# SCIENTIFIC NOTEBOOK # 727

## Validation of MT3DMS: Modular Three-Dimensional Multispecies Transport Model

*by*

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# 1. INITIAL ENTRIES

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This computerized Scientific Notebook is intended to address the criteria of CNWRA QAP-001.

[Anna Buseman-Williams, July 15, 2005]

## 1.1. Objectives

The objective of this study is to verify the accuracy of MT3D by developing relatively simple test cases and comparing analytical and numerical solutions of each contaminant transport and to determine the most accurate advection solution scheme to use for any particular transport problem. MT3D will be used for the purpose of simulating the transport of potentially highly contaminated groundwater through areas that surround the waste repository at Yucca Mountain.

## 1.2. Computers, Computer Codes, and Data Files

MT3DMS Version 4.5, the computer code used to simulate solute transport, was originally developed by Chunmiao Zheng at S.S. Papadopulos & Associates, Inc., and subsequently documented for the Robert S.Kerr Environmental Research Laboratory of the U.S. Environmental Protection Agency. The code is discussed in the user's manual *MT3DMS: A Modular Three-Dimensional Multispecies Transport Model for Simulation of Advection, Dispersion, and Chemical Reactions of Contaminants in Groundwater Systems; Documentation and User's Guide* written by Zheng and P. Patrick Wang at the University of Alabama and dated December 1999. The MT3D simulations were carried out in GMS 5.1, Groundwater Modeling System, built on February 24, 2005. The analytical solutions were coded using MATLAB Version 7.0.1.

# 2. Introduction

MT3D, Modular 3-Dimensional Transport model, is a mass transport model capable of simulating advection, dispersion/diffusion, and chemical reactions of contaminants in groundwater flow systems and is commonly used by hydrogeologists to simulate solute transport. The model is based on the assumption that changes in the concentration field will not significantly affect the flow field, therefore MT3D does not have the capability of simulating groundwater flow (Zheng and Wang 1999). MT3DMS may be linked to any blockcentered finite-difference, but for this case, MODFLOW was used. GMS will provide a graphical interface and will serve as a link between MODFLOW and MT3D with no user specified code required.

It includes three major classes of transport solution techniques, standard finite-difference method, particle-tracking-based Eulerian-Lagrangian methods, and the higher-order finite-volume TVD method, in a single code. Because no single technique has been effective for all transport conditions, using a combination of these techniques is believed to offer the best approach for solving transport problems (Zheng and Wang 1999).

MT3D can be used to simulate changes in concentrations of groundwater contaminants considering advection, dispersion, and some basic chemical reactions. The chemical reactions present in the model are equilibrium controlled or rate-limited linear or nonlinear sorption and first-order irreversible or reversible kinetic reactions.

## 3. Theoretical/Computer Analyses

Numerical and analytical models were completed for a one-dimensional transport in a uniform flow field, as well as a three-dimensional transport in a uniform flow field, both with continuous sources. In both cases, it was expected that the analytical solutions would agree with the results of the numerical solution created by MT3D. For one-dimensional transport, a variety of different solution schemes were used in the advection package for both an advection dominated case and a non-advection dominated case. It was expected that after comparison with the analytical solution, the MOC would by far the most effective scheme for the advection dominated case, while in the non-advection dominated case the MOC solution will only be slightly more accurate.

3.1 One-Dimensional Transport in a Uniform Flow Field

A slightly modified version of a simple benchmark problem entitled *One-Dimensional Transport in a Uniform Flow Field* from the MT3DMS User's Guide was used (Zheng and Wang 1999) for the first test case. The initial and boundary conditions are as followed:

$$C(x,0) = 0$$
$$C(0,t) = C_o \qquad t > 0$$
$$\frac{\partial C}{\partial x}(\infty,t) = 0 \qquad t > 0$$

Three cases of the problem were completed.

The following parameters were used to complete each case, where $\alpha_L$ is the dispersivity, $R$ is the retardation faction, and $\lambda$ is the decay rate constant.

Case 1a (Advection and dispersion): $\alpha$=10 m, $R$ = 0, $\lambda$= 0
Case 1b (Advection, dispersion, and sorption): $\alpha$=10 m, $R$ = 5, $\lambda$ = 0
Case 1c (Advection, dispersion, sorption, and decay): $\alpha$=10 m, $R$ = 5, $\lambda$ = 0.002 $d^{-1}$

Groundwater seepage velocity $(v)$ = 0.24 m/day

Porosity ($\theta$) = 0.25
Simulation time ($t$) = 2,000 days

Numerical Solution:
The first and last columns were constant-head boundaries, designated in MODFLOW with IBOUND values less then zero. Arbitrary head values were to be selected to establish a uniform hydraulic gradient. Using Darcy's Law, $v\theta = K(dh/dL)$, where $K$ is the hydraulic conductivity, $h$ is the hydraulic head, and $L$ is the total length and assuming $K$=1, a $dh$ value of 60 meters was found. Concentration values were entered in terms of relative concentration. Case 1a was solved using the MOC option in the advection package with DCEPS=$10^{-5}$, NPLANE=1, NPL=0, NPH=4, NPMIN=0, and NPMAX=8, while Cases 1b and 1c were solved using the MMOC option with NLSINK and NPSINK equivalent to NPLANE and NPC for the MOC option. In all cases, the fixed pattern and one vertical plane were chosen for initial particle placement. When the chemical reaction package was required, a linear sorption isotherm was assumed.

Analytical Solution:
The following analytical solutions may be found in Domenico and Schwartz (1990).

Case 1a

$$C(x,t) = \left(\frac{C_o}{2}\right)\mathbf{erfc}\left[\frac{(x - vt)}{2\sqrt{(\alpha_x vt)}}\right]$$

Case 1b

$$C = \frac{C_o}{2}\mathbf{erfc}\left[\frac{(Rx - vt)}{2\sqrt{(\alpha_x vtR)}}\right]$$

Case 1c

$$C = \left(\frac{C_o}{2}\right)\exp\left\{\left(\frac{x}{2\alpha_x}\right)\left[1 - \sqrt{\left(\frac{1+4\lambda\alpha_x}{v}\right)}\right]\right\}\mathbf{erfc}\left[\frac{x - vt(1+4\lambda\alpha_x / v)^{1/2}}{2\sqrt{(\alpha_x vt)}}\right]$$

The MATLAB code was designed to insert the necessary parameters for each case from $x$=5 m to $x$=1005 m for 10 m intervals at a time of $t$=2000 days and output a plot of the relative concentration vs. distance.

The approach used in this analysis is summarized as follows:

(I) A grid consisting of 101 columns, 1 row, and 1 layer with total lengths in the $x$, $y$, and $z$ dimensions of 1010 m, 1 m and 1 m, respectively, was created.

(ii) MODFLOW was used to input head and hydraulic conductivity information, as detailed above. The model created groundwater flow patterns, and all three cases were based on the same MODFLOW simulation saved under the file name *Ch. 7 Examples\One-Dimensional Transport in a Uniform Flow Field\grip.gpr.*

(iii) Data regarding the contaminant was entered into MT3D for each case, and the results were extracted from the OUT file.

(iv) The results from the numerical solution were inputted into MATLAB to compare with the results of the analytical solution computed in MATLAB, found under file name *Ch. 7 Examples\One-Dimensional Transport in a Uniform Flow Field\Matlab Solution\Conc.m.* .

3.2 Three Dimensional Transport in a Uniform Flow Field

A modified version of Example 17.6 provided by Domenico and Schwartz (1990) was used to compare analytical and numerical solutions for three-dimensional transport. The parameters used for the study may be found below. It can be noted that some parameters differ from those stated by Domenico and Schwartz (1990), and while sorption is present in Example 17.6, the chemical reaction package was not used in this study.

Longitudinal dispersivity ($\alpha_x$) =1.0 m
Transverse dispersivity ($\alpha_y$) =0.1 m
Vertical dispersivity ($\alpha_z$) =0.01 m
Groundwater seepage velocity ($v$) = 1 x $10^{-6}$ m/sec = 0.0864 m/day
Porosity ($\theta$) = 0.3
Simulation time ($t$) = 15 years = 5475 days
Source Size in Y (Y) = 15 meters
Source Size in Z (Z) = 10 meters

Numerical Solution:
A grid consisting of 700 columns, 14 rows, and 10 layers with total lengths in the *x*, *y*, and *z* dimensions of 700 m, 105 m and 50 m, respectively, was created. As in the one-dimensional study, the first and last column were designated as constant-head boundaries. *K* was again assumed to be one and a *dh* value of 18 meters was found based on Darcy's Law calculations. Four continuous sources were placed in the center of the first row (layers 5 and 6, columns 7 and 8) in order to most accurately simulate a contaminant along the plane of symmetry of the plume, as addressed in the problem statement. The third order TVD solution scheme (ULTIMATE) was used in the advection package, and concentration values were entered as relative concentrations.

Analytical Solution:
The analytical solution for three-dimensional transport with a continuous source, below, was found in Domenico and Schwartz (1990).

$$C(x,y,z,t) = \left(\frac{C_o}{2}\right)\operatorname{erfc}\left[\frac{(x-vt)}{2\sqrt{\alpha_x vt}}\right]\operatorname{erf}\left[\frac{Y}{4\sqrt{\alpha_y x}}\right]\operatorname{erf}\left[\frac{Z}{4\sqrt{\alpha_z x}}\right]$$

As in the case of the one-dimensional study, the MATLAB code inserts the parameters found above into the equation for $x$ values from 5 to 705 meters for 10 meters intervals.

The approach used in this analysis is similar to that used in the one-dimensional transport. However, because concentrations extracted from the OUT file in MT3D was so large, it was necessary to save this information in a new MATLAB m-file titled *concentrations.m* The numerical solution may be found under the file name *Ch. 17 Examples_DomenicoSchwartz\Three Dimensional Transport_Ex_17.6\Modflow _4\m4f.gpr,* and the analytical solution may be found under the file name*Ch. 17 Examples_DomenicoSchwartz\Three Dimensional Transport_Ex_17.6\Matlab Solution\exam.m.* The file *Ch. 17 Examples_DomenicoSchwartz\Three Dimensional Transport_Ex_17.6\Matlab Solution\concentrations.m*contains the concentrations obtained from the OUT file of MT3D.

3.3 Solution Scheme Comparisons: Advection Dominated Case

As in the one-dimensional transport problem, the benchmark problem provided by Zheng and Wang (1999) was used. For this study, the advection only case was used ($\alpha$=0, $R$ =0, $\lambda$= 0) with the same parameters described above.

Numerical Solution:
The grid set-up and MODFLOW run remained the same as described above. First the simulation was run using the MOC option in the advection package with DCEPS=$10^{-5}$, NPLANE=1, NPL=0, NPH=4, NPMIN=0, and NPMAX=8. Then it was solved with the Third Order TVD Scheme (ULTIMATE) solution with the maximum number of cells any particle will be allowed to move per transport step set as one. Finally it was solved using the standard finite difference model with upstream weighting, again with one as the maximum number of cells a particle can move.

Analytical Solution:
The analytical solution provided by Domenico and Schwartz (1990) that was used for Case 1a in the one-dimensional transport problem was used in this study. The equation was solved for $x$ values from 5 meters to 1005 meters at 10 meter intervals and the longitudinal dispersivity was set to 0.0001 rather than zero to avoid division by zero.

The approach used in this analysis was similar to that used in the following two studies. For graphing purposes rather than importing MT3D data into MATLAB, the plot was completed in Excel. The grid used for the numerical solutions may be found under the file name *Ch. 7 Examples\One- Dimensional Transport in a Uniform Flow Field\grip.gpr,* and the analytical solution can be found under the file name *Validation of MT3D\Solution Scheme Comparison_Advective\analyticalsolution..m.*

3.4 Solution Scheme Comparisons: Non-Advective Dominated Case

As in the one-dimensional transport problem, the benchmark problem provided by Zheng and Wang (1999) was used. For this study, the advection and dispersion case was used (Case 1a above) with the same parameters described above.

Numerical Solution:
The grid set-up and MODFLOW run remained the same as described above. In MT3D, the solution schemes were set up the same as described above.

Analytical Solution:
The analytical solution provided by Javendel et. al (1984) that was used for Case 1a in the one-dimensional transport problem was used in this study. The equation was solved for $x$ values from 5

meters to 1005 meters at 10 meter intervals and the longitudinal dispersivity was set to 10 meters.

The approach used in this analysis was similar to that used in the following three studies. For graphing purposes rather than importing MT3D data into MATLAB, the plot was completed in Excel. The grid used for the numerical solutions may be found under the file name *Ch. 7 Examples\One- Dimensional Transport in a Uniform Flow Field\grip.gpr,* and the analytical solution can be found under *Validation of MT3D\Solution Scheme Comparison_NonAdvective\analyticalsolutionnonadvective..m.*

## 4. Theoretical/Computer Analyses Activities

This section summarizes the theoretical/computer analysis attempted, descriptions of the problems encountered and documentation of the changes made.

4.1 One-Dimensional Transport in a Uniform Flow Field

After doing more research, it was determined that the analytical solution originally used for comparison had some errors. Another solution was provided by Bear (1979), which can be found below.

$$C(x,t) = \frac{C_o}{2}\exp\left\{\frac{qx}{2nD_h}\left[1 - \sqrt{\left(1 + \frac{4\lambda D_h n^2}{q^2}\right)}\right]\right\} \times$$
$$\mathbf{erfc}\left\{\frac{x - (q/n)\left[1 + 4\lambda D_h n^2 / q^2\right]^{1/2} t}{2\left[D_h t\right]^{1/2}}\right\}$$

After comparing the Bear (1979) solution to the Domenico and Schwartz (1990) solution, the necessary changes were made to the latter. To ensure the accuracy of this new solution, for all three cases a form of the analytical solution provided by Javandel, et al. (1984) was used.

$$\frac{C}{C_o} = \frac{v}{v+U}\exp\left[\frac{x(v-U)}{2D}\right]\operatorname{erfc}\left[\frac{Rx - Ut}{2\sqrt{DRt}}\right] + \frac{v}{v+U}\exp\left[\frac{x(v+U)}{2D}\right]\operatorname{erfc}\left[\frac{Rx + Ut}{2\sqrt{DRt}}\right] +$$
$$\frac{v^2}{2DR\lambda}\exp\left[\frac{vx}{D} - \lambda t\right]\operatorname{erfc}\left[\frac{Rx + vt}{2\sqrt{DRt}}\right]$$

where

$$U = \sqrt{\left(v^2 + 4DR\lambda\right)} \quad \text{and} \quad D = \alpha_x v$$

For each case, R, $\alpha$, and $\lambda$ were set to the values found above. In Cases 1a and 1b, where decay was not present, $\lambda$ was set to 0.000000001 $d^{-1}$ in order to avoid division by zero.

4.2 Three-Dimensional Transport in a Uniform Flow Field

Upon completing of the comparison of the numerical solution with that of an analytical solution with four continuous point sources, shown by Figure 1, it became clear that the area within the 15 by 10 meter zone was not concentrated enough.

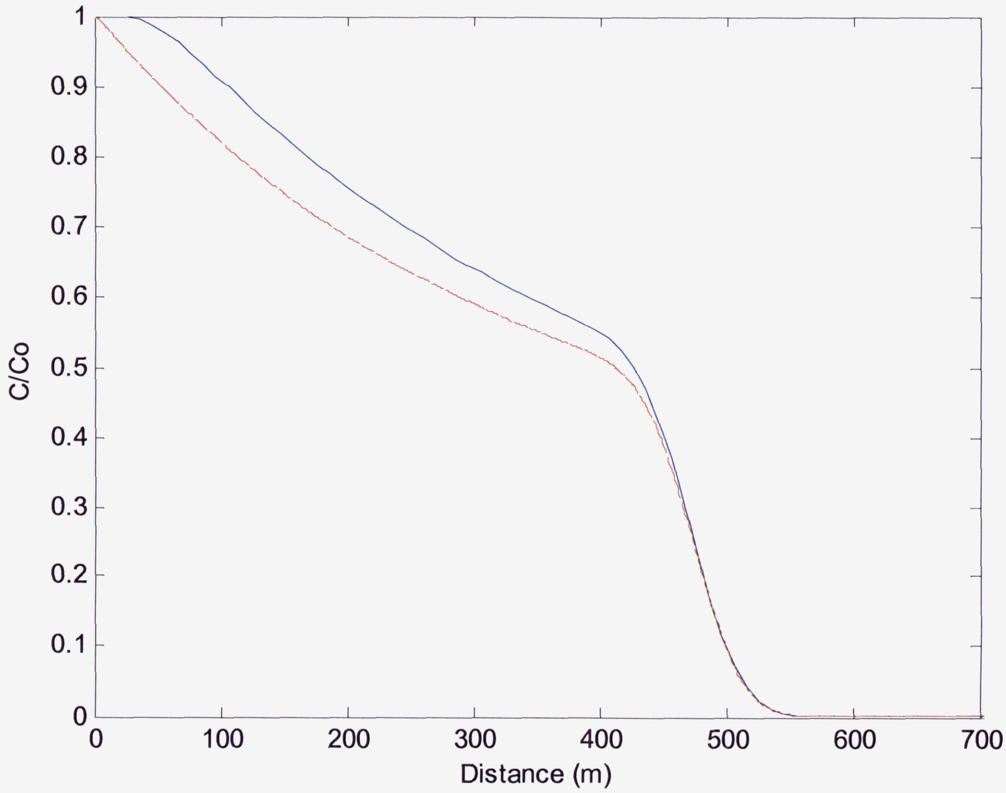


Figure 1. Comparison of the analytical solution (blue) with a numerical solution with four sources (red)

The resolve this issue, it was concluded that the need for a finer grid existed. Rather than four continuous sources, nine continuous sources were inserted in the new grid. To ensure the source size and total grid lengths remained consistent, a grid consisting of 700 columns, 21 rows, and 15 layers was created. A grid with 16 sources with 700 columns, 28 rows, and 20 layers was constructed as well. Because of the large amount of data in the OUT file, the concentrations resulting from the MT3D simulations with four, nine and sixteen sources were stored in separate MATLAB m-files entitled *concentrations.m*, *concentrations9.m*, and *concentrations16.m* , respectively. All of these files are saved in the directory *Ch. 17 Examples_DomenicoSchwartz\Three Dimensional Transport_Ex_17.6\Matlab Solution* .

## 5. Analyses and Results

Figure 2 displays the results of numerical and analytical solutions for one-dimensional transport in a uniform flow field.

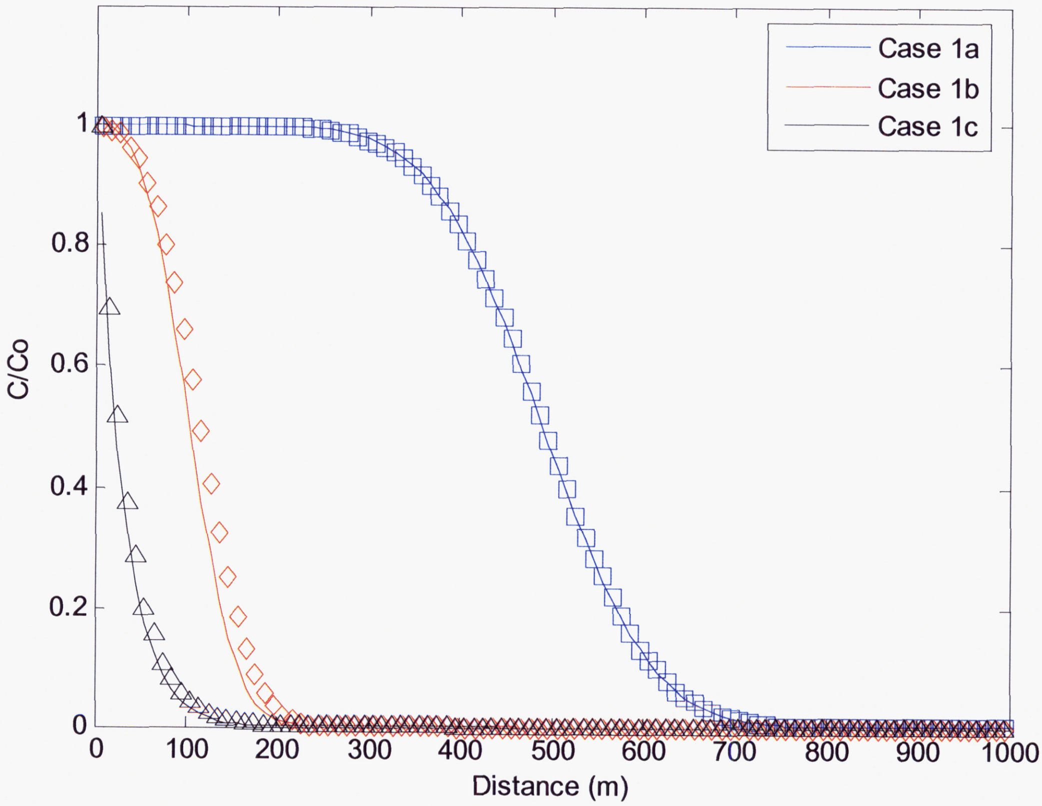


Figure 2. Comparison of concentrations calculated by analytical solutions (solid lines) and numerical solutions (symbols) for each case of the one-dimensional problem

The general results are as expected. When decay and retardation are not present, as in Case 1a, the contaminant travels a further distance, and as decay and retardation are introduced into the problem, the transport is slower.

For all cases, the relative concentration versus distance curve for the numerical and analytical solutions follow the same general path. The analytical and numerical solutions for Case 1a, where advection and longitudinal dispersion were present, produce almost identical results. The concentrations calculated from the numerical model are slightly higher than those results from the analytical solution for the remaining cases, particularly in Case 1b. Although these results are consistent with results provided by Zheng and Wang (1999), the difference between analytical and numerical results is slightly greater in this study. This variance may be due to a discrepancy in the $x$ values inputted into the models. Solving for $x$ values of 5 to 1005 meters at intervals of 10 meters in the analytical model was meant to best represent the fact that MT3D calculates information at the center of each cell. However the use of these particular values could have resulted in overestimation of concentration values in the analytical model. The $x$ values used for the analytical model were the same distances used to plot the concentration values extracted from the OUT files. These values may not be necessarily agree exactly with what MT3D used and when other values are used to plot the numerical solution, such as $x = 0\text{-}1000$, the graph is naturally affected. Either or both of these two factors may have provided a source of error.

Figure 3 shows the comparison of the calculated concentrations from the analytical solution and the numerical solutions with four, nine and sixteen sources in the three-dimensional transport model.

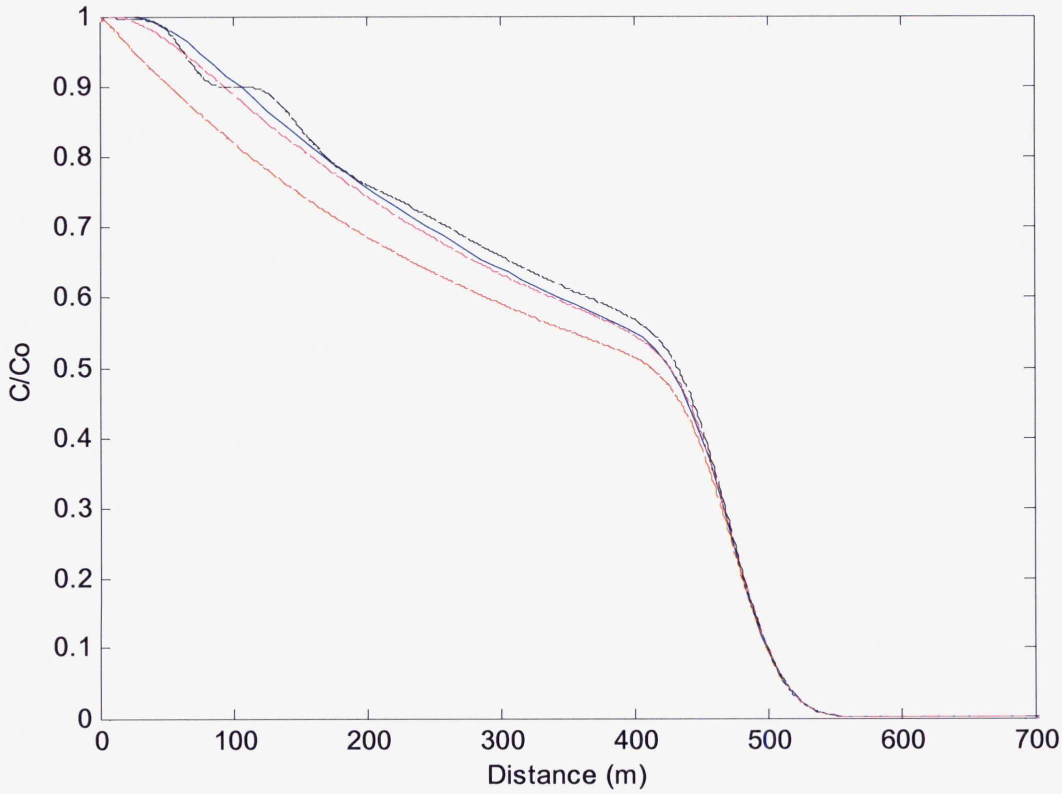


Figure 3. Comparison of concentrations calculated by analytical solutions (blue line) and numerical solutions with four sources (red line), nine sources (black line) and sixteen sources (magenta line) for the three-dimensional problem

As discussed earlier, the MT3D simulation containing four sources was not very accurate. As expected, the simulation containing nine sources (black line) was closer to the analytical solution, however the results are still off. The simulation containing sixteen sources (magenta line) closely matches the results of the analytical solution. Based on the trend illustrated in Figure 3, it is expected that if simulations were run in MT3D with 25 and 36 sources, the calculated concentrations would be almost identical to that of the analytical solution. However because of the resources available, these simulations could be completed at this time.

Figure 4 displays relative concentration vs. distance for the three advective solution schemes and the analytical solution for a purely advective case.

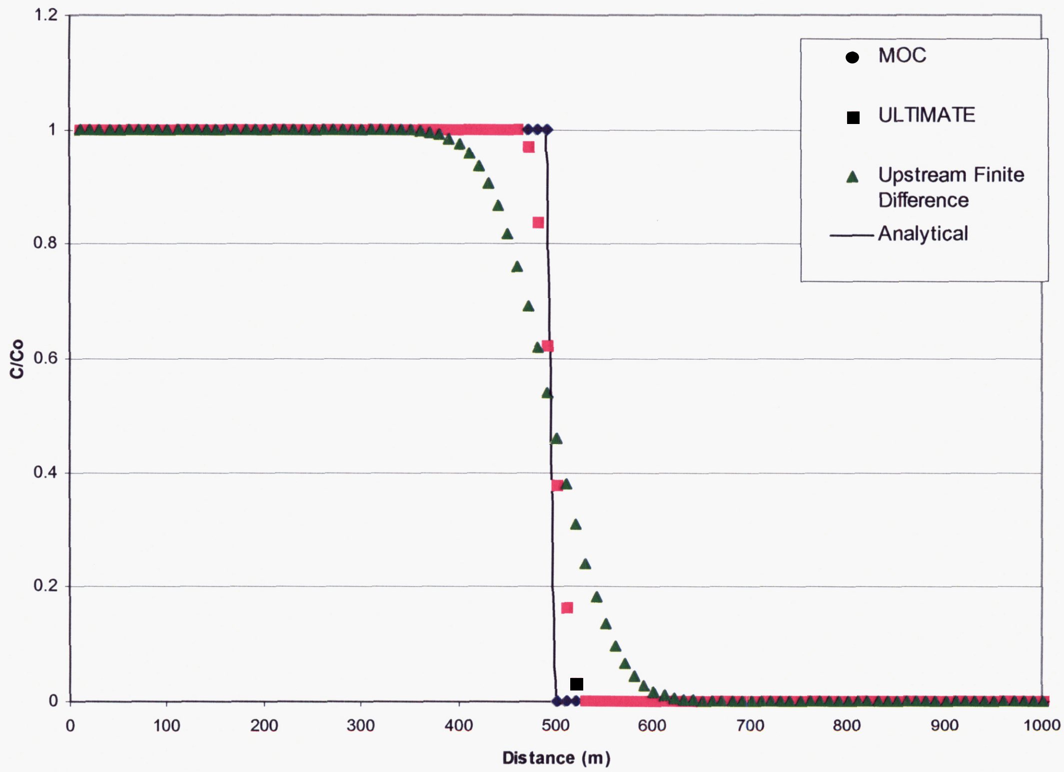


Figure 4. Comparison of solution schemes (symbols) and analytical solution (solid line): advection dominated

While both the the MOC and ULTIMATE solution schemes are within 5 percent of the analytical solution, the MOC solution provides nearly identical results and is the most accurate for purely advective cases. Based on these results, the upstream finite difference solution scheme does not provide a sufficient solution for advection dominated cases and should be used.

Figure 5 illustrates a comparison of advection solution schemes and the analytical solution for smooth case.

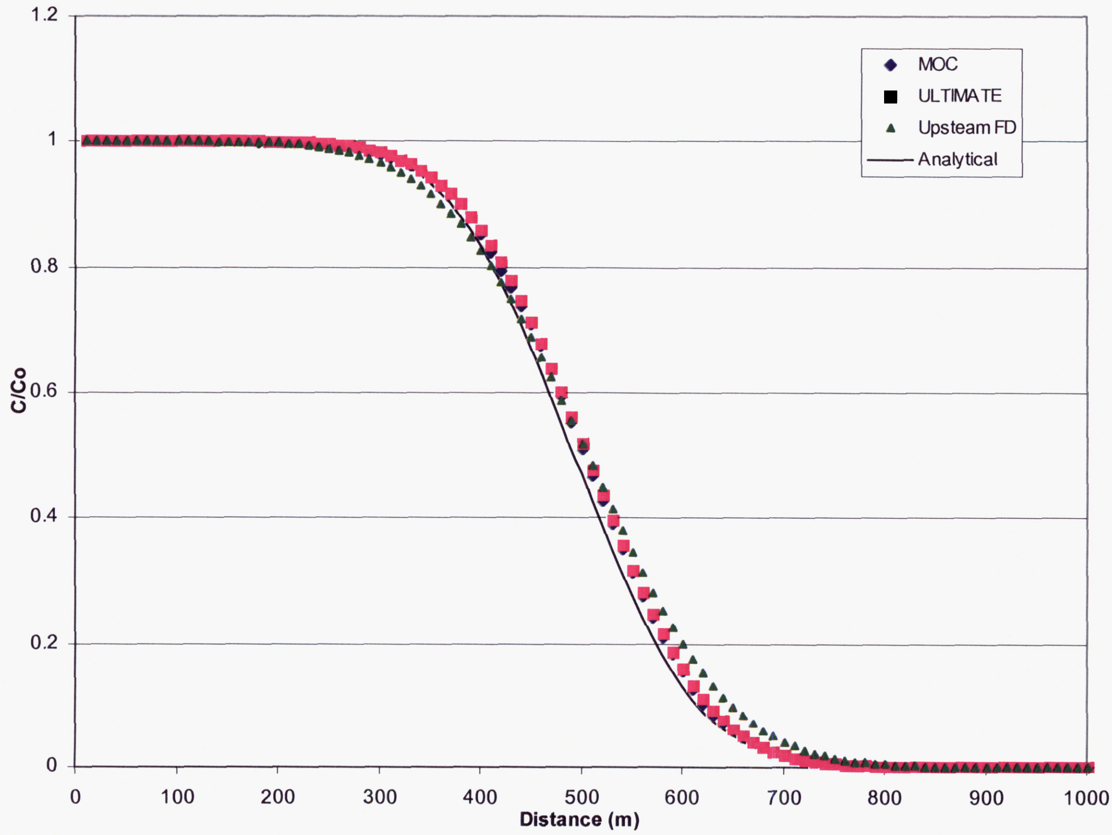


Figure 5. Comparison of solution schemes (symbols) and analytical solution (solid line): non-advection dominated

All results calculated by the numerical models in different solution schemes are a close match to the analytical solution. The MOC and ULTIMATE solutions are more accurate than the standard finite difference model. However the standard finite difference model with upstream weighting is more accurate in the case of a non-advection dominated model than a purely advective case. From these results, it can be concluded that any solution scheme is acceptable for use in a non-advection dominated transport simulation, however the MOC is the most accurate. Additional investigations and conclusions regarding advection solution schemes are given by Prommer et. al (2002).

**Close - out of Electronic Notebook 727**
No further entries will be made to this electronic notebook after July 28, 2005. Any further work on this project will be done in the form of journal articles or CNWRA/NRC publications.

Entries into Scientific Notebook No. 727 for the period July 13, 2005 to July 28, 2005 have been made by Anna Buseman-Williams.

## 6. References


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I have reviewed this scientific notebook and find it in agreement with QAP-001.

Gordon Wittmeyer
8/11/2005