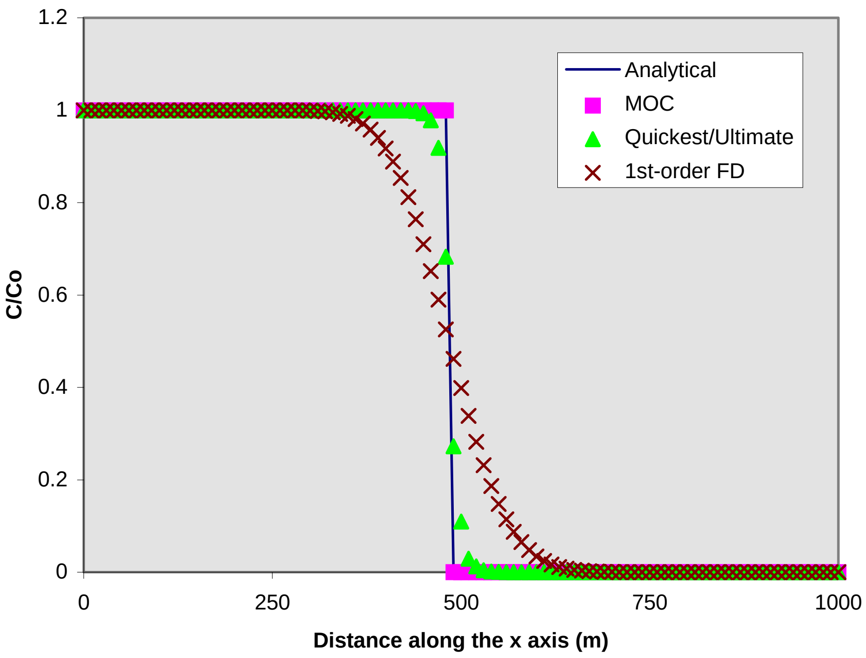
MT3DMS

A Modular Three-Dimensional Multispecies Transport Model for Simulation of Advection, Dispersion, and Chemical Reactions of Contaminants in Groundwater Systems

A Progress Report



The Hydrogeology Group
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A Progress Report

Prepared for

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April 1997

INTRODUCTION

The MT3D contaminant transport model was originally developed by the Principal Investigator at S. S. Papadopulos & Associates, Inc. and subsequently documented for the Robert S. Kerr Environmental Research Laboratory of the U. S. Environmental Protection Agency (USEPA) in Ada, Oklahoma. Since the initial release in early 1990, MT3D has become one of the most commonly used contaminant transport models with which other transport codes are often compared. The existence of MT3D and its availability in public domain has benefited the government agencies and private sectors working for prevention and mitigation of groundwater contamination problems.

The USEPA version of the MT3D code was selected by the U. S. Army Engineer Waterways Experiment Station (WES) as part of the Department of Defense Groundwater Modeling System (GMS). The primary objectives for the first phase of this project are to 1) develop MT3D into a multi-species code for linking with other bioreactive and geochemical models, 2) add a higher order finite-difference scheme that is mass conservative but without excessive numerical dispersion and artificial oscillations, and 3) implement an implicit matrix solver to remove any stability constraints as needed. The first phase of work has been completed and is described in the subsequent sections. Additional work for the second phase of the project is underway to add a new interface to a finite-element flow model such as FEMWATE, and to include a first-order reversible reaction that can be applied to model non-equilibrium sorption, NAPL dissolution, and mass transfer between “mobile” and “immobile” domains.

MULTI-SPECIES STRUCTURE

Overall Design Goals

One of the main objectives for the next generation of the MT3D model is to simulate contaminant fate and transport in the presence of multi-species biological and geochemical reactions. To that end, a new multi-species structure has been developed and implemented on this new version of MT3D, referred to as MT3DMS. The multi-species structure has been designed with two primary goals in mind. First, the new structure must remain compatible with the original modular structure to take full advantage of the existing graphical interface and other companion software developed for the original single-species MT3D code. Second, the new structure must be flexible enough to accommodate future new reaction modules with little or no modification at all.

Changes to the Existing Structure

Several changes were made to achieve the overall design goals. First, two new global initialization variables were added, `ncomp` for the total number of species, and `mcomp` for the number of mobile components. For single-species simulation, `ncomp` and `mcomp` shall both be equal to 1; the required input files for single-species simulation using MT3DMS would be identical to those of the original single-species MT3D.

The second change involves the assignment of starting concentrations (initial condition) and sink/source concentrations. In MT3DMS, depending on the value of `ncomp`, multiple starting concentration arrays must be specified in the input file of the basic transport (BTN) package, one species at a time. In the input file of the sink/source mixing (SSM) package, depending on the value of `mcomp`, the concentration data for the recharge fluxes must be defined `mcomp` times, one species at a time. The same procedure must be repeated for the evapotranspiration fluxes. To specify concentrations for point sources such as wells and river nodes, the concentrations for all species at the source location must be defined.

The third change involves the chemical reaction (RCT) package. With the new structure in MT3DMS, all the chemical reaction constants must be specified `ncomp` times, one species at a time. Each species can undergo equilibrium-controlled sorption (linear, Freundlich or Langmuir) and/or first-order irreversible decay. A new rate-limited mass transfer reaction between species will be added. For multi-species simulation using RT3D, SEAM3D, or other add-on codes as the reaction simulator inside MT3DMS, the RCT input file for MT3DMS will be replaced by one specific to an add-on module.

For output, MT3DMS generates a standard output file which contains the echoes of input data and mass budget summaries. In addition, it generates a set of optional output files named,

`MT3D???.UCN` (unformatted concentration file)
`MT3D???.OBS` (observation point file)
`MT3D???.MAS` (mass balance summary file)

where `???` is the species index number.

The formats and structures of these files are identical to those of the original single-species MT3D code so that they can be processed by the existing graphical interface software without any changes. For more information on the changes in the program and input/out structure, refer to Attachment A.

Comparison with the Single-Species Version

Numerous tests have been performed to check the correctness of the new multi-species structure. An example is shown in Figure 1. A contaminant source with a specific strength is continuously injected into a uniform flow field. The three plots on the left column, which show the plume configurations at the end of two years after the injection has begun, are based on three individual simulation runs using the single-species MT3D code. The three plots on the right column are based on one single simulation run using the multi-species MT3DMS code. Cases I(b) and II(b) are identical to cases I(a) and II(a) except for the reduced source strength for the latter. Cases I(c) and II(c) are also identical to cases I(a) and II(a) except for the presence of a first-order decay for the latter. Since no inter-component reaction is simulated, the three plots on the left should be identical to their corresponding plots on the right, as indicated in Figure 1.

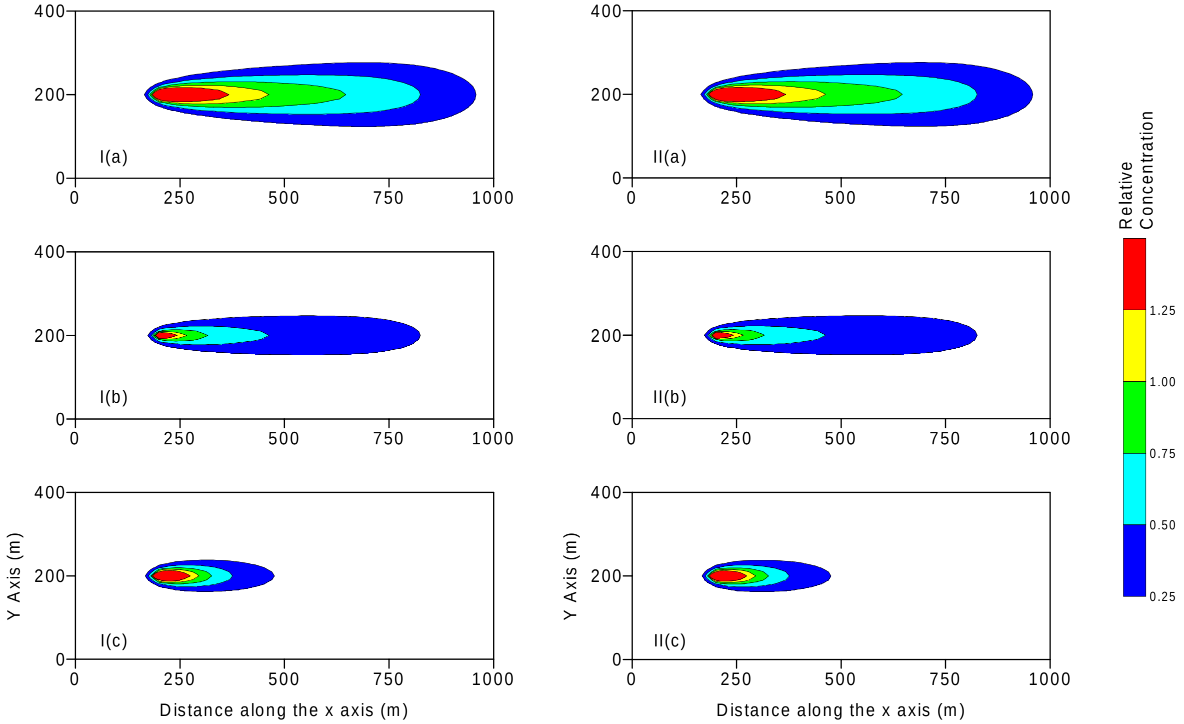


Figure 1. Two-dimensional transport from a continuous source in a uniform flow field. The three plots on the left are based on three simulation runs of the single-species MT3D code while the three plots on the right are based on a single simulation run of the multi-species MT3DMS code. Cases I(b) and II(b) are identical to cases I(a) and II(a) except for the reduced source strength for the latter. Cases I(c) and II(c) are also identical to cases I(a) and II(a) except for the presence of a first-order decay for the latter.

THE “ULTIMATE” MASS CONSERVATIVE SOLUTION SCHEME

Background

Despite numerous new techniques, numerical solution of advection-dominated solute transport remains an “embarrassingly” difficult problem because of the often contradictory needs to suppress numerical dispersion, avoid artificial oscillations and conserve mass. The method of characteristics (MOC) and its variants as implemented in the original MT3D code are extremely effective in virtually eliminating numerical dispersion. However, several problems exist under various circumstances. First, the MOC scheme and its variants are not strictly mass conservative. While various empirical solution parameters can be adjusted to achieve minimum mass balance errors, there are situations where a small mass balance descrepany is not attainable, especially when the model grid is highly irregular. Second, the MOC scheme and its variants may yield concentration solutions that have a “rough” appearance due to the discrete nature of particle-based techniques. Although this is normally not a significant problem, it presents a difficulty for certain parameter estimation procedures and sensitivity analysis. Finally, the MOC scheme and its variants generally require significantly more computer memory than does the standard finite-difference method or finite-element method. While memory requirement is generally not a problem for single-species simulation, it can become a limiting factor for multi-species simulation involving a large number of species.

Leonard (1988) presents the one-dimensional form of a third-order upwind finite-difference scheme, called QUICKEST. To avoid artificial oscillations, the QUICKEST scheme is used with a Universal Limiter for Transient Interpolation Modeling of the Advective Transport Equations, or ULTIMATE. This QUICKEST/ULTIMATE scheme is mass conservative, free of excessive numerical dispersion and artificial oscillations, and relatively efficient in terms of memory use and execution speed. These properties make the QUICKEST/ULTIMATE scheme an attractive alternative for solving three-dimensional multicomponent advective-dispersive-reactive transport equations.

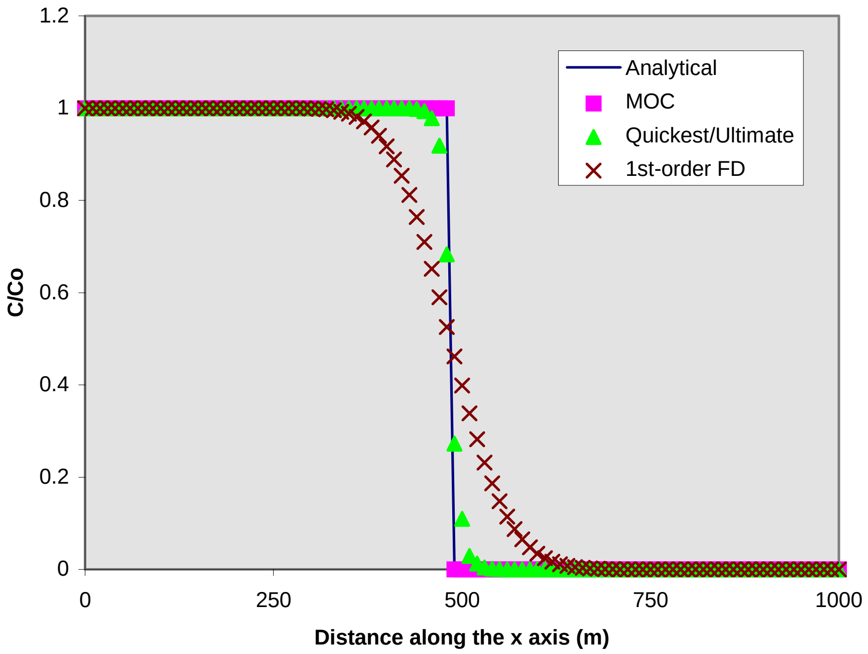
We have implemented the QUICKEST/ULTIMATE scheme as an additional solution option in MT3DMS for solving the advection term. The implementation has involved detailed derivation of the general, three-dimensional, non-uniform equations for the QUICKEST/ULTIMATE scheme (see Attachment B), and comprehensive testing based on numerous benchmark problems. Two examples are presented in the next section. Other examples and field-scale test problems will be presented in the final program documentation along with detailed theoretical background and numerical implementation.

Test Examples

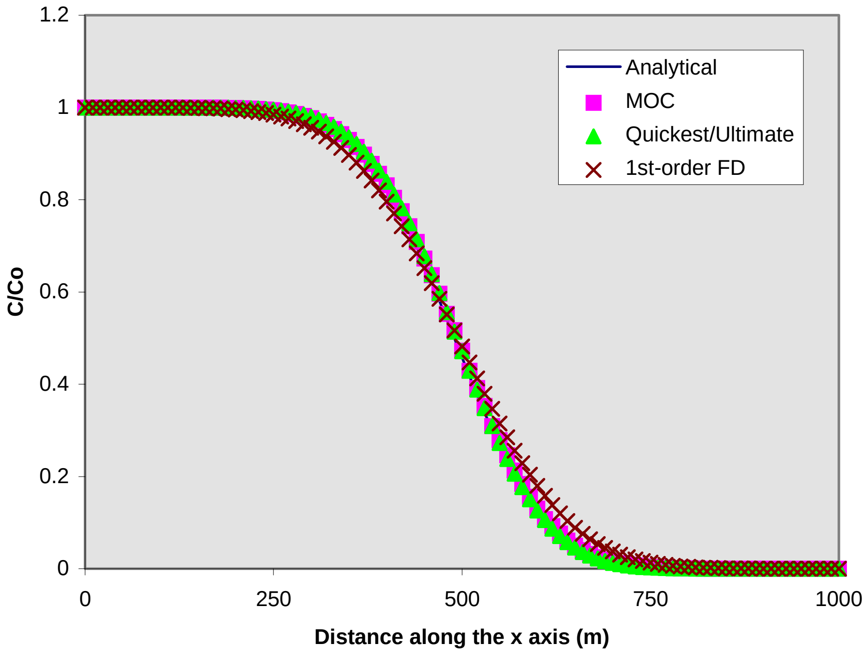
The first example is flow and transport in a one-dimensional uniform flow field. Two cases are considered. In case 1, the transport problem is purely advective, i.e., the grid Peclet number is infinity (the grid Peclet number is a measure of the domination of advection over dispersion for a given grid spacing). This case represents the most severe test for the various transport solution techniques. In case 2, the grid Peclet number is one, which indicates that the transport problem is no longer advection-dominated and can be solved by most transport techniques without any major difficulty.

Figure 2(a) shows the comparison of the analytical solution with numerical solutions based on the method of characteristics (MOC), the first-order upwind (upstream) finite-difference method , and the new third-order QUICKEST/ULTIMATE (3QU) scheme, respectively. The MOC solution yields a solution identical to the analytical solution, This is not unexpected considering that the MOC scheme is most effective for this type of problems completely dominated by advection. While the 3QU scheme is not as close to the analytical solution as the MOC solution, it is noted that the 3QU scheme leads to dramatic improvement over the conventional first-order upstream finite-difference solution.

Figure 2(b) shows the same comparison, but with the grid Peclet number equal to one. Because the transport problem is no longer dominated by advection, the standard finite-difference method works fine, as shown in the figure. The more computationally intensive MOC and 3QU schemes lead to marginal gains in solution accuracy. Clearly, for problems that are not dominated by advection, the standard finite-difference method can be used effectively.



(a) Purely advective case (Pe= ∞)



(b) Smooth case (Pe=1)

Figure 2. Comparison of the analytical solution with various numerical solutions based on different solution schemes for the advection term.

The second example is flow and transport from a continuous source in a uniform flow field with the flow direction at a 45 degree angle to the x and y axes. The grid Peclet number for this problem is 5 in the longitudinal direction, and 50 in the transverse direction, respectively. This problem represents a challenging test for any transport solution technique because of the grid effect compounded by the sharpness of the concentration front. Figures 3(a) through 3(d) show the analytical solution, compared with the numerical solutions based on the MOC scheme, the first-order upstream finite-difference scheme, and the third-order QUICKEST/ULTIMATE scheme, respectively.

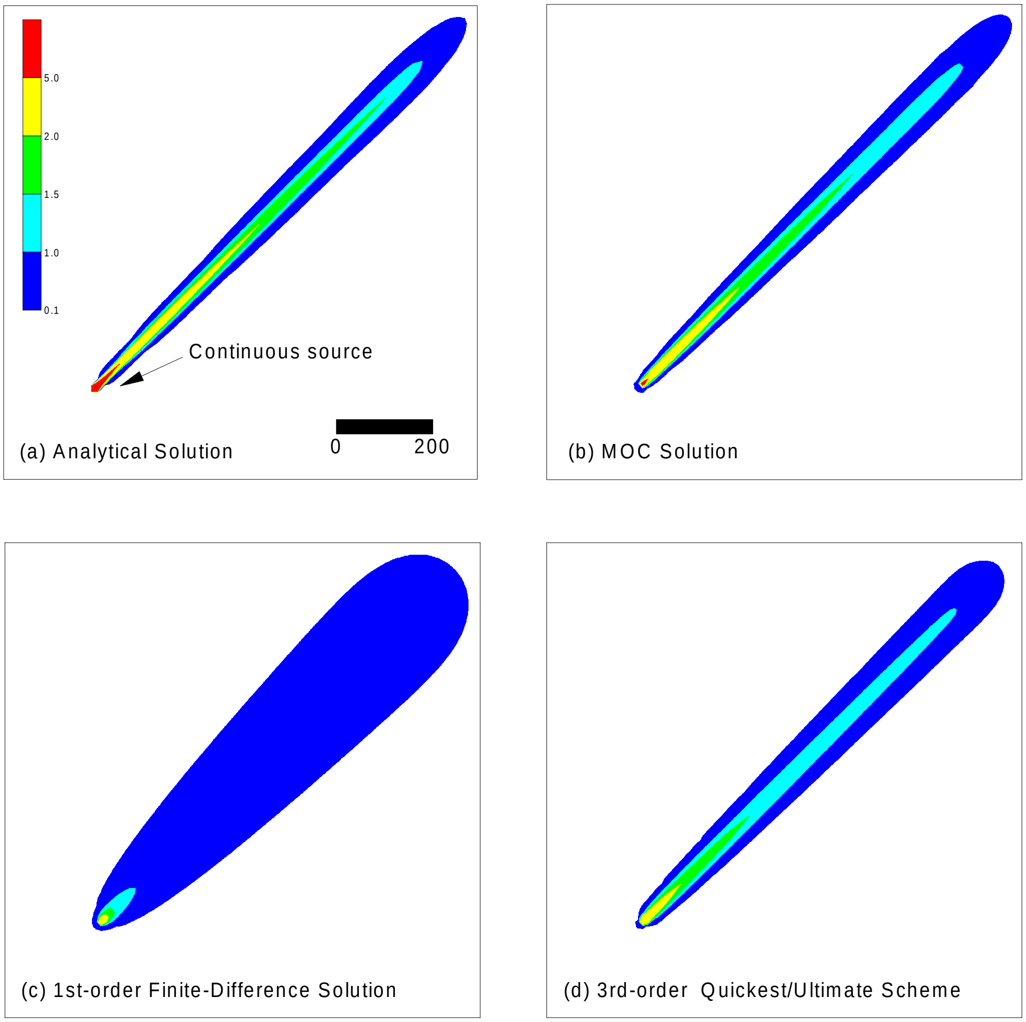


Figure 3. Comparison of the analytical solution with numerical solutions based on different solution schemes for the advection-dominated problem. The flow field is uniform with the flow direction at a 45 degree to the x and y axes. The grid Peclet number of the transport problem is 5 in the longitudinal direction and 50 in the transverse direction.

As seen from Figure 3(b), the solution based on the MOC scheme is very close to the analytical solution. The solution based on the first-order upstream finite-difference scheme, Figure 3(c), yields excessive numerical dispersion. While the solution based on the QUICKEST/ULTIMATE scheme, Figure 3(d), contains more numerical dispersion than the MOC solution, it represents a significant improvement over that based on the first-order upstream finite-difference scheme. Given the same transport step size, the computation times for different transport options are shown in Table 1. The memory requirements for the QUICKEST/ULTIMATE scheme and the first-order finite-difference scheme are identical. The MOC scheme requires additional memory equal to the number of particles needed multiplied by a factor of six (or nine for three-dimensional problems).

Table 1. Comparison of computation times for different solution options.

Solution Scheme	MOC	3rd-order QU	1st-order FD
Computation Time (Seconds)	202	83	30

IMPLICIT MATRIX SOLVER

Motivation for an Implicit Matrix Solver

In the original MT3D code, the dispersion, sink/source and reaction terms are solved using the explicit finite-difference method. As a result, the time step size for a transport solution may be limited by the stability criteria associated with these terms. This may be not a problem for many field problems dominated by advection, because for this type of problems the transport step size is often constrained by the accuracy requirement which stipulates that the advective movement in one time step should not exceed the length of one model cell. However, the transport time step allowed for a particular problem with small grid spacing, large dispersion coefficients, and large sink/source terms might lead to exceedingly small transport steps using the explicit method. This is because the stability criteria are proportional to grid spacing, and inversely proportional to the dispersion coefficients and the sink/source flux. Thus, it is desirable to have an implicit matrix solver with no stability constraint for solving those problems that are not advection dominated or for solving local scale models where a fine grid is used. Even for advection dominated problems, it may be worthwhile to make a few initial trial runs with large time steps for testing purposes.

Implementation

As the third major task of this project, we have developed an implicit matrix solver for MT3DMS using highly efficient generalized conjugate gradient (GCG) methods with Lanczos/ORTHOMIN acceleration (see Attachment C). The implicit matrix solver is implemented in MT3DMS through a new package named GCG with three preconditioning options to choose from: Jacobi, Symmetric SOR (SSOR), and Modified Incomplete Cholesky

(MIC). If the user selects the GCG package, dispersion, sink/source, and sorption/decay terms are solved implicitly without any stability constraints. For the advection term, the user has the option to use any of the schemes available, including the method of characteristics (MOC) and its variants (HMOC and MMOC), the first-order upstream finite-difference method, and the new mass conservative third-order QUICKEST/ULTIMATE scheme. If the MOC or one of its variants is selected, the transport time size is controlled by a user-specified Courant number, or the number of model cells a particle is allowed to move in one time step. If the first-order upstream finite-difference method is selected, the user can define an initial step size and a multiplier for successively steps. Alternatively, the user can let the program automatically decide the initial step size based on the accuracy requirement. Finally, if the third-order QUICKEST/ULTIMATE scheme is selected, the program will automatically determine a step size that meets the special requirement of this scheme.

If the GCG package is not selected, the explicit method is automatically used in MT3DMS to solve dispersion, sink/source, and sorption/decay terms. The transport step size will be subject to the usual stability constraints. As pointed out previously, the explicit method is an efficient choice for advection-dominated problems. The explicit method is also desirable when the implicit solver requires a large number of iterations or fails to converge under certain circumstances. Moreover, the implicit solver requires a significant amount of computer memory to operate. Thus, for computer systems without sufficient memory, the explicit method may become the only option.

An Evaluation Example

This section demonstrates the use of the implicit solver in solving a field-scale model as presented in the original MT3D manual (Figure 4). The finite-difference mesh for the flow and transport model consists of four layers, 61 rows and 40 columns. Using the explicit, first-order finite-difference option, a total of 890 transport steps are required to obtain the solution at the end of 2000 days. The uniform transport step size of 2.25 days used is determined by to meet the various stability constraints. The total computation time for the explicit solution is 128 seconds (Table 2). Using the implicit solver with the modified incomplete Cholesky preconditioner, the transport step size can be relaxed, thus shortening the computation time required. However, it should be noted that as the step size increases, the solution accuracy, as measured by the calculated total mass removal at the end of the simulation, gradually deteriorates, as the time step sizes far exceed the Courant number of one.

The GCG solver as used in the test example with the modified incomplete Cholesky preconditioner is very efficient. Given a concentration closure criterion of 10^{-6}, the number of iterations required for each implicit step in Runs #1 and #2 ranges from four to 15. For Run #3, which uses only one step, the total number of iterations is 25.

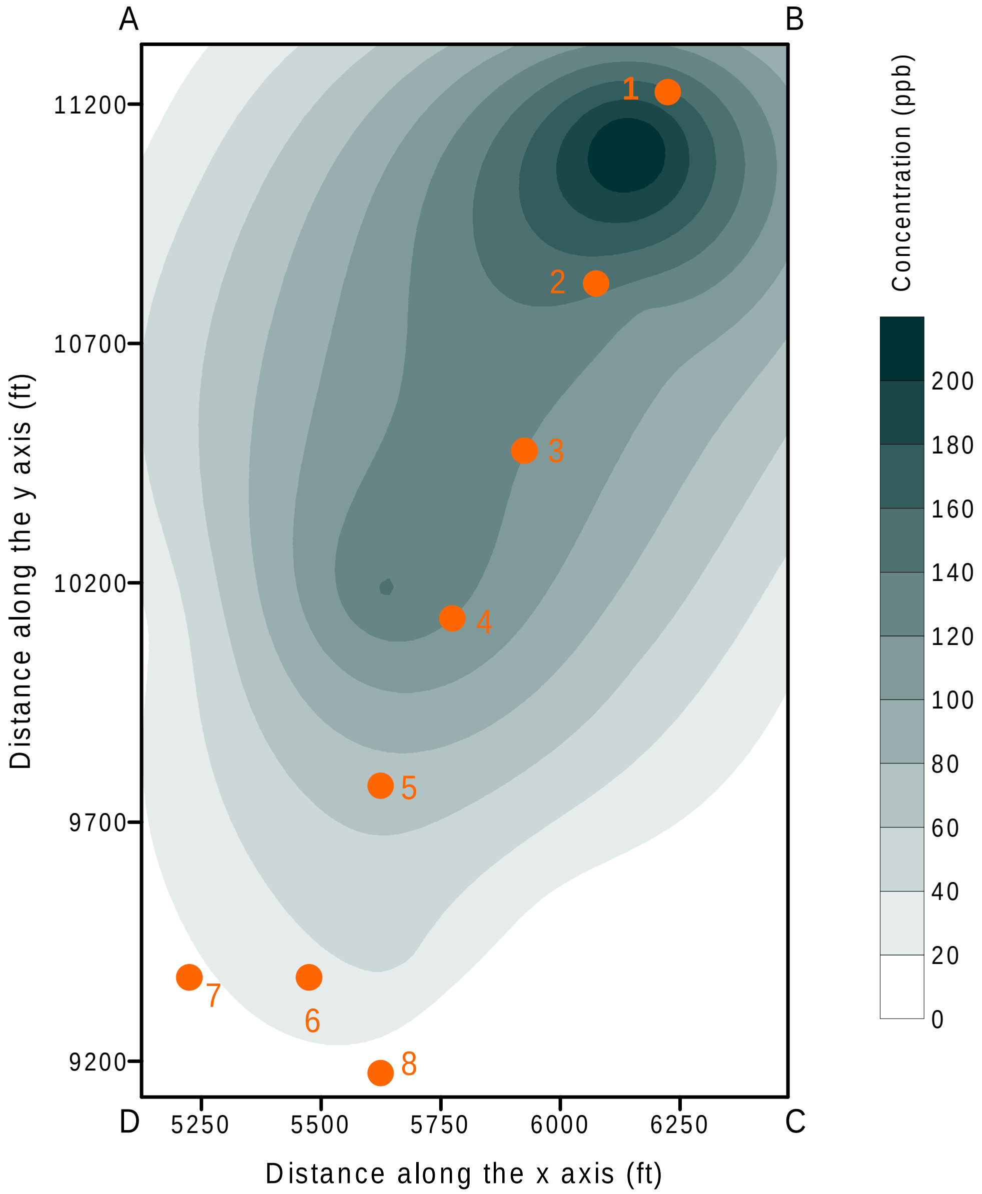


Figure 4. The example problem used to test the implicit matrix solver. The initial concentration distribution and pumping well locations are shown on the map (ABCD indicates the detailed study area located in the center of a larger model area).

Table 2. Comparison of computation times using explicit and implicit schemes.

Explicit and Implicit Schemes	Initial Transport Step Size	Transport Step Multiplier	Total Number of Steps Used	Total Computation Time (Seconds)	Relative Mass Removed
Explicit	2.25	n/a	891	128	1.00
Implicit Run #1	2.25	1.5	16	43	0.95
Implicit Run #2	2.25	2.0	10	30	0.93
Implicit Run #3	2000	n/a	1	8	0.79