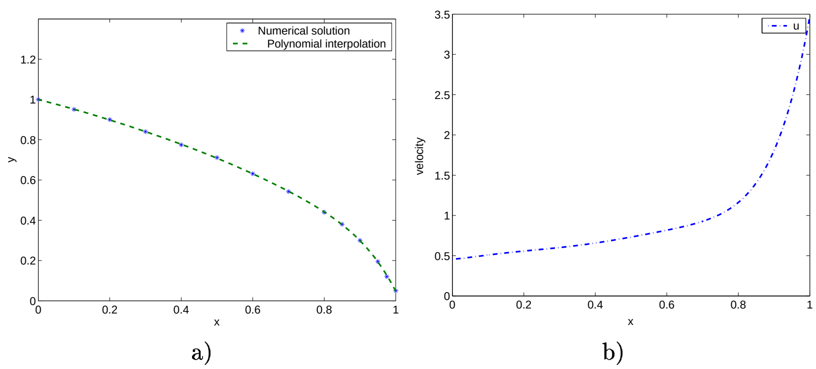

Figure 2. Numerical solutions: a) numerical solution for the phreatic surface $y = h_1(x)$, height of seepage face is $y = 0.05$, b) velocity in the horizontal direction.

It can be deduced from (2.1) and (2.2) that: $u \approx -h_{1x}$ and $v \approx \delta^2 y h_{1xx}$ which relates the velocity to the location of the free surface. Fig.2 shows the free surface and velocity in the x direction.

3. Bioremediation Model

We now consider the transport equations following Molz et al. (1986) [4] and Odencrantz et al. (1993) [5], for the degradation of the pollutant s^* by biomass m^* and consumption of the nutrient a^*. For the purpose of developing a numerical algorithm, we reformulate the model equations and put: $S^* = \theta_\ell s^*,\ A^* = \theta_\ell a^*$ and $M^* = m^*$.

3.1. Dimensionless model

When the contaminant enters the saturated aquifer, a plume will develop spreading in all directions. For the purposes of investigating the progress of the concentration profiles in the x direction we assume that the aquifer is sufficiently narrow that the concentrations in the y direction are approximately constant (smoothed via diffusion effects). We thus consider concentrations $S(x,t)$, $A(x,t)$ and $M(x,t)$.

Hence we obtain the reduced dimensionless system of equations:

$$R_s \frac{\partial S}{\partial t} = -u\frac{\partial S}{\partial x} + \frac{1}{Pe_L}\frac{\partial}{\partial x}\left(\theta_\ell \frac{\partial}{\partial x}\frac{S}{\theta_\ell}\right) - \lambda_1 r(x,t), \tag{3.1a}$$

$$\frac{\partial A}{\partial t} = -u\frac{\partial A}{\partial x} + \frac{1}{Pe_L}\frac{\partial}{\partial x}\left(\theta_\ell \frac{\partial}{\partial x}\frac{A}{\theta_\ell}\right) - \lambda_2 r(x,t), \tag{3.1b}$$

$$\frac{\partial M}{\partial t} = -\lambda_4(M-1) + \lambda_3 r(x,t), \tag{3.1c}$$

where $r(x,t)$ is the double Monod kinetics term. Initially we have a pollutant and nutrient free porous medium with a constant indigenous biomass concentration. The boundary conditions are: $S(0,t) = s_0\theta_\ell$ and $A(0,t) = a_0\theta_\ell$. Also the flux at the outflow boundary is zero.

3.1.1. The liquid fraction

We adopt the macroscopic approach. The volumetric fraction of the liquid phase in the medium is:

$$\theta_\ell = n - \hat{\kappa} m \tag{3.2}$$

where $\hat{\kappa}$ is the ratio of initial biomass mass per unit volume of the porous medium and the density of biomass and $n = 1-\theta_s$ is the constant medium porosity neglecting the presence of the microbes. Thus (3.2) assumes all biomass responsible for degradation is attached to the soil matrix.

4. Asymptotics based on $\hat{\kappa} \ll 1$

Consider a model where $\hat{\kappa} \ll 1$: i.e. there is little clogging due to biomass growth. We look for solutions to (3.1) as expansions of the form:

$$S = \phi_0 + \hat{\kappa}\phi_1 + \cdots, \quad A = \psi_0 + \hat{\kappa}\psi_1 + \cdots, \quad M = \omega_0 + \hat{\kappa}\omega_1 + \cdots \tag{4.1}$$

so that $\theta_\ell = n - \hat{\kappa}\omega_0 - \hat{\kappa}^2\omega_1 + \cdots$.

4.1. O(1) equations

The leading order governing equations are given by:

$$R_s\frac{\partial \phi_0}{\partial t} = -u\frac{\partial \phi_0}{\partial x} + \varepsilon\frac{\partial^2 \phi_0}{\partial x^2} - \lambda_1 r_0(x,t), \quad (4.2a)$$

$$\frac{\partial \psi_0}{\partial t} = -u\frac{\partial \psi_0}{\partial x} + \varepsilon\frac{\partial^2 \psi_0}{\partial x^2} - \lambda_2 r_0(x,t), \quad (4.2b)$$

$$\frac{\partial \omega_0}{\partial t} = -\lambda_4(\omega_0 - 1) + \lambda_3 r_0(x,t), \quad (4.2c)$$

where $\varepsilon = 1/Pe_L$ and

$$r_0(x,t) = \omega_0\frac{\phi_0}{K_s+\phi_0}\frac{\psi_0}{K_a+\psi_0}, \quad (4.3)$$

with inlet boundary conditions $\varepsilon\frac{\partial\phi_0}{\partial x}(0,t) = u(\phi_0 - n), \varepsilon\frac{\partial\psi_0}{\partial x}(0,t) = u(\psi_0 - n)$, $\frac{\partial\phi_0}{\partial x}(1,t) = 0,\ \frac{\partial\psi_0}{\partial x}(1,t) = 0$ and initial conditions $\phi_0(x,0) = 0,\ \psi_0(x,0) = 0,\ \omega_0(x,0) = 1$.

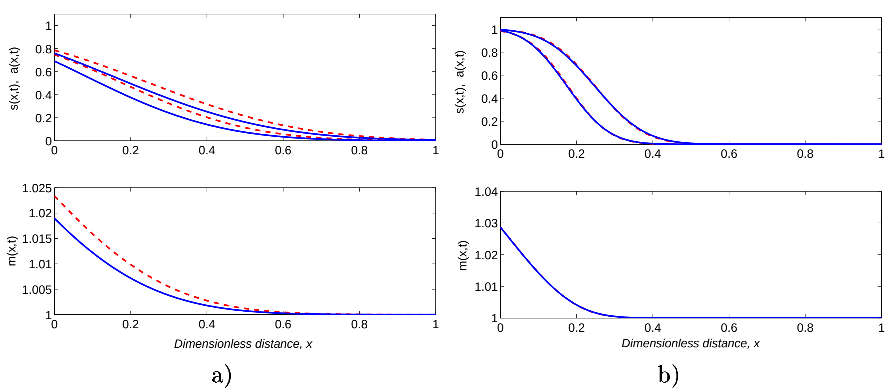

Figure 3. The numerical solution (solid curves) and the asymptotic solution (dashed curves).

We check the accuracy of our numerical solution by obtaining approximate solutions in the limit of large Peclet number, $Pe_L \equiv 1/\varepsilon \gg 1$, choosing realistic distinguished limits where $\lambda_i = O(\sqrt{\varepsilon})$. The solution to (3.1) is obtained in the form: $s(x,t) = \phi_0/n$, $a(x,t) = \psi_0/n$ and $m(x,t) = \omega_0$. The approximate analytical solutions are:

$$s(x,t) = \frac{1}{2}\left(1 - \text{erf}\left[\frac{x - ut/R_s}{\sqrt{\varepsilon}}\sqrt{\frac{R_s}{4t}}\right]\right), \quad (4.4a)$$

$$a(x,t) = \frac{1}{2}\left(1 - \text{erf}\left[\frac{x - ut}{\sqrt{\varepsilon}}\sqrt{\frac{1}{4t}}\right]\right) \quad (4.4b)$$

and

$$m(x,t) = 1 + \lambda_3 \int_0^t \frac{s(x,t)}{K_s + s(x,t)} \frac{a(x,t)}{K_a + a(x,t)} dt. \tag{4.5}$$

Fig.3 is a plot of the asymptotic solution and the numerical solution for different values of ε. The width of the shock layer is of $O(\sqrt{\varepsilon})$. The sharpening of the shock layer as ε decreases is evident in the figures.

The $O(\hat{\kappa})$ equations can only be solved numerically.

5. Summary and Conclusion

In this paper we developed an analytical and numerical approach to approximate an in situ bioremediation of a contaminated phreatic aquifer. The mathematical derivation of the flow velocity involved an assumption that the aquifer is thin and long. This assumption and dimensional analysis helped us reduce the two dimensional problem to a one dimensional problem. Excessive biomass concentration near the entrance boundary motivated us to express the medium porosity as a function of biomass concentration assuming that all biomass grows in colonies attached to soil particles.

In the above model, the pore clogging is assumed to be small. A model fully incorporating finite pore clogging, and the actual mechanism of pore clogging is currently under development.

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References

[1] M. Chapwanya and S.B.G. O'Brien. Corner and start-up singularities in porous flow. *Journal of Computational and Applied Mathematics*, **176**(1), 163 – 177, 2005.

[2] A.C. Fowler. *Mathematical models in the applied sciences.* Cambridge University Press, 1997.

[3] K.T.B. MacQurrie, Sudicky E.A. and Frind E.O. Simulation of biodegradable organic contaminants in groundwater:1. Numerical formulation in principal directions. *Water Resourses Research*, **26**(2), 207 – 222, February 1990.

[4] F.J. Molz, M.A. Widdowson and L.D. Benefield. Simulation of microbial growth dynamics coupled to nutrient and oxygen transport in porous media. *Water Resources Research*, **22**(8), 1207 – 1216, August, 1986.

[5] J.E. Odencrantz, A.J. Valocchi and Rittmann B.E. Modelling the interaction of sorp- tion and biodegradation on transport in groundwater in situ bioremediation systems. In: *Proceeding of the ground water modelling conference.* Colorado School of Mines Campus, 1993. June 9-12