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Project Summary

Denitrification in Nonhomogeneous Laboratory Scale Aquifers: 4. Hydraulics, Nitrogen Chemistry, and Microbiology in a Single Layer

F.T. Lindstrom, L. Boersma, D. Myrold, and M. Barlaz

A two-dimensional mathematical model for simulating the transport and fate of organic chemicals in a laboratory scale, single layer aquifer is presented. The aquifer can be nonhomogeneous and anisotropic with respect to fluid flow properties. The physical model for which this mathematical model has been developed is assumed to have open inlet and outlet ends and to be bounded by impermeable walls on all sides. The mathematical model allows placement of fully penetrating injection and/or extraction wells anywhere in the flow field. The inlet and outlet boundaries have user prescribed hydraulic pressure fields. The steady state hydraulic pressure field is obtained first, by using the two-dimensional Darcy flow law and the continuity equation.

Separate dynamic transport and fate equations are then set up for each of four dissolved chemicals, which include a substrate, nutrients, oxygen, and nitrate. Two equations, modeling the local growth and decay of two microbial populations, one operating with either oxygen or nitrogen, the other only with oxygen, are coupled to the transport and fate equations. The four chemical transport and fate equations are then solved in terms of user prescribed initial conditions. Boundary conditions are zero flow at the top, bottom, and sidewalls and accounting of mass at the inlet and exit ports. The model accounts for the major physical processes of dispersion and advection, and also can account for linear equilibrium sorption, four first order loss processes, including irreversible chemical reaction and/or dissolution into the organic phase, and irreversible binding in the sorbed state. The loss of substrate, nitrate, nutrient, and oxygen is accounted for by modified Monod kinetic type rate rules. The chemical may be released internally by distributed sources that do not perturb the flow field, or from fully penetrating injection wells. Chemical compound may also enter at the inlet boundary. Chemical mass balance type inlet and outlet boundary conditions are used. The solution to the field equation for hydraulic pressure is approximated by the space centered finite difference method using the strongly implicit procedure (SIP) with a user specified heuristic for choosing the iteration parameter. A solution to the transport and fate equations is approximated with a forward in time Euler-Lagrange time integrator applied to the chemical transport and fate semi-discretization.

This Project Summary was developed by EPA's Robert S. Kerr Environmental Research Laboratory, Ada, OK, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

Laboratory scale, physical models of aquifers are increasingly being used for the study of aquifer processes. Often it is less expensive to evaluate hypotheses for restoration procedures using laboratory scale models than to work under field conditions. Aquifer restoration methods are not without hazards. Biorestoration processes may alter the hydraulic properties of the aquifer.

Furthermore, numerical models of the transport and fate of chemicals in aquifers are now rapidly coming within the reach of environmental scientists. These models, once validated for the systems they are designed to simulate, are often cheaper and much faster to operate in real time response than the physical models. Thus the combination of mathematical models and laboratory scale models presents a cost effective and time efficient method for the study of bioremediation of contaminated aquifers.

In this report a mathematical models for denitrification processesin non–homogeneous, laboratory scale aquifers is described. The nitrogen chemistry and microbiological processes that occur in a single layer, saturated, aquifer are included in this model. A physical model aquifer is used at the USEPA Laboratory at Ada, Oklahoma for testing bioremediation processes for denitrification. This model will be used to evaluate data generated by this aquifer.

The success of biological denitrification methods depends on availability of a fundamental understanding of the transport and fate processes. In addition, knowledge about the important limiting factors, or limiting system properties must be acquired. Therefore, the immediate objective was to develop a preliminary mathematical model and associated computer code to describe substrate injection into a single layer, laboratory scale aquifer and to use the model in a sensitivity manner to assess the magnitude of the physical and biological factors controlling aquifer denitrification processes and identify those which can be manipulated to enhance the process.

One of the long-term goals of this study is development of a mathematical model of aquifer denitrification processes enhanced by stimulation of microbial populations. The experience gained from developing the preliminary model was used to develop the two-dimensional model for the simultaneous transport and fate of nitrate, and oxygen, substrate, e.g., methanol and inorganic nutrients, in the single layer aquifer, described in this report. Two independently operating microbial populations are included in the model, both using modified Monod kinetics. The model, called LT3VSI, is described in this report.

Physical Aquifers at RSKERL

Two large (4 ft wide, 4 ft high, 16 ft long) physical aquifers were constructed at the USEPA Robert S. Kerr Environmental Research Laboratory in Ada, Oklahoma. Each aquifer contains three horizontal layers of material, with each layer assumed to be homogeneous and isotropic with respect to water flow. These systems can be used for validation of mathematical models that simulate the hydrodynamic pressure distribution for the study of transport and fate of chemicals, and for evaluation of the growth characteristics of indigenous microbial populations. The physical aquifers are also used for the study of proposed physical and biological remediation schemes.

Long-term Goals of the Mathematical Modeling Effort

The goal of the present mathematical modeling effort is to describe the fate and transport of contaminants in the physical models. This work includes two-dimensional mathematical modeling of the steady state hydraulics and simultaneous transport and fate of the dissolved oxygen, nutrients (such as phosphorus), a carbon based substrate (for example methanol), and dissolved nitrate. Also included are two microbial populations which change in space and time. The mathematical model will be used to study scenarios for biorestoration of aquifers contaminated with nitrates.

The procedures being followed to achieve these goals include several steps. The first step was development of a preliminary model of the transport and fate of chemical compounds, with constant first-order loss processes and linear equilibrium sorption assumptions. This model is for two space dimensions and simulates only the "aquifer" slab of the physical model. The second step was to use the preliminary, two-dimensional model, called LT2VSI, for preliminary numerical studies of several scenarios for injection and/or extraction well placement. The third step was to expand LT2VSI by including four chemical compounds and two microbial populations. This model, referred to as LT3VSI, is the subject of this report.

Assumptions Underlying Model LT3VSI

The RSKERL physical models have been constructed in such a way that homogeneous and isotropic soil slabs were obtained. They have impermeable (no flow) side walls, an open top, partially open ends, and an impermeable lower or bottom boundary. The assumptions regarding the walls and the bottom made in the preliminary mathematical model LT2VSI reflect these conditions with the exception that the top boundary was assumed to be a "no flow" boundary. The hydraulic head distributions at the completely open inlet and exit boundaries are prescribed in model LT2VSI and fully penetrating injection and extraction wells may be present. Model LT2VSI was developed for a single-layer of soil representing the aquifer part of the three soil layers making up the RSKERL aquifers.

This report describes an extension of the preliminary model which is referred to as LT3VSI. The hydraulics in LT3VSI are the same as in LT2VSI. LT3VSI uses a Two-dimensional, horizontal, steady state, fluid flow field defined by a hydraulic head field which depends on appropriate Dirichlet and Neumann boundary conditions and characterizing the spatial dependency of the longitudinal and transverse components of the hydraulic conductivity tensor at saturation. The model determines simultaneous two-*dimensional* transport and fate of four dissolved chemicals, i.e.: oxygen, substrate, nutrient, and nitrate in the nonhomogeneous aquifer. The distribution of chemicals is affected by advection and dispersion in both the longitudinal and transverse directions. Linear equilibrium adsorption/desorption processes on each of the porous medium fractions is permitted. Three different first-order loss processes 1) chemical reaction with other soil components in the free phase, 2) other irreversible processes in the free phase, 3) chemical reaction in the sorbed phase. Modified Monod microbial degradation kinetics of the substrate system including oxygen, nutrients, and nitrate in addition to two microbial populations is also permitted. Zero order sources of the chemicals can be simulated. Appropriate Dirichlet and no flux Neumann boundary conditions with a provision for nonzero initial distribution of the chemicals is another feature of the model. Fully penetrating injection and/or extraction wells are allowed.

It is assumed that most, if not all, of the chemical and biological process coefficients are at least once continuously differentiable functions of the transverse coordinate x and the longitudinal coordinate y.

Fluid Flow Field

The porous medium may be nonhomogeneous and anisotropic with respect to fluid flow properties and has impervious walls on all sides. These conditions allow evaluation of two-dimensional transport and fate. It is assumed that the fluid flow field operates at steady state conditions at all times. Also it is assumed that any fluid flow perturbations introduced at the flow boundaries propagate extremely rapidly throughout the flow field, so that a new steady state is achieved instantly. Under these conditions the fluid storativity term in the fluid flow model may be neglected as shown for aquifers of the size considered here. The aquifer material can be nonhomogeneous as well as anisotropic, with the principal components of the saturated hydraulic conductivity tensor assumed to be once continuously differentiable over the interior of the flow domain. Dirichlet boundary conditions hold at both the inlet and outlet ends. Hydraulic heads at the inlet and outlet ends are specified. No-flow Neumann or flux type boundary conditions are specified along the walls. The Darcy velocity field components of the flow vector are defined by the transverse and longitudinal components of the saturated hydraulic conductivity in the aquifer. For isotropic and homogeneous porous media an analytical representation of the hydraulics in terms of a double sum infinite series of trigonometric functions, i.e., an eigenfunction solution procedure is possible. However, even in the very special isotropic case, the solutions are usually very slow to converge. Thousands if not millions of terms are necessary to achieve the required number of significant digits in each velocity component. Thus, the hydraulic head field on the interior of the flow domain, is usually approximated by means of finite difference or finite element methods.

Approximation of the Fluid Flow Equations

The method chosen for the solution of the flow equations is the Strongly Implicit Procedure (SIP). A heuristic for choosing the "cancellation of terms" parameter is included in the models SIP subroutine.

Velocity Components

Once all components of hydraulic head are known, the x and y components of the Darcy fluid velocity field, and also the effective pore velocities, can be estimated. However, since the hydraulic head field is known only approximately and only on a finite set of grid points, the two velocity components must be numerically estimated by interpolation.

Chemical Transport and Fate Model

The assumptions, which form the basis for the transport and fate model and which hold for each one of the four chemical compounds, i.e., substrate, nutrient, oxygen, and nitrate are: 1) Mass transport is via advection (convection) and dispersion. 2) The x and y dispersion components are linearly dependent upon the moduli of the velocity components of the flow field for two-dimensional flow in an isotropic and nonhomogeneous aquifer. 3) The porous medium can be partitioned into three distinct fractions sorbing particles (clay minerals and small silt particles), weakly sorbing particles (large silt and sand particles), and strongly sorbing organic matter with linear equilibrium sorption rule assumed for the porous medium. 4) Chemicals can be introduced into the aquifer with the feed stream at the inlet end or from constantly emitting sources in the aquifer. Fluids added by these methods must have a low volumetric concentration and the flow rates must be low enough so that the previously established fluid flow field is not disturbed. It is assumed that density gradients, density stratification, or local changes in the transport and/or fate properties of the porous medium do not occur in time. 5) Water containing chemicals can be introduced via fully penetrating injection wells or extracted from similar wells by pumping. 6) Loss of chemical can occur via first order irreversible loss processes such as chemical transformations and precipitation in both the free and sorbed phases in addition to loss via microbial degradation. 7) Microbiological processes are modeled using modified Monod kinetics. The model developed here includes two microbial populations, utilizes substrate under both aerobic and anaerobic conditions.

Consideration of the balance of chemical mass leads to the coupled system of four nonlinear, two-dimensional, transport and fate equations as the generic transport and fate equation. This equation is used to describe the transport and fate of each compound in the aquifer. Closed form solutions such as combinations of elementary functions or eigenfunctions do not exist for the system of equations. Therefore an approximate solution must be obtained using numerical procedures. The procedure used here is a type of finite difference Euler-Lagrange procedure, which is a modification of the method of characteristics.

Conclusions for the Model

Methods were developed for solving equations that describe transport and fate of chemicals in laboratory scale models of aquifers. The mathematical model is for aquifers consisting of a single layer of material, which can be either heterogeneous or homogeneous and anisotropic or isotropic with respect to the water flow field and heterogeneous or homogeneous but isotropic with respect to the chemical transport field properties.

The two-dimensional transport and fate model can be used for study of the important aspects of bioremediation of aquifers contaminated with nitrogen. A broad range of aquifer remediation scenarios may be considered. These scenarios could include studies of placement of injection/extraction wells to induce plume spreading or plume shaping and the effects of regions of varying hydraulic conductivity on the shape of the plumes. The comprehensive treatment of the inlet and exit port induced boundary conditions, included with the analysis represents a significant step forward in modeling the transport and fate of chemicals in laboratory scale physical aquifers.

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F.T. Lindstrom, L. Boersma, D. Myrold, and M. Barlaz are with Oregon State University, Corvallis, OR 97331.
Thomas E. Short is the EPA Project Officer (see below).

The complete report, entitled ""Dentrification in Nonhomogeneous Laboratory Scale Aquifers: 4. Hydraulics, Nitrogen Chemistry, and Microbiology in a Single Layer," (Order No. PB91-182345/AS; Cost: $17.00, subject to change) will be available only from:

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Robert S. Kerr Environmental Research Laboratory
U.S. Environmental Protection Agency
Ada, OK 74820

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