Original Software Publication

HYDROSCAPE: A new versatile software program for evaluating contaminant transport in groundwater

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ABSTRACT

HYDROSCAPE is a MATLAB®-based software program compiled as an executable file that uses an analytical solution to the advection–dispersion equation (ADE) to solve solute contaminant transport problems. It has an easy-to-use, intuitive user interface that produces high-quality outputs, includes a parameter estimator algorithm, and allows the user to upload maps from Google Maps™. Furthermore, the ADE solution is modified in two important, novel ways that greatly broaden its application to contaminant transport problems in hydrogeology. The user may: (1) customize the source region; and (2) implement horizontal geological units within the domain ("simple geology"). Through comparisons to numerical simulations, we demonstrate that although our novel simple geology feature is heuristic, because the plume shape, size, mass/volume, and concentrations are similar to numerical simulations, the feature is a useful screening-level tool.

Software metadata

Current software version	1.0
Permanent link to executables of this version	https://github.com/ElsevierSoftwareX/SOFTX-D-17-00026
Legal Software License	MIT
Computing platform / Operating System	Windows
Installation requirements & dependencies	MATLAB Runtime R2015a required
If available Link to user manual–if formally published include a reference to the publication in the reference list	https://www.eas.ualberta.ca/download/
Support email for questions	sfunk@ualberta.ca

1. Introduction

Modeling how contaminants are transported in the subsurface is an important aspect in contaminant hydrogeology due to its application in developing proper remediation strategies. The complexities associated with most contaminated sites may include geological heterogeneities, material variability, and spatial and temporal changes in both the source region and groundwater flow. Therefore, numerical simulations are often used to predict the fate and transport of contaminants in the subsurface. However, numerical simulations can be costly, require copious amounts of data, are time consuming to construct, and may be subject to

errors such as numerical dispersion, oscillations, non-convergence and truncation errors [1]. Analytical solutions to the advection–dispersion equation (ADE; Eq. (1)), a partial differential equation that describes the transport of a solute through advection, dispersion and diffusion, are therefore invaluable for rapid and inexpensive assessments of contaminant scenarios [2], determining the mechanisms for transport [3] and verifying numerical codes [2].

$$R\frac{\partial C}{\partial t} = D_L\frac{\partial^2 C}{\partial x^2} + D_{TH}\frac{\partial^2 C}{\partial y^2} + D_{TV}\frac{\partial^2 C}{\partial z^2} - v\frac{\partial C}{\partial x} - \lambda C \qquad (1)$$

Notation and terms are defined in Appendix A.

HYDROSCAPE uses an analytical solution to Eq. (1) ([4]; hereafter referred to as "the solution"), and packages it into an easy-to-use interactive graphical user interface (GUI) that produces high-quality outputs, includes a parameter estimator for inverse modeling, and allows the user to upload maps from Google Maps™.

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Table 1
Comparison of some key features of HYDROSCAPE to other programs that use analytical solutions to the ADE.

Program	Reactions			Aquifer	Map Overlay	Customized Source Region		Heterogeneity	
	First-order Decay	Zeroth-order rxn	Inst. Bio. rxn	Finite Dim.		Shape/ Conc.	Source Function	Vertical (Simple Geol.)	Horiz.
HYDROSCAPE	X				X	X	X	X	
3DADE/N3DADE	X	X							
AT123D-AT	X			X	X				
BIOSCREEN / BIOCHLOR	X		X			X			
ATRANS	X			X			X		
ArcNLET	X				X				X

Furthermore, we have modified the solution to allow users to: (1) build a customizable source region; and (2) implement horizontal geological units, each having different hydraulic and transport parameters, within the domain ("simple geology"). These novel features allow hydrogeologists to simulate quickly more complex scenarios that would otherwise be impossible with conventional analytical solutions. As a screening-level tool, HYDROSCAPE is more versatile and more broadly applicable than other programs currently available (see below). Ultimately, HYDROSCAPE may expedite the evaluation of remediation strategies for contaminated sites by hydrogeologists and environmental scientists. Additional details are provided in Supplementary Material and the User's Manual (https://www.eas.ualberta.ca/download/).

2. Comparison with related programs

Windows-based software programs utilizing analytical solution to the ADE have been developed in the past, and are briefly described below.

The FORTRAN-based computer program 3DADE and N3DADE were developed by the US Department of Agriculture [5], based on the solutions of Leij et al. [6] and [7]. However, these programs come with the disclaimer "The code lacks the versatility to handle a wide variety of transport scenarios, whereas computational efficiency and user-friendliness were not a major concern during code development" [5].

The code for AT123D was developed based on the semi-analytical solutions in Yeh et al. [8]. The AT123D models have been used to simulate 3D transport of dissolved contaminants (e.g. Sinton et al. [9]), with a variety of source region configurations to choose from, within semi-infinite or finite aquifers. The use of Green's functions in AT123D allows for the user to choose from simple geometric sources, including point, line, plane or prismatic sources, and allows for either semi-infinite or finite aquifers [8]. Improvements made in the numerical integration and infinite series schemes [10] and the introduction of a GUI [11] have subsequently improved the code (now called AT123D-AT).

Perhaps the most well-known analytical solution-based computer program is the Domenico [12] family of software programs (i.e. BIOSCREEN and BIOCHLOR), which were developed by the US EPA (Environmental Protection Agency) for the simulation of either hydrocarbon-based contaminants (BIOSCREEN; [13]) or chlorinated solvents (BIOCHLOR; [14]) through natural attenuation. The benefit of BIOSCREEN (and its updated counterpart BIOSCREEN-AT; [4]) and BIOCHLOR is that the code is readily available as an easy-to-use Microsoft Excel®-based program. Similar to BIOSCREEN, Neville [15] developed ATRANS for a continuous patch source in a finite-thickness aquifer. Using the principle of superposition, ATRANS allows the user to create an arbitrary source function, whereas BIOSCREEN allows for a "layer cake" source region ([16]; discussed more in Section 4.4.1.). Recently, an extension of ArcGIS called ArcNLET was developed for simulating nitrate load in groundwater [17]. ArcNLET uses the Domenico [12] solution to solve the transport module of the program. ArcNLET first solves the flow module using a digital elevation map (DEM) and a map of the distribution of hydraulic conductivities and porosities [17]. Using some simplifying assumptions, particle tracking is used to generate a representation of the groundwater flow field [17]. ArcNLET then solves the transport of nitrate by superimposing the plume onto the flow field such that the centerline of the plume conforms with the flow paths of the field [17]. Comparisons with numerical simulations shows that the ArcNLET implementation is adequate for a screening-level tool [17].

Table 1 highlights some of the key features of the abovementioned programs and compares them to HYDROSCAPE. Most of the programs mentioned are largely constrained by the limitations and simplifications of the analytical solutions on which they are based (e.g. 3DADE/N3DADE and AT123D-AT). Other than BIOSCREEN [13] and ATRANS [15], the analytical solutions used remain unaltered. However, a feature that most programs lack is the ability to simulate horizontal layers within the domain (i.e. simple geology). ArcNLET allows its users to simulate horizontal heterogeneity, whereas HYDROSCAPE allows for vertical heterogeneity; however, ArcNLET lacks the customizability of the source region (Table 1).

3. HYDROSCAPE architecture

HYDROSCAPE is a MATLAB®-based program that uses a modified solution to the ADE to solve solute transport problems. To increase accessibility, HYDROSCAPE has been compiled into an executable file, allowing the user to run the program without MATLAB®. User-friendliness, versatility and computational efficiency were of primary concern during the development of the code and interface (Fig. 1). HYDROSCAPE was created to be used in two ways: (1) to solve a forward problem whereby parameters are known, and the user is interested in predicting the fate of the plume; or (2) to solve the inverse problem, whereby the user has some experimental or field data and wants to estimate what set(s) of parameters can reproduce the data (outlined in Section 4.2).

For the forward problem, users work through HYDROSCAPE's tab structure, inputting the requisite parameters in each tab (Fig. 1). Each tab (and certain buttons) is color coded to emphasize what parameters are required to be inputted and accepted. HYDROSCAPE then produces a simulation for the user to review. Standard outputs include surface and contour maps in map and cross-sectional views, three-dimensional contour volumes, concentration profiles (along an arbitrary transect), and breakthrough curves, all of which can be animated. Multiple breakthrough curves and concentration profiles can be plotted together for comparison. HYDROSCAPE also calculates a variety of parameters associated with the plume (e.g. plume dimensions, mass and volume). HYDROSCAPE allows the user to import and overlay a map by accessing Google Maps™, allowing for a quick assessment of the real-world extent of a plume (Fig. 1).

For the inverse problem, users may select the "Parameter Estimator" feature in HYDROSCAPE. Users must input the patch source geometry, the free-solution diffusion coefficient and "control points", known values of concentration at specified locations in