Comparison of Three Numerical Models for Chain-Decay Transport Simulation at a Closed AFB in Texas

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ABSTRACT

Numerical schemes of three codes, MODFLOW-SURFACT, MT3D99, and RT3D, were compared for simulation of chain decay of PCE at a decommissioned Air Force Base in central Texas, to explore the implications of simulation code and solution scheme selection. The flow field generated by MODFLOW-SURFACT was used by MT3D99 and RT3D for transport simulation. Nine different transport models were developed incorporating three solution methods in combination with different time-stepping schemes. The solution methods examined within MODFLOW-SURFACT were TVD/Crank-Nicolson, upstream finite-difference/Crank-Nicolson and upstream finite-difference/fully implicit-in-time weighting. Upstream weighting and fully implicit finite-difference schemes were used for inter-code comparisons. The results obtained with MT3D99 were closer to MODFLOW-SURFACT than to RT3D. RT3D incorporates the implicit assumption that decay reactions occur only in the dissolved phase so it predicts slower overall degradation. The results of the sensitivity analysis confirm that MODFLOW-SURFACT is capable of reproducing results obtained with public-domain transport simulators, and offers increased flexibility in the use of solution methods and time-stepping schemes.

INTRODUCTION

Biodegradation modeling is a useful tool for predicting the attenuation of organic contaminants in groundwater. Currently available MODFLOW-format numerical models for the simulation of a straight chain biodegradation of chlorinated ethenes (PCE→TCE→DCE→Vinyl Chloride) include MODFLOW-SURFACT (HydroGeoLogic, 1998), MT3D99 (SSPA, 2000), and RT3D (Clement, 1997). The unsaturated zone over the study area of the decommissioned base is highly complex; therefore, MODFLOW-SURFACT was used to simulate groundwater flow because it can obtain physically realistic solutions without encountering numerical convergence problems with drying and re-wetting. MODFLOW-SURFACT is a fully integrated groundwater flow and solute transport code developed as an extension to MODFLOW (McDonald and Harbaugh, 1988). Since the source code of MODFLOW-SURFACT is not publicly available, it is valuable to examine its performance on real site simulations against other transport simulators that are in the public domain. For this study, transport results obtained with MODFLOW-SURFACT were compared with the results from MT3D99 and RT3D (version 2.5), using a flow-field generated by MODFLOW-SURFACT.

This study is based on the Zone 4 off-base groundwater flow and transport zoom model for a decommissioned AFB developed by HydroGeoLogic, Inc. The model was extracted from the March 2001 basewide flow model and used to evaluate different remediation alternatives for the removal of the chlorinated solvents tetrachloroethene (PCE), trichloroethene (TCE), 1,2-dichloroethene (DCE) and vinyl chloride (VC). The objective of the analyses was to estimate the time required to meet the maximum contaminant levels (MCLs) mandated under federal drinking water standards. The MCLs for PCE, TCE, 1,2-cis DCE and VC are 5 parts per billion (ppb), 5 ppb, 70 ppb and 2 ppb, respectively.

PROBLEM DESCRIPTION

Figure 1 displays the numerical grid for the zoom model overlain on the basewide flow model. The surface area of the zoom model is approximately 28.6 square miles. The zoom model has a minimum grid spacing of 50 feet, occurring in the vicinity of the remediation system (pumping wells) and consists of 220 rows and 241 columns in each of 4 model layers. A period of 15 years is considered in the transport simulations.

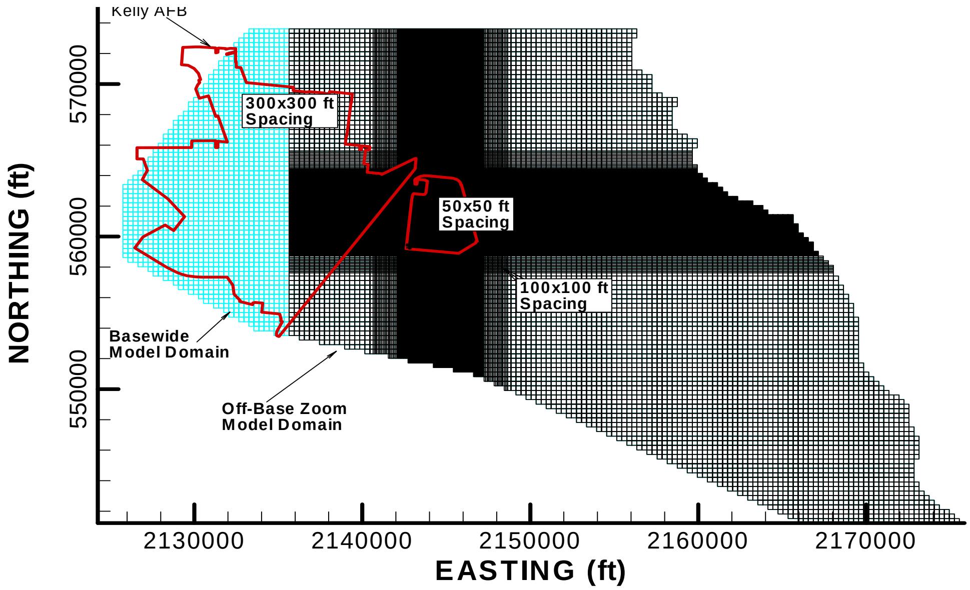

Figure 1. Numerical Grid of Zone 4 Off-Base Zoom Model Embedded within the March-2001 Basewide Model.

Prior to conducting simulations with MT3D99 and RT3D, several simulations were conducted with the various transport options within MODFLOW-SURFACT to better understand the factors controlling model performance. For spatial discretization of the advection term, upstream weighting, midpoint weighting, or the Total Variation Diminishing (TVD) method may be used. These schemes behave as follows: upstream weighting schemes tend to disperse sharp advective concentration fronts; midpoint weighting may create unphysical oscillations; and recently developed TVD schemes provide improvements to both problems but are computationally more demanding.

For the temporal discretization of the transport equations, explicit, Crank-Nicolson (also called centered-in-time weighting) and implicit schemes can be used. Explicit time-weighting schemes are subject to stringent stability criterion that must be satisfied to ensure stable solutions. Although both Crank-Nicolson and fully implicit schemes are not constrained by stability criteria, the selection of time-step size may affect the accuracy of the simulations.

In the current evaluation, TVD and upstream weighting schemes were selected for spatial discretization, and Crank-Nicolson and fully implicit schemes were chosen for temporal discretization. Nine different transport models were developed incorporating three solution methods in combination with time-step sizes of 2, 20, and 200 days. The solution methods examined were TVD/Crank-Nicolson, upstream finite-difference/Crank-Nicolson and upstream finite-difference/fully implicit-in-time weighting.

According to Zheng and Bennett (2002), the combination of TVD and Crank-Nicolson weighting is reportedly the most accurate available. The results obtained with MODFLOW-SURFACT using a time step size of 20 days were used as the benchmark against which the results with different solution schemes were compared. For inter-code comparisons, the TVD scheme implemented in MT3DMS (Zheng and Wang, 1999) and its successors MT3D99 and RT3D was not selected because it is based on explicit-in-time weighting with associated stability constraints which were severely limiting. In this study, the maximum allowable transport step was 6.0E-4 days. This small time-step size precluded feasible simulations with the MT3D99 TVD solution option. Although MT3D99 also offers the user an option to over-ride the automatic setting of transport time-step sizes for the TVD scheme, the simulations collapsed completely due to instability when time step sizes of 5 and 10 days were specified. The Eulerian-Lagrangian methods of MT3D99 were also not selected for this study because of excessive simulation times. Therefore, only the upstream weighting scheme for spatial discretization with fully implicit temporal discretization was used.

The simulation results for all cases examined were evaluated based on the reduction of contaminant area and total mass where the solvent compounds were above MCLs. As shown in Figure 2, the results obtained with upstream/Crank-Nicolson and upstream/fully implicit time weighting are close to those obtained from TVD/Crank-Nicolson. The results also demonstrate that a larger time-step size of 200 days also yields acceptable results for this study.

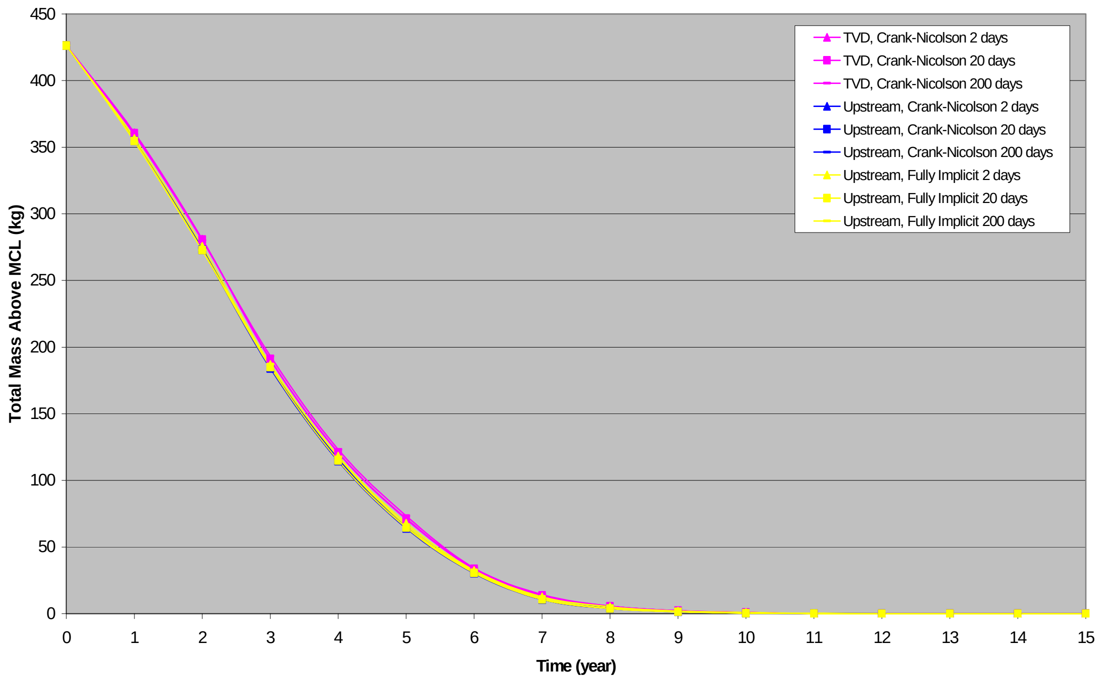

Figure 2. Transport Parameter Sensitivity for Pumping Condition: Predicted Evolution of Total Mass of PCE, TCE and VC Above MCLs for Different Schemes and Transport Step Sizes

TCE concentration distributions calculated after 5 years with the three simulation codes are shown in Figures 3a-c. The contours of dissolved phase concentrations calculated with the three codes are very similar. The estimated times required to achieve clean up are also similar. The plumes above MCLs for PCE, TCE, DCE, and VC become negligible after 9 years.

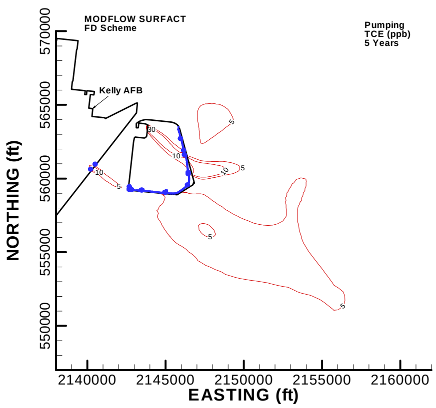

Figure 3a

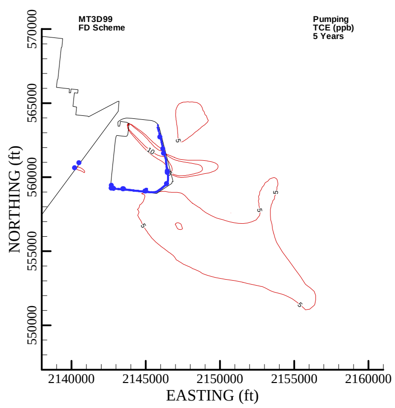

Figure 3b

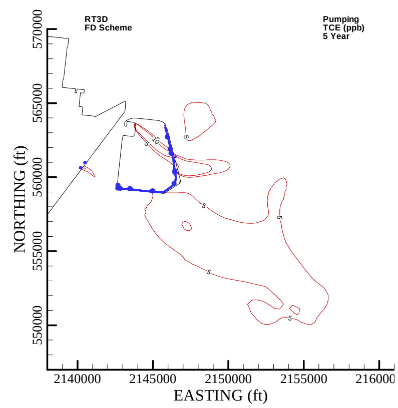

Figure 3c

Figures 3a, 3b, and 3c. Model Comparison: Simulated TCE Contours for Pumping at 5 Years from, a) MODFLOW SURFACT b) MT3D99 and c) RT3D.

The total masses of PCE, TCE, and VC remaining in the dissolved and sorbed phases are shown in Figure 4. The MT3D99 results agree closely with MODFLOW-SURFACT. The RT3D results suggest slightly higher mass in the system; the higher mass persists also at later times, i.e., greater than 10 years. The reason for this difference is that RT3D assumes that degradation reactions along a decay chain occur only in the dissolved phase (Clement, 1997). At this site, it is more likely that decay reactions occur at the same rate in the dissolved and sorbed phases, and this can be accommodated by MODFLOW-SURFACT and RT3D. The effect of this assumption in the RT3D results is that the solvent plumes are predicted to persist slightly longer.

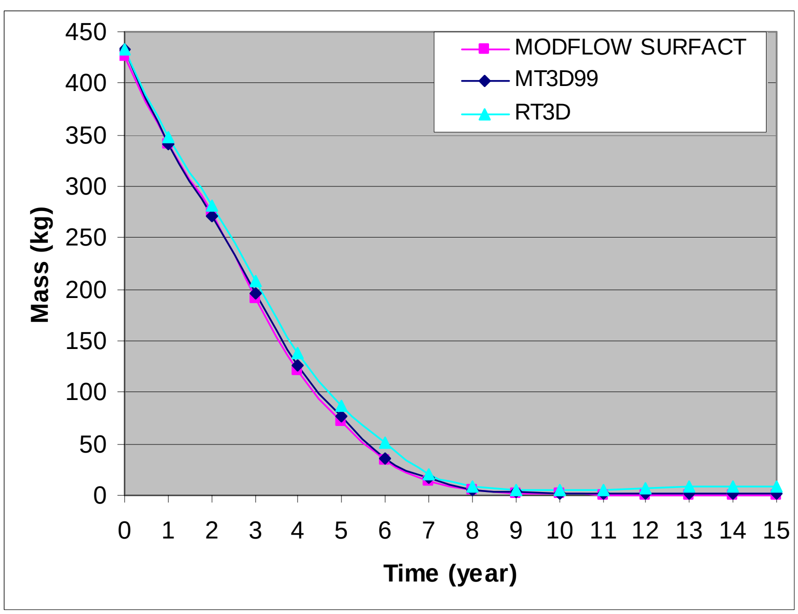

Figure 4. Model Comparison for Pumping Condition: Predicted Evolution of Total Mass of PCE, TCE and VC Above MCLs for Different Models.

SUMMARY

The main features of MODFLOW-SURFACT, MT3D99, MT3DMS, and RT3D that are related to this study are summarized in Table 1. Since MT3DMS is incapable of simulating chain biodegradation, it was not selected for this study. For the model considered in this study, it was only feasible to execute simulations with the TVD solution option as implemented in MODFLOW-SURFACT. The MODFLOW-SURFACT TVD results were used as a benchmark for evaluating the results of MT3D99 and RT3D Similar simulation results were obtained from three numerical schemes: TVD/Crank-Nicolson, upstream/Crank-Nicolson and upstream/fully implicit at time-step sizes of 2, 20 and 200 days. Special considerations for higher resolution of sharp fronts were therefore not important for this case. For the inter-code comparison, similar simulation results were obtained for MODFLOW-SURFACT, MD3T99 and RT3D using the same upstream/fully implicit schemes. Compared to those of MODFLOW-SURFACT and MT3D99, contaminant reduction is slower for RT3D because it does not account for decay in the sorbed phase.

Table 1. Main features related to this study of the listed models

	MODFLOW-SURFACT	MT3D99	MT3DMS	RT3D
Advection Solution	• TVD • Upstream FD	• TVD* • Upstream FD • MOC • HMOC	• TVD* • Upstream FD • MOC • HMOC	• TVD* • Upstream FD • MOC • HMOC
Chained Decay	Yes	Yes	No	Yes
First-order Decay	Yes	Yes	Yes	Yes
Multi-species	Yes	Yes	No	Yes

*TVD based on explicit-in-time weighting

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