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BIOSCREEN, AT123D AND MODFLOW/MT3D, A COMPREHENSIVE REVIEW OF MODEL RESULTS

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ABSTRACT

The Domenico equation is commonly used to evaluate long term risks associated with contaminated groundwater. Numerous groundwater models are based on it, including BIOSCREEN and BIOCHLOR. This paper compares the results from BIOSCREEN, AT123D and MODFLOW/MT3D groundwater models. Results from the AT123D and MODFLOW/MT3D models indicate that BIOSCREEN significantly under estimates contaminant mobility and thus exposure risks. This was unexpected as BIOSCREEN results are commonly assumed to be extremely conservative. In fact BIOSCREEN did produce the highest downgradient concentrations; however it took unreasonable long periods of time to achieve them. Such lengthy time periods are not typically evaluated as part of a risk evaluation. Even more surprisingly BIOSCREEN produced the same peak concentration for all contaminants and for all aquifer types tested. Both contaminant concentration and travel times from AT123D and MODFLOW/MT3D models were almost identical. Furthermore these results varied with contaminants and aquifer properties as expected. The influence of biodegradation was also evaluated. Inclusion of conservative biodegradation rates made BIOSCREEN the least conservative model by far. This is because the lengthy travel times produced by BIOSCREEN provide a longer period of time over which biodegradation works.

Keywords: AT123D, BIOSCREEN, MODFLOW, MT3D

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1. INTRODUCTION

Groundwater transport modeling can be useful in making informed and defensible remedial decisions. Often this involves the use of a simple transport model, such as the Domenico equation, as a first step of the decision process. Selection of an appropriate transport model is of paramount importance in this process, as capabilities and ease of use can vary greatly. This paper compares three commonly used transport models, BIOSCREEN, AT123D, and MODFLOW/MT3D. These models are used to predict groundwater contaminant concentrations, which, in turn can determine the amount of contamination that can remain in place, while assuring the protection of human health and environment. The three models reviewed in this paper were selected based on their past use and availability.

2. MODEL DESCRIPTIONS

There are two basic types of computer-based groundwater transport models, analytical and numerical.

2.1 BIOSCREEN

BIOSCREEN (Newell et al., 1996) is based on the Domenico equation (Domenico, 1987), and was developed for the US Air Force by Ground Water Services, Inc. With over 6,000 downloads, it may be the most widely used analytical groundwater model in the world. BIOSCREEN is a public domain, two-dimensional screening level groundwater fate and transport model, which is used by many regulatory agencies. Contaminant transport is simulated under one-dimensional horizontal groundwater flow. Version 1.4 of the BIOSCREEN model was utilized to perform the modeling in this review.

The BIOSCREEN load can only be simulated as a plane perpendicular to groundwater flow. Processes simulated in this model are advection, dispersion, adsorption, and biological decay (Table 1). Biodegradation can be simulated as either a first-order decay, or an instantaneous reaction process. The results can be displayed as both area and centerline graphs. However, BIOSCREEN cannot produce a point of compliance report, which presents a graphical representation of constituent concentrations over time at a specific point.

The Domenico equation, on which the BIOSCREEN model is based, assumes that the source contaminant concentration remains constant through time (i.e., the source mass is infinite) (Figure 1). This means that the source concentration remains constant no matter how long the model is run. The infinite source is an inherent limitation of the Domenico equation. It does however simplify the algebraic solution, thus significantly reducing the computational time. In an attempt to overcome this limitation of the Domenico equation, a declining source concentration term was added to BIOSCREEN. This was accomplished by reducing the source concentration at a rate based on an estimate of the total mass in the source volume (even though actual load is still only a plane). However, the rate at which the source declines is not explicitly determined based on contaminant migration. As stated in the BIOSCREEN User's manual: *"this is an experimental relationship, and it should be applied with caution."*

2.2 AT123D

AT123D (Yeh 1981) is an acronym for the Analytical Transient 1-, 2-, and 3-Dimensional Simulation of Waste Transport in the Aquifer System. It is a public domain three-dimensional analytical groundwater transport model. Contaminant transport is simulated under one-dimensional horizontal groundwater flow. Transport processes simulated are advection, dispersion, adsorption, diffusion, and biodegradation (Table 1). The aquifer can be simulated as either confined or unconfined.

On the surface AT123D and BIOSCREEN appear to be similar, yet there are significant differences in the basic model assumptions. For instance BIOSCREEN is written in Excel, which although powerful is not designed to optimize mathematical calculations. On the other hand, AT123D and MODFLOW/MT3D are all written in FORTRAN, which is specifically created for the development of scientific applications. The use of FORTRAN provides a dramatic improvement in performance and flexibility of application, which allows AT123D and MODFLOW/MT3D to simulate a wider array of processes and load configurations.

There are a total of eight load configurations in AT123D, in which the load can be established as a point, line, area or volume. The source concentration in AT123D declines as contamination migrates downgradient (Figure 1). In addition to simulating a single instantaneous release, a separate load can be applied for each time-step. This feature allows AT123D to be linked to the SESOIL (Bonazountas and Wagner 1981) vadose zone model. Modeling was performed using Version 6.0 of AT123D in the SEVIEW 6.3 Integrated Contaminant Transport and Fate Modeling System (Schneiker 2005).

2.3 MODFLOW and MT3D

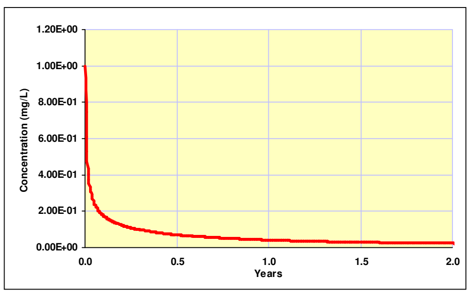
MODFLOW (McDonald and Harbaugh 1988) is a public domain, three-dimensional numerical groundwater flow model. Groundwater flow can be simulated for both steady state and transient conditions. It can also simulate flow based on external stresses, such as wells, recharge, evapotranspiration, rivers, and lakes. Hydraulic conductivities, storage coefficients, and groundwater flow parameters may differ spatially, thus accounting for anisotropic conditions (heterogeneous aquifers). The aquifer can be simulated as confined or unconfined. MODFLOW is currently the most

Table 1. Models Processes

Process	BIOSCREEN	AT123D	MODFLOW/MT3D
Volume source		✓	✓
Declining source		✓	✓
Advection	✓	✓	✓
Dispersion	✓	✓	✓
Adsorption	✓	✓	✓
Biological Decay	✓	✓	✓
Water Diffusion		✓	✓

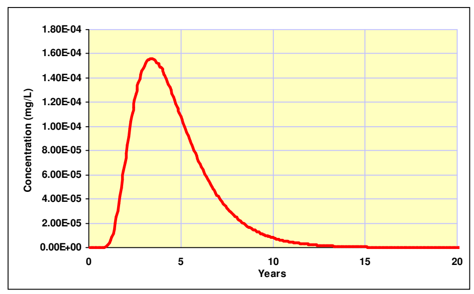
Instantaneous Load (AT123D and MODFLOW/MT3D)

Source Concentration



Declining source concentrations as predicted by the AT123D and MT3D models. The source is depleted as the contamination migrates downgradient.

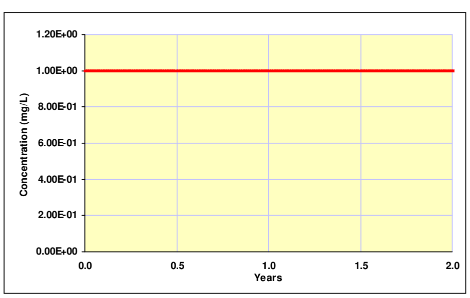
Downgradient Concentration



Resulting downgradient contaminant concentrations reach a peak value then decline due to depletion of the source.

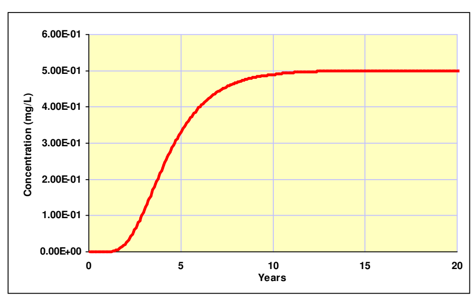
Infinite Load (BIOSCREEN)

Source Concentration



The BIOSCREEN source concentration remains constant through time.

Downgradient Concentration



Downgradient concentrations reach a peak value but never decline.

Figure 1. Models Loads

widely used numerical model in U.S. for groundwater flow problems.

MT3D (Zheng 1990) is a public domain three-dimensional groundwater transport model. It was developed independently from MODFLOW, and was designed to work with any cell-centered numerical groundwater flow model. Transport processes simulated are advection, dispersion, adsorption, diffusion, and biodegradation (Table 1). As with AT123D a separate contaminant load can be applied for each time step. The feature means that MT3D can also be linked to the SESOIL model. Contaminant load can be established as a volume of contaminated groundwater in any of the cells, or as a plane at the top of the water table. As with AT123D, MT3D simulates a declining source as an integral part of the fate and transport process.

3. FATE AND TRANSPORT PROCESSES

Groundwater models use various methods to simulate contaminant fate and transport processes. A summary of fate and transport processes simulated by the models is displayed in Table 1. There can be substantial differences in the total number of processes simulated, and in the methods used to simulate a particular process. All of the models tested simulate advection, dispersion, adsorption and biological decay processes. The AT123D and MT3D models simulate two additional processes. The first is the declining source concentration as the contamination mass migrates downgradient. The second is the water diffusion process. Water diffusion produces migration of contamination from areas of higher concentration to areas of lower concentration. This process is not dependent upon groundwater flow, and as such it even occurs in stagnant groundwater. Diffusion becomes progressively more important as groundwater flow decreases. Inclusion of this process means that AT123D and MODFLOW/MT3D can be used for lower permeability aquifers than BIOSCREEN.

3.1 Input Parameters

This evaluation consisted of determining predicted groundwater concentrations at a point ten meters (32 feet) downgradient of the source. Hydraulic conductivities simulated ranged from 1.0E+1 cm/sec to 1.0E-6 cm/sec. A total of 54 model scenarios were completed to evaluate results over a wide range of conditions.

The source dimensions were set to 6 by 10 by 5 feet in AT123D and MT3D, while the source in BIOSCREEN was set to a plane perpendicular to groundwater flow with a width of 10 feet and a depth of 5 feet (Table 2). Modeling was performed using an initial concentration of 1.0 ppm.

Results were evaluated at a point located 10 meters (32 feet) downgradient from the source. The 10-meter distance was selected as some regulatory agencies have used this distance in the development of default cleanup objectives.

Model input parameters (Tables 3 and 4) were obtained from default values specified by the Ohio Department of Commerce, Bureau of Underground Storage Tank

Regulations (BUSTR 2003). These input parameters were designed for use in the BUSTR Screen transport and fate model. BUSTR Screen is a variation of BIOSCREEN specifically developed for BUSTR. A tight clay aquifer scenario was added. This produced a wider range of conditions over which model responses could be evaluated. A gradient of 0.001 ft/ft was used for all aquifers. Modeling was performed for benzene and methyl tertiary-butyl ether (MTBE). We decided to use these chemicals as they often control remediation of contaminated sites. Chemical specific parameters for organic carbon partition coefficient (Koc) and water diffusion coefficient were obtained from the SEVIEW 6.3 chemical database. Biodegradation rate values were also obtained from the BUSTR (2003) data. Biodegradation of MTBE was not considered, as it is not assumed to readily degrade. Dispersivity values utilized in this evaluation are presented on (Table 5). AT123D and BIOSCREEN input parameters are almost identical with the exception of two additional parameters in AT123D: the distance of the load in the x direction and the water diffusion coefficient (Table 6).

Table 2. Contaminant Load Coordinates

Models	**AT123D & MODFLOW/MT3D**	**BIOSCREEN All**
units	**ft**	**ft**
x-axis*	-6.0	0.0
y-axis	10.0 (± 5.0)	
z-axis	-5.0	

***Table 3.* Aquifer Parameters**

Aquifer Type	**Hydraulic Conductivity**	**Porosity**	**Bulk Density**	**Soil Organic Carbon**	**Gradient**
units	**cm/sec**	**dimensionless**	**kg/L**	**fraction**	**ft/ft**
Tight Clay	1.0E-6	0.20	1.9	0.001	0.001
Clay	1.0E-5	0.20	1.8	0.001	0.001
Silt	1.0E-3	0.30	1.7	0.001	0.001
Silty Sand	1.0E-1	0.30	1.6	0.001	0.001
Clean Sand	1.0E+0	0.30	1.5	0.001	0.001
Gravel	1.0E+1	0.35	1.4	0.001	0.001

Table 4. Chemical Parameters

Chemical of Concern	Partition Coefficient (K_{oc})	Solute Half-Life	Water Diffusion Coefficient	Maximum Contaminant Level (MCL)
units	L/kg	years	cm^2/sec	mg/L
Benzene	58.9	1.97	9.80E-6	0.005
MTBE	6.0	- -	8.70E-6	0.040

Table 5. Aquifer Dispersivities

units	ft
Longitudinal	3.28
Transverse	0.328
Vertical	0.0328

Table 6. AT123D and BIOSCREEN Input Parameters

Parameter		BIOSCREEN	AT123D	MODFLOW /MT3D
Hydraulic Conductivity		✓	✓	✓
Gradient		✓	✓	✓
Dispersivities		✓	✓	✓
Porosity		✓	✓	✓
Bulk Density		✓	✓	✓
Organic Carbon Content		✓	✓	✓
Partition Coefficient		✓	✓	✓
Bio degradation	**Half-Life**	✓	✓	✓
	Instantaneous Reaction	✓		
Water Diffusion Coefficient			✓	✓

3.2 Model Setup and Run Times

It took less than 5 minutes to setup each of the BIOSCREEN and AT123D scenarios. It took about two hours to setup the MODFLOW/MT3D models. Modeling was performed using a 2.4 GHz Pentium 4 computer using the Microsoft Windows XP operating system. BIOSCREEN was run in Microsoft Excel 97. Among all three models, BIOSCREEN was the fastest, producing almost instantaneous results for all aquifer types. AT123D took a maximum of 10 seconds to run. It took MODFLOW/MT3D up to 28 minutes to run the tight clay simulations.

3.3 Model Reports

All three models are capable of presenting the results as area reports (Table 7). These reports depict concentrations over the entire area at a specific time. In MODFLOW/MT3D area results can also be displayed for a cross section. Although the area reports look nice, they provide minimal data for evaluating exposure risk. Results can also be displayed as centerline reports. These reports are useful when calibrating contaminant concentrations to measured values.

Table 7. Model Reporting Capabilities

Parameter	BIOSCREEN	AT123D	MODFLOW/MT3D
Area	✓	✓	✓
Centerline	✓	✓	
Point of compliance		✓	✓

Both AT123D and MT3D present results at a point of compliance. Called an observation point in MT3D, this report depicts predicted concentrations over time at a specific location, which meets the requirement for the development of risk-based evaluations. BIOSCREEN does not contain a point of compliance report and as such, it had to be run repeatedly until sufficient data was produced to generate a point of compliance report, thus making BIOSCREEN the most time consuming model evaluated.

4. RESULTS

Modeling results are presented as both peak groundwater concentrations, and maximum allowable source concentrations. The resulting groundwater concentrations are shown in Tables 8 and 9 (as well as in Figures 2a, 2b, 3a and 3b). Due to the significant difference between the BIOSCREEN results and the other models, concentrations are displayed as both linear and logarithmic plots. Travel times to the peak concentrations are presented in Tables 10 and 11.

Results show a strong agreement in the peak concentrations and travel times produced by AT123D and MODFLOW/MT3D. These models produced almost identical peak concentrations and at nearly the same time. Observed variations may be related to differences in the way results are generated. For example results in AT123D are calculated for a specific point, whereas results in MODFLOW/MT3D are generated for an entire cell.

Table 8. Benzene Peak Concentrations

Permeability	**BIOSCREEN**		**AT123D**		**MODFLOW/MT3D**	
	No Bio	**w/Bio**	**No Bio**	**w/Bio**	**No Bio**	**w/Bio**
cm/sec	**mg/L**	**mg/L**	**mg/L**	**mg/L**	**mg/L**	**mg/L**
1.0E+1	0.724	0.724	0.0985	0.0985	0.0791	0.0791
1.0E+0	0.724	0.721	0.0982	0.0978	0.0934	0.0931
1.0E-1	0.724	0.694	0.0982	0.0943	0.0817	0.0788
1.0E-3	0.724	0.0277	0.0543	0.00293	0.0836	0.00581
1.0E-5	0.724	1.37E-23	0.00272	3.96E-11	0.0108	1.05E-12
1.0E-6	0.724	8.47E-78	0.00108	8.47E-15	0.00242	1.48E-15

Table 9. MTBE Peak Concentrations

Permeability	**BIOSCREEN**	**AT123D**	**MODFLOW/MT3D**
cm/sec	**mg/L**	**mg/L**	**mg/L**
1.0E+1	0.724	0.116	0.0791
1.0E+0	0.724	0.116	0.0934
1.0E-1	0.724	0.116	0.0817
1.0E-3	0.724	0.0676	0.0847
1.0E-5	0.724	0.00415	0.0120
1.0E-6	0.724	0.00136	0.00251

Predicted BIOSCREEN groundwater concentrations were at least one order of magnitude higher than the other models for hydraulic conductivities between 1.0E+1 cm/sec and 1.0E-3 cm/sec. Concentrations produced by BIOSCREEN and the other models diverged further as hydraulic conductivities were reduced, reaching a maximum of three orders of magnitude at a hydraulic conductivity of 1.0E-6 cm/sec. It should be noted that peak concentrations produced by BIOSCREEN did not vary at all. In fact, BIOSCREEN produced the same peak downgradient concentration for all aquifer types and chemicals tested (Figures 2a, 2b, 3a and 3b). We tested this conclusion by performing additional modeling for benzo-a-pyrene, and obtained the same results. Based on our evaluation it appears that BIOSCREEN produces the same peak concentration regardless of the contaminant or aquifer properties.

Travel times to peak downgradient concentrations predicted by BIOSCREEN were significantly longer, reaching a maximum of 39,000 years for benzene with a hydraulic conductivity of 1.0E-6 cm/sec. However, based on AT123D and MODFLOW/MT3D predicted travel times were 310 and 572 years respectively. According to BIOSCREEN it would take benzene 40 years to reach a point 10 meters downgradient with a hydraulic conductivity of 1.0E-3 cm/sec. However, the other two models indicate it would only take 10 years for benzene to reach this point. BIOSCREEN produced a travel time for benzene of 3,980 years at a hydraulic conductivity of 1.0E-5 cm/sec. While the other models indicated that it would only take between 311 and 329 years to reach the peak concentration.

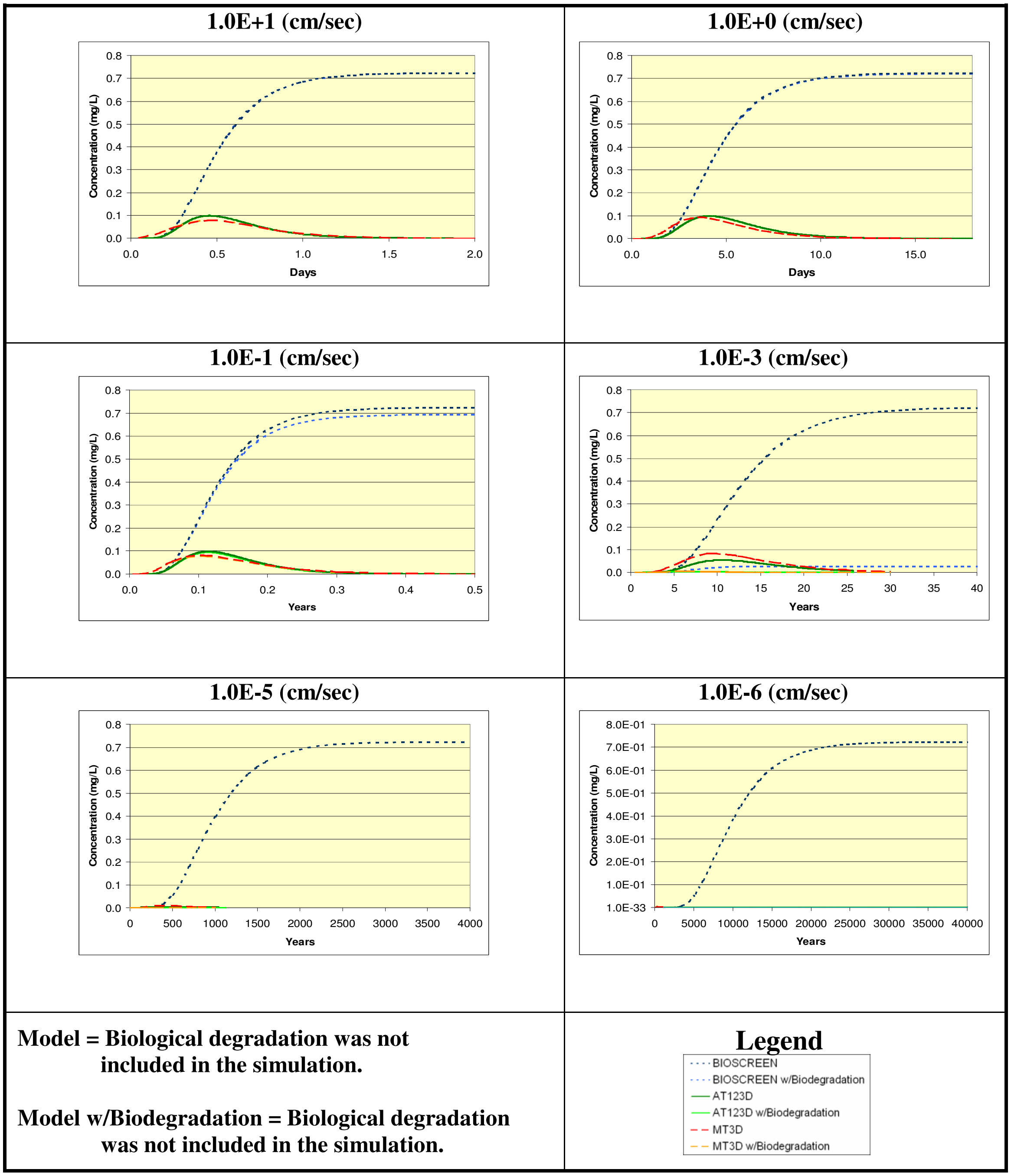
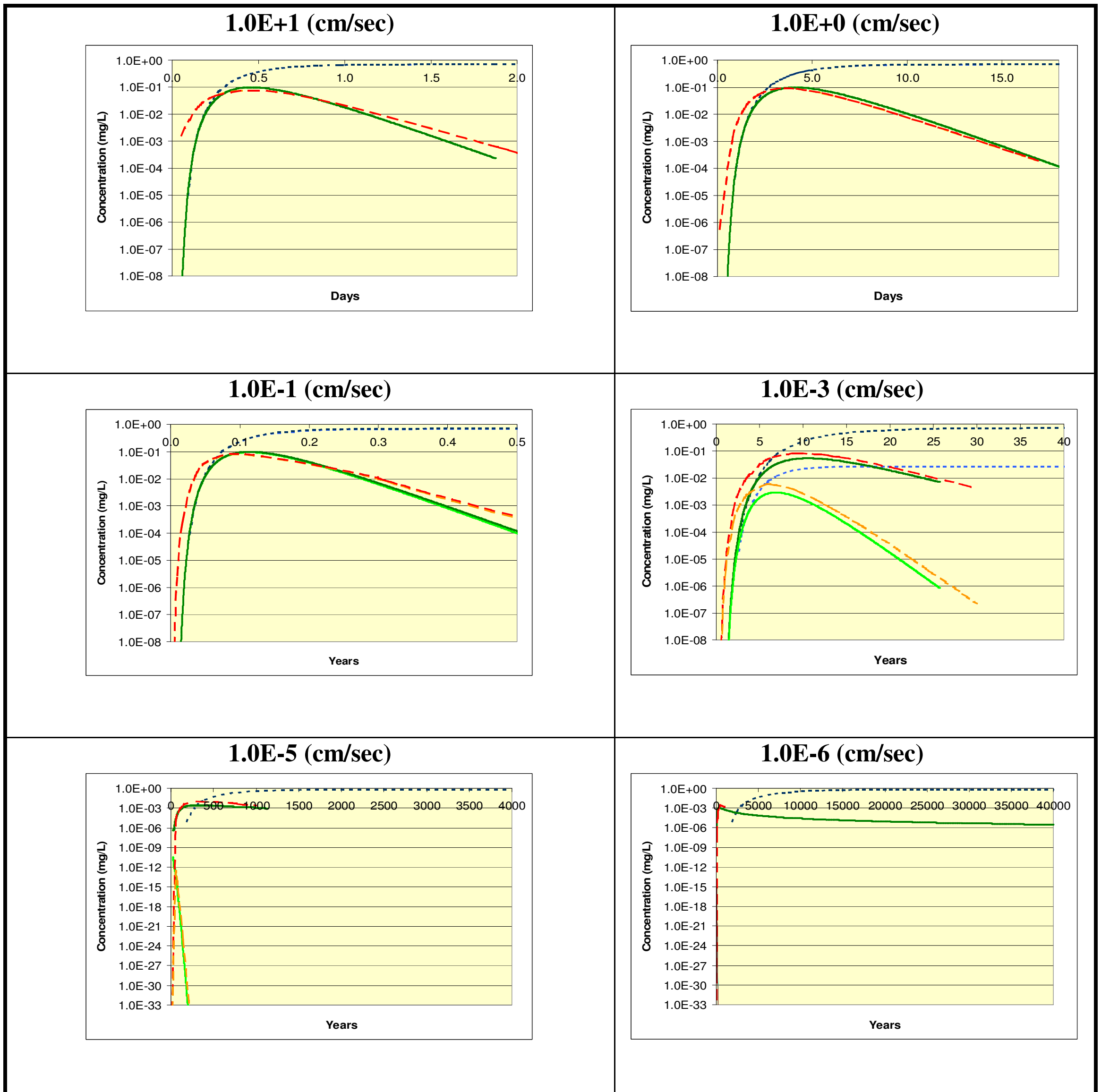


Figure 2a. Linear Plots
Benzene Results for Varying Hydraulic Conductivities



Model = Biological degradation was not included in the simulation.

Model w/Biodegradation = Biological degradation was not included in the simulation.

Legend

- BIOSCREEN
- BIOSCREEN w/Biodegradation
- AT123D
- AT123D w/Biodegradation
- MT3D
- MT3D w/Biodegradation

Figure 2b. Logarithmic Plots
Benzene Results for Varying Hydraulic Conductivities

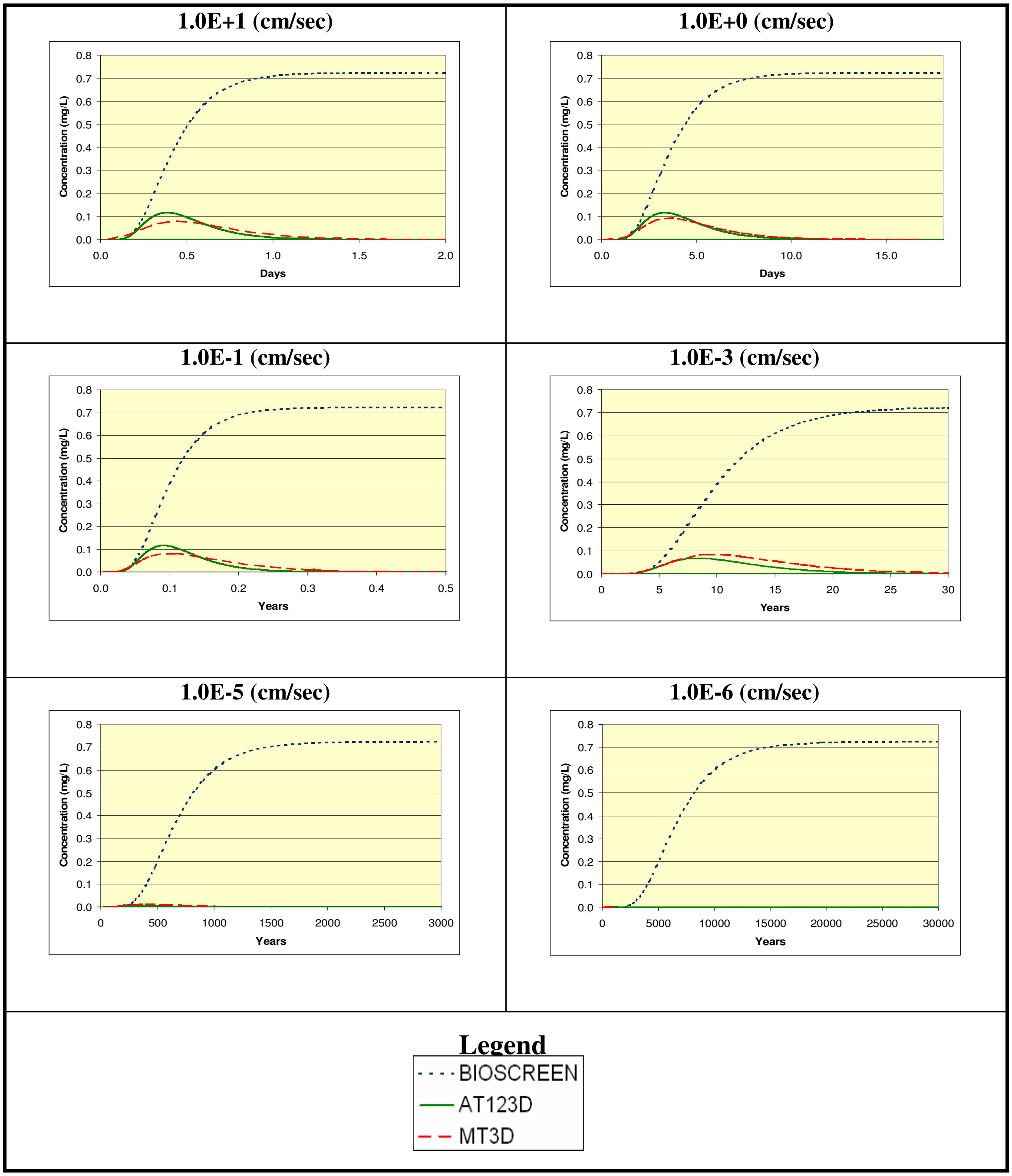


Figure 3a. Linear Plots
MTBE Results for Varying Hydraulic Conductivities

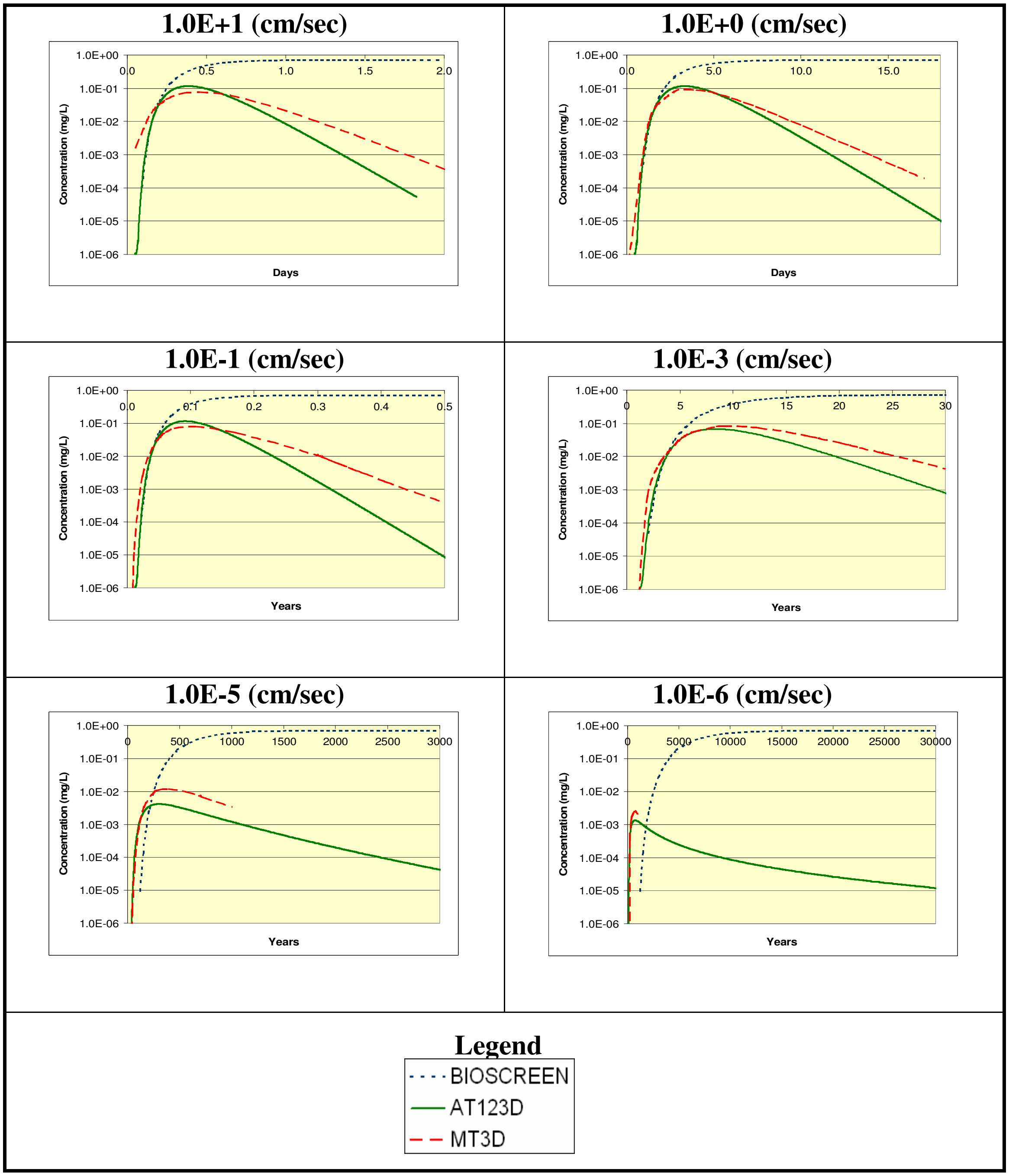


Figure 3b. Logarithmic Plots
MTBE Results for Varying Hydraulic Conductivities

Biodegradation had almost no impact on results for hydrologic conductivities from 1.0E+1 cm/sec to 1.0E-1 cm/sec in any of the models. This is not surprising as it took less than half a year to reach the peak concentration at a point 10 meters downgradient in these aquifers. Such short time frames do not provide enough time for any significant amount of biodegradation. However, at hydraulic conductivities of 1.0E-3 cm/sec and below, biodegradation significantly reduced the resulting peak downgradient concentrations. This is due to the longer travel times associated with lower permeabilities, providing a longer period of time over which biodegradation works. Given that BIOSCREEN produced the longest travel times, it produced the highest amounts of biodegradation.

Table 10. Time to Peak Benzene Concentrations

Permeability cm/sec	**units**	**BIOSCREEN**		**AT123D**		**MODFLOW/MT3D**	
		No Bio	**w/Bio**	**No Bio**	**w/Bio**	**No Bio**	**w/Bio**
1.0E+1	days	1.82	1.82	0.45	0.45	0.45	0.45
1.0E+0	days	17.3	17.3	4.05	4.05	3.57	3.57
1.0E-1	years	0.48	0.47	0.11	0.11	0.11	0.11
1.0E-3	years	40	23.4	10.5	6.70	9.67	6.22
1.0E-5	years	3980	105	311	26.3	329	31.5
1.0E-6	years	39000	600	310	50.0	572	35.9

Table 11. Time to Peak MTBE Concentrations

Aquifer Type cm/sec	**units**	**BIOSCREEN**	**AT123D**	**MODFLOW/MT3D**
1.0E+1	days	1.82	0.36	0.45
1.0E+0	days	15.7	3.15	3.57
1.0E-1	years	0.43	0.089	0.107
1.0E-3	years	43.0	8.25	9.67
1.0E-5	years	2940	289	359
1.0E-6	years	29300	680	630

4.1 Maximum Allowable Concentrations

The maximum allowable contaminant concentration in the source area is another key point in comparing the results of the three models. Regulations typically require that the predicted groundwater concentrations do not exceed the Maximum Contaminant Level, MCL, at the point of compliance. As demonstrated in Tables 12 and 13, AT123D and MODFLOW/MT3D allow at least one order of magnitude more benzene and MTBE to remain in place in the source, than BIOSCREEN for aquifers with hydraulic conductivities of between 1.0E+1 cm/sec and 1.0E-1 cm/sec. As hydraulic conductivities were lowered to 1.0E-6 cm/sec, AT123D and MODFLOW/MT3D allowed up to three orders of magnitude more contamination to remain in the source than BIOSCREEN did.

Table 12. Maximum Allowable Benzene Source Concentrations

Permeability	MCL	BIOSCREEN		AT123D		MODFLOW/MT3D	
		No Bio	w/Bio	No Bio	w/Bio	No Bio	w/Bio
cm/sec	Mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L
1.0E+1	0.005	0.00691	0.00691	0.0508	0.0508	0.0632	0.0632
1.0E+0	0.005	0.00691	0.00693	0.0509	0.0511	0.0535	0.0537
1.0E-1	0.005	0.00691	0.00720	0.0509	0.0530	0.0612	0.0634
1.0E-3	0.005	0.00691	0.180	0.0921	1.71	0.0598	0.860
1.0E-5	0.005	0.00691	3.65E+20	1.84	1.26E+08	0.463	4.76E+09
1.0E-6	0.005	0.00691	5.90E+74	4.63	5.90E+11	2.07	3.38E+12

Table 13. Maximum Allowable MTBE Source Concentrations

Permeability	MCL	BIOSCREEN	AT123D	MODFLOW/MT3D
cm/sec	mg/L	mg/L	mg/L	mg/L
1.0E+1	0.040	0.0552	0.345	0.506
1.0E+0	0.040	0.0552	0.345	0.428
1.0E-1	0.040	0.0552	0.345	0.490
1.0E-3	0.040	0.0552	0.592	0.472
1.0E-5	0.040	0.0552	9.64	3.33
1.0E-6	0.040	0.0552	29.4	15.9

Inclusion of biodegradation for benzene had no effect on the maximum allowable source concentration for hydraulic conductivities between 1.0E+1 cm/sec and 1.0E-1 cm/sec in any of the models. This is because the travel times were too short for biodegradation to produce any effect. However, the influence of biodegradation increased significantly as hydraulic conductivity was lowered. This is due to lengthy travel times associated with the lower hydraulic conductivities.

4.2 Influence of Model Capabilities

Discrepancies observed between BIOSCREEN and the other models are not a result of the input parameters. Instead the differences are a result of the original model design specifications. BIOSCREEN was designed for ease of use and computational speed. This goal was achieved by limiting contaminant load options, as well as the transport and fate processes. Computational speed was deemed an important design criterion due to limited computer capabilities at the time it was developed. Other models, such as AT123D and MODFLOW/MT3D, were initially designed with increased model capabilities, such as additional load options, and additional fate and transport processes.

Inclusion of these processes in AT123D and MODFLOW/MT3D means that they can be confidently used over a wider range of aquifer types and release scenarios, which in turn, improves confidence in the results. Only recently have computer capabilities improved to the point where run times are no longer an issue for AT123D. Although there has been a significant improvement in performance, model setup and run times, the time involved still restricts the use of MODFLOW and MT3D.

5. DISCUSSION

With its infinite source concentration, BIOSCREEN produced the highest concentrations, if run until the peak downgradient concentration is observed. However, even with the infinite source, inclusion of biodegradation caused BIOSCREEN to produce the lowest downgradient concentrations. Travel times to peak the downgradient concentrations predicted by BIOSCREEN were significantly longer than in AT123D and MODFLOW/MT3D. This is because BIOSCREEN does not simulate diffusion, which can become a significant process as gradients and hydraulic conductivities are lowered. Under such conditions BIOSCREEN significantly under estimates contaminant mobility thus increasing travel times and the amount of biodegradation. Perhaps the most interesting observation is that BIOSCREEN produced the same peak downgradient concentrations for all aquifers and chemicals tested. This appears to be inaccurate and suggests review of the basic model assumptions and solutions.

There was a strong correlation between the AT123D and MODFLOW/MT3D results. As aquifer and chemical properties changed so did the results.

Ease of use has always been a concern in the process of model selection. Of the three models tested, BIOSCREEN was slightly easier than AT123D to setup and run, while MODFLOW/MT3D was the most challenging. It has often been assumed that more accurate modeling would need additional site characterization to obtain the required input parameters. However, even though AT123D and BIOSCREEN use almost identical input parameters they produce different results.

6. CONCLUSIONS

BIOSCREEN results are not consistent with the other models tested. When compared to AT123D and MODFLOW/MT3D it significantly underestimates contaminant mobility and overestimates downgradient concentrations. Furthermore, given the lengthy travel times, inclusion of biodegradation significantly reduces downgradient concentrations, thus, making BIOSCREEN the least conservative model evaluated. Lengthily travel times produced by BIOSCREEN may generate a false sense of security, which may underestimate exposure risks. Exposure risk is often considered inconsequential at sites where modeling predicts that it will take more than 100 years to reach a downgradient point of compliance. Based on our results BIOSCREEN may not be an appropriate model to evaluate such risks.

Risk-based evaluations are established using the peak concentrations and the travel times to reach those peak concentrations. It is typically assumed that risks to groundwater quality decrease as contaminant travel times increase. Therefore BIOSCREEN, which underestimates contaminant mobility, may not provide an adequate assessment of downgradient risks. Given the lengthy travel times produced by BIOSCREEN, it should always be run until the peak concentration is observed. Even conservative biodegradation rates should be used with caution in BIOSCREEN, as the lengthy travel times generate significantly lower peak downgradient concentrations than the other models evaluated. On the other hand, cleanup objectives based on peak downgradient concentrations from BIOSCREEN in which biodegradation is not used maybe too conservative. This could result in costly remedial actions, which may not be justified.

Discrepancies are not a result of the model input parameters as AT123D and BIOSCREEN use almost identical parameters. Rather they are a result of inherent limitation associated with BIOSCREEN model and the Domenico equation. Given today's powerful computers, it is difficult to justify the use of Domenico equation based models, especially when analytical models such as AT123D can be safely used over a wider range of aquifer conditions. AT123D results are comparable to MODFLOW/MT3D, yet it takes much less time to use. MODFLOW/MT3D modeling could be performed as an alternative to AT123D modeling especially at sites with complex conditions.

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