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An open-source, generic, environmental model for chemical fate and transport analysis in multi-media systems

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ABSTRACT

A new, open-source, software tool, the Generic Environmental Model (GEM) is summarized and illustrated herein. The GEM is a numerical approach to solving the classical, advective-dispersive, partial differential equations describing chemical fate and transport in environmental media. Its generic capabilities are due to the flexible compartment approach for spatial discretizations as well as an architecture that makes it amenable to a wide variety of environmental problems. Theoretical underpinnings and capabilities are described in this paper and are illustrated with a multi-media example using a holistic approach to multi-media modeling that includes both feedforward and feedback processes among media. The holistic approach is compared to results that might arise from a more conventional approach using a set of single-media models coupled together in a feedforward-only fashion. The GEM is open-source and was developed to facilitate rapid model-building for a wide variety of environmental contamination problems. The authors encourage users to download and use the tool.

1. Introduction

This paper introduces a new software tool designed to facilitate fate and transport (F&T) modeling of toxic chemicals in a wide variety of environmental settings. The software, named the Generic Environmental Model (GEM), is flexible, mathematically rigorous, based on fully numerical solutions to the underlying partial differential equations (PDEs), and available on-line as open-source (link: https://github.com/keithwlittle/GEM). It is written in the Java language. The GEM is intended as a tool that allows users to quickly develop accurate solutions to PDEs that are unique to their chemicals, environmental settings, and spatial/temporal resolution of interest. The architecture allows the user to build that set of PDEs of particular interest and obtain solutions to *those* PDEs, rather than the classical approach of force-fitting the problem into an existing black box model, which may not honor all of the F&T features of interest. The GEM is extensively documented, including detailed user instructions and examples in Little (2012).

Regarding a literature review of similar models and comparative differences, we are not aware of another, open-source, environmental modeling platform that has these generic features. Goldsim (http://www.goldsim.com/Web/Products/GoldSimPro/) is an environmental modeling platform that has F&T capability, but is proprietary. In the public domain, several of the fugacity models originally developed by Mackay (1991) have generic capability and are typically being used for regional, multi-media modeling applications. However, they operate on fugacity-based PDEs and seem more generally applicable to low spatial and temporal resolution applications.

Following a description of the GEM tool's theoretical basis, functionality, and a summary of verification/validation exercises, its use is illustrated via a multi-media, chemical F&T example. The multi-media domain is hypothetical, but realistic, and comprises soil, aquifer, surface water, and air media. A holistic, GEM-based model is set up and dynamically executed and includes feedforward and feedback processes (e.g., volatilization, settling, dispersion) both within and among the media. A second simulation is performed wherein inter-media processes are included only in a feedforward manner, i.e. from one medium to another – to mimic conventional multi-media modeling tools that couple single medium models with outputs from one model becoming inputs to another in one direction only. The holistic results are compared to feedforward-only results.

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2. Functionality, design motivation, and numerical approach

2.1. Overview of functionality

The "generic environmental" attribute of the GEM tool arises from several design features:

- It is designed as an environmental modeling platform, or framework, rather than a model with specific functionality. Users enter their specific data regarding state variables (SVs), environmental topology, parameters, and processes and the corresponding PDEs are then assembled and solved.
- It is based on the generalized PDE describing advective - dispersive F&T of chemical mass in porous media, which can be simplified to surface water or air media.
- The numerical approximation to the spatial derivatives uses the "compartment" method, which is mathematically equivalent to standard finite difference approximations, with the exception that the spatial domain itself is discretized rather than the spatial derivative terms in the underlying PDE. This seemingly trivial difference has the practical benefits of being both highly intuitive to the user as well as being robust to alternative dimensionalities. Thus a 1-D problem is easily converted into 2- or 3-D simply by adding more compartments in those dimensions. Temporal derivatives are approximated by standard finite difference methods.
- The spatial discretization options are either "back space" (BS) or "center space" (CS). Temporal discretization options are forward time (FT), back time (BT), or center time (CT). The choices have implications for allowable time step sizes and compartment volumes vis a vis avoidance of numerical errors (numerical dispersion, wiggle/negativity).
- Complete parameterization of the model is achieved through straightforward, comma-separated value (CSV), text files. Fate processes types and parameterization are highly flexible and provided by the user. The CSV files are readily generated by the user using a spreadsheet. CSV files for most of the examples mentioned later are available on-line (https://github.com/keithwlittle/GEM). In particular, a set of input files for a relatively simple, soil column application is included along with a tutorial describing the structure of the associated input files. (See "Start Here" folder.) The new user is encouraged to first become familiar with this example and make sequential changes to its files as needed to build input files for new applications.
- Multiple, interacting SVs are possible, including specification of the compartmental relevancy of each SV.
- A quasi-Newton iterative algorithm is included allowing nonlinear capability. Although designed to build systems of equations describing F&T of chemical mass in environmental systems where hydrodynamic flows among compartments are user inputs, the GEM can also be used to solve the PDEs describing the hydrodynamic movement of water itself by a suitable change of variables and reinterpretation of parameters. Indeed, the GEM can be used either in "Environmental System" mode, where it assumes the user is building environmental F&T – type PDEs, or in "Equation Solver" mode. Equation Solver mode is completely general and the user enters the equations of interest – that may have nothing to do with environmental modeling – and the GEM subsequently solves those equations.

2.2. Underlying PDE

The GEM is designed primarily for chemicals that, among other processes, partition between liquid, solid, and gaseous phases in surface water and/or porous media domains. Despite the fact that the underlying PDEs describing these partitioning processes in water/porous media domains are remarkably similar, the historical development of F&T software has almost exclusively been compartmentalized into separate surface water models (e.g., WASP https://www.epa.gov/exposure-assessment-models/water-quality-analysis-simulation-program-wasp]) and porous media models (e.g., HYDRUS [http://www.groundwatersoftware.com/hydrus.htm]). This departure in software tools is principally because the underlying PDEs describing system hydrodynamics are quite different between these two media. However, once the flows are known, the F&T PDEs can be shown to be equivalent and can be used for either medium. This commonality is the motivating principle behind the GEM, which receives spatial and temporal flow distributions as user inputs to the F&T PDEs. The underlying PDE solved numerically by the GEM is summarized below.

The classical advective - dispersive equation describing chemical mass balance in a 1-dimensional (x), porous medium with equilibrium partitioning can be written as (e.g., Schnoor, 1996; or Fetter, 1993)

$$R\frac{\partial C_d}{\partial t} = -u_x\frac{\partial C_d}{\partial x} + D_x\frac{\partial^2 C_d}{\partial x^2} \quad (1)$$

where

C_d is solute (dissolved) concentration (M_c/L_w^3)
U_x is the advective, pore water velocity (L_w/T)
D_x is the diffusive/dispersive mixing coefficient through the pore water (L_w^2/T)
R is the dimensionless "retardation" coefficient defined as

$$R = 1 + \frac{K_d \rho_b}{\theta} \quad (2)$$

where

K_d is the solids/liquid partitioning parameter (L_w^3/M_s)
ρ_b is the bulk density of the solids (M_s/L_T^3)
Θ is the porosity or water content (L_w^3/L_T^3)

We are distinguishing between chemical and solids mass by using subscripts "c" and "s", respectively, and water and total volume by subscripts "w" and "T", respectively.

For water containing sorbing chemicals flowing through porous media, the retardation parameter, R, acts to slow down the movement of the chemical relative to the water itself, because it is being retarded by sorption onto the immobile solid media. In addition, in ground water applications one is typically more interested in the chemical concentration in the flowing water than in the concentration of chemical on the solids which have been left behind. Hence, the SV, C_d, in equation (1) is dissolved concentration.

Equation (1) is the underlying PDE (in 1-D) solved numerically by the GEM. Although commonly associated with contamination in porous media, the equation is extremely flexible. For example, consider partitioning chemicals flowing in a surface water medium containing suspended solids. The chemical is partitioning between solid and liquid phases just as in the porous medium scenario. However, it is typical for toxic surface water models to simulate total (dissolved plus sorbed) chemical as the SV rather than dissolved chemical. This is because the sorbed chemical is not being "left behind" in space and time (retarded) on the solids as on immobile porous media, but rather exists in the same location in