# LABORATORY NOTEBOOK

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NOTEBOOK NO.

CONTINUED FROM NOTEBOOK NO. CONTINUED TO NOTEBOOK NO.

**ASSIGNED TO:**


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Data and Results from Validation Test of SLIM
IM 20.06002.01.272.804
WordPerfect and ASCII formats

(rjl 6/4/2007)

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Project Title: Validation of SLIM

| PAGE 4 | SUBJECT | DATE |
|---|---|---|
| 1 | Objectives | 06/14/06 |
| 2 | This notebook documents work performed | aMJ |
| 3 | for the validation ~~for~~ of SLIM. (aMJ 6.14.06) The objective | |
| 4 | of the study is to verify the accuracy of | |
| 5 | SLIM by developing simple test cases and | |
| 6 | comparing the analytical and numerical | |
| 7 | solutions of each contaminant transport. | |
| 8 | SLIM will be used for the purpose of simulating | |
| 9 | the transport of potentially highly | |
| 10 | contaminated groundwater through areas | |
| 11 | that surround the waste repository at | |
| 12 | Yucca Mountain. This notebook uses | |
| 13 | ~~previous~~ aMJ 6.14.06 analytical solutions performed | |
| 14 | previously for the validation of MT3D found | |
| 15 | in Scientific Notebook 727E. The validation | |
| 16 | will be used to support project # 06002.01.282 | |
| 17 | and is intended to address the criteria of | |
| 18 | CNWRA QAP-001. | |
| 19 | Computers, Computer Codes, & Data Files | |
| 20 | SLIM, the computer code used to simulate | |
| 21 | solute transport, was originally developed by | |
| 22 | Andrew F.B. Tompson at M.I.T (Massachusetts | |
| 23 | Institute of Technology) and was later | |
| 24 | developed at Lawrence Livermore National | |
| 25 | Laboratory. | |
| 26 | The analytical solutions were coded using | |
| 27 | MATLAB Version 7.0.1. | |
| 28 | The SLIM code was slightly modified by | |
| 29 | David Farrell for SwRI's applications. These | |
| 30 | modifications are detailed in Scientific | |
| 31 | Notebook 735. | |
| 32 | | |

| | SUBJECT | DATE |
|---|---|---|
| 33 | Introduction | |
| 34 | SLIM is a general purpose three-dimensional | 6.15.06 |
| 35 | particle-grid transport model for saturated | aRW |
| 36 | or unsaturated flows with reactions. It | |
| 37 | solves the three-dimensional advective- | |
| 38 | dispersive-reactive equation describing | |
| 39 | solute transport using the random-walk | |
| 40 | particle algorithm. This method represents | |
| 41 | the solute mass as a large collection of | |
| 42 | particles, each of which is moved by random | |
| 43 | displacement over discrete increments | |
| 44 | of time. The magnitudes of each displace- | |
| 45 | ment depend directly on the velocity | |
| 46 | and dispersion tensor. | |
| 47 | SLIM was chosen for use in this project in | |
| 48 | an attempt to reduce run time. | |
| 49 | | |
| 50 | | |
| 51 | | |
| 52 | | |
| 53 | | |
| 54 | | |
| 55 | | |
| 56 | | |
| 57 | | |
| 58 | aRW 6.15.06 | |
| 59 | | |
| 60 | | |
| 61 | | |
| 62 | | |
| 63 | | |
| 64 | | |



| | SUBJECT | DATE |
|---|---|---|
| 65 | Theoretical/Computer Analyses: Results | 6.15.06 |
| 66 | Numerical ~~and analytical models~~ models were aRW 6.15.06 | aRW |
| 67 | completed for a one-dimensional flow field, | |
| 68 | as well as a three-dimensional, both w/ ~~a~~ aRW 6.15.06 | |
| 69 | continuous sources. It was expected that ~~both~~ all aRW 6.15.06 | |
| 70 | numerical solutions would agree with the | |
| 71 | analytical solutions generated for the | |
| 72 | validation of MT3D (Scientific Notebook | |
| 73 | 727E). | |
| 74 | | |
| 75 | - One-dimensional Transport in a Uniform Flow- | |
| 76 | Field: Procedure | |
| 77 | | |
| 78 | In order to compare results w/ already | |
| 79 | completed analytical solutions, SLIM will be | |
| 80 | used to complete a simulation of a simple | |
| 81 | benchmark problem from MT3DMS User's | |
| 82 | Guide (Zheng & Wang 1999). | |
| 83 | | |
| 84 | The parameters are as follows: | |
| 85 | v (groundwater seepage velocity) = 0.24 m/day | |
| 86 | n (porosity) = 0.25 | |
| 87 | t (simulation time) = 2000 days | |
| 88 | L (length) = 1010 meters | |
| 89 | | |
| 90 | Two cases of one-dimensional flow ~~will be~~ aRW 6.15 | |
| 91 | were completed. In the first, Case 1a, advection | |
| 92 | and dispersion were present ($\alpha_x = 10$ m, $R=0, \lambda=0$), | |
| | while the second added in decay as | |
| | well ($\lambda = 0.002\ d^{-1}$). | |

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Because SLIM does not have the capability to input the decay rate constant, $\lambda$, the decay case output is found by multiplying the advection & dispersion case by $e^{-\lambda t}$. Therefore it was only necessary to simulate one one-dimensional case in SLIM. — 6.15.06 aaw

The approach in this analysis is summarized below: — 6.19.06 aaw

It was first necessary to change the parameters in the input files to the values indicated on the previous page. These input files are "rxn.1.dat", "rxn.2.dat", "poros," and "files.dat."

In "poros" the values were changed to 0.25. It was ensured that the number of data changed was sufficient enough to cover the size of the whole grid.

"Files.dat" is found below:

Software Validation_SLM\Code\1d run\files.dat

```
rxn.1.dat
rxn.2.dat
slim3.log
slim3.err
plotm.dat
plotM1.dat
plotc.dat
plotC1.dat
plotp.capture
plotb.dat
plotw.dat
poros

KD_FILE
365.0E+07 FLUXZ
```

note: all electronic files are contained on the Software Validation-SLM disc



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6.19.06 aaw

The majority of the input paraments are found in "rxn.1.dat". Below is the file used for the one-dimensional flow cases.

```
1                                   ! run number
102,2,2                             ! nx,ny,nz: discretization (128,128,64)
10.,1.,1.                           ! dx,dy,dz: discretization increment (feet)
1,0,0                               ! mx,my,mz: specify dimensions of the
problem (1,1,1) ⟶ indicates only 1-d flow (1,0,0)
10.,0.0,0.0                         ! al,ath,atv: dispersivities (1.0,0.1)
8000000                             ! npmax: max. num. particles per component
(19000)
0.,2000,10.,2000      ! t-init,t-max,dt,tcut: initial time, max time
lim., time step, cutoff time for inflow mass (0,50000,10.,100000)
0                                   ! itime (0): controls time step
1,0,1,0 ⟶ 1 Dirichlet boundary!     ! ibounc1(0),ibounc2(0),nbounc (0),initpar
(1): Dirichlet, Neuman, tot. bound. cond.s, initial part. distrib.
0,0                                 ! ixm,ixp (0,0): boundary reflection
indicators
0,0                                 ! iym,iyp (0,0): boundary reflection
indicators
0,0                                 ! izm,izp (0,0): boundary reflection
indicators
560,350                             ! iup,iud (210467,361223): particle
displacement seed, particle dispersion seed ⟶ random
10,10                               ! interv,intervp (10,201): printout interval for
end-of-time-step results, printout interval for end-of-time-step plot
data
1,1,1,1,0                           ! iplotm,iplotb,iplotc,iplotp,iplocp
(0,0,1,0,1): moment plot, breakthrough plot, contour plot, particle
point plot, conc. vs time plot
1.,0                                ! ver (0-1),isvel (1-2): dispersion scaling
factor, spatially variable velocities
1                                   ! intrp
1,0,1                               ! ncomp,ncomps,nr (125,1250,1000)
0,0                                 ! irxn,issorb
1                                   ! iplace (0 - account for particles
remaining in the source cell at the end of the time step)
```

Software Validation_SLM\Code\1d run\rxn.1.dat

Because the "isvel" value is set to 0, this indicates that the velocity will be explicitly defined in subroutine input3. So in the file "slim3z-por-disp-update.for" on line 1383 the value for vel(1,j) was set to 0.24.

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6.19.06 aBW

In the "rxn.2.dat" file data regarding phase ~~of~~ aBW 6.19.06 components and boundary conditions are inputted. Below is the "rxn.2.dat" input file for the one-dimensional flow test cases:

```
-----------------------------------------------
solid phase mineral data
-----------------------------------------------

MINERAL A
0    0    0                                (3)
0. .0    0                               (1.0)
0. .0    .0                              (1.5)

-----------------------------------------------
liquid phase component data
-----------------------------------------------

COMPONENT A
1.0 0.

-----------------------------------------------
initial liquid phase component mass distribution
-----------------------------------------------

0, 0.00
0, 0.00
-----------------------------------------------
specified dirichlet boundary conditions
-----------------------------------------------
cell #   mass into cell
1, 0, 100000.00, 0.00, 0.00
0, 0, 0., 0.00, 0.00
0, 0, 0., 0., 0.

-----------------------------------------------
specified neuman boundary conditions
-----------------------------------------------

0, 0, 0.00, 0.00, 0.00
```

Software validation-SLIM\Code\1d run\rxn.2.dat

The first line of information under "specified durichlet boundary conditions" indicates that 100,000 particles are inputted into cell 1.





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According to Tompson et. al (1987), as the number of particles increases the noise is reduced. Therefore it is expected that if excess noise is present, increasing that value will mitigate this error.

After it was ensured that the initial parameters were inputted correctly, "slim3z-por-disp-update.for" was compiled by typing LF95 slim3z-por-disp-update.for at the DOS command prompt. This produces a new application, MAP & OBJ files. Now the file was run by typing "slim3z-por-disp-update.exe" at the command ~~plot~~ prompt. aBW 6.19.06 Upon completion of running the application, new plotp (CAPTURE file), plotm.dat, plotC1.dat, plotc.dat, and plotb.dat files ~~are~~ we aBW 6.19.06 produced. A text document entitled "slum3" was also produced. It contains parameters, time steps, errors, and other data associated with the run completed. plotc.dat ~~plotp.capture~~ aBW 6.19.06 is the output file of concern because it contains the concentration at each printout time. However because plotc is a binary file it must be ~~re-run~~ aBW 6.19.06 compiled using the slum2tec_3d_update.for file in order to have the ability to read it.

The output file resulting from this will contain the concentrations at a given distance and can then be compared with the analytical solutions in MATLAB.

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In summary the procedure is as follows:

(1) input initial parameters in appropriate files.

(2) compile & execute slim3z-por-disp-update.

(3) compile & execute slim2tec-3d-update. to obtain the plotc OUT file at the necessary times.

(4) plot numerical solution in MATLAB ($c/c_0$ vs. distance) for comparison with the analytical solution from scientific notebook 727E.

7.10.06 aBW

## One-Dimensional Transport in a Uniform Flow Field: Results

Figure 1 displays a relative concentration vs. time graph for the analytical & numerical solution for 1-d transport w/ advection & dispersion. Some "noise" is present for the first ~300 meters, but it is expected that further increasing the number of particles would reduce this, as stated earlier. aBW 7.10.06 The analytical and numerical solution are very similar, and the root mean square values were calculated to be less than 1%. aBW 7.10.06 Figure 2 displays the plot with the addition of decay. The numerical and analytical solutions are very close, as expected, and the root mean square values are below 1% as well. From these results it can be concluded that SLIM is an accurate model for one-dimensional transport w/ advection, dispersion, and decay.





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from: Software Validation - SLIM\Code\1d run\Final Results\no decay\oned_comparisons MATLAB

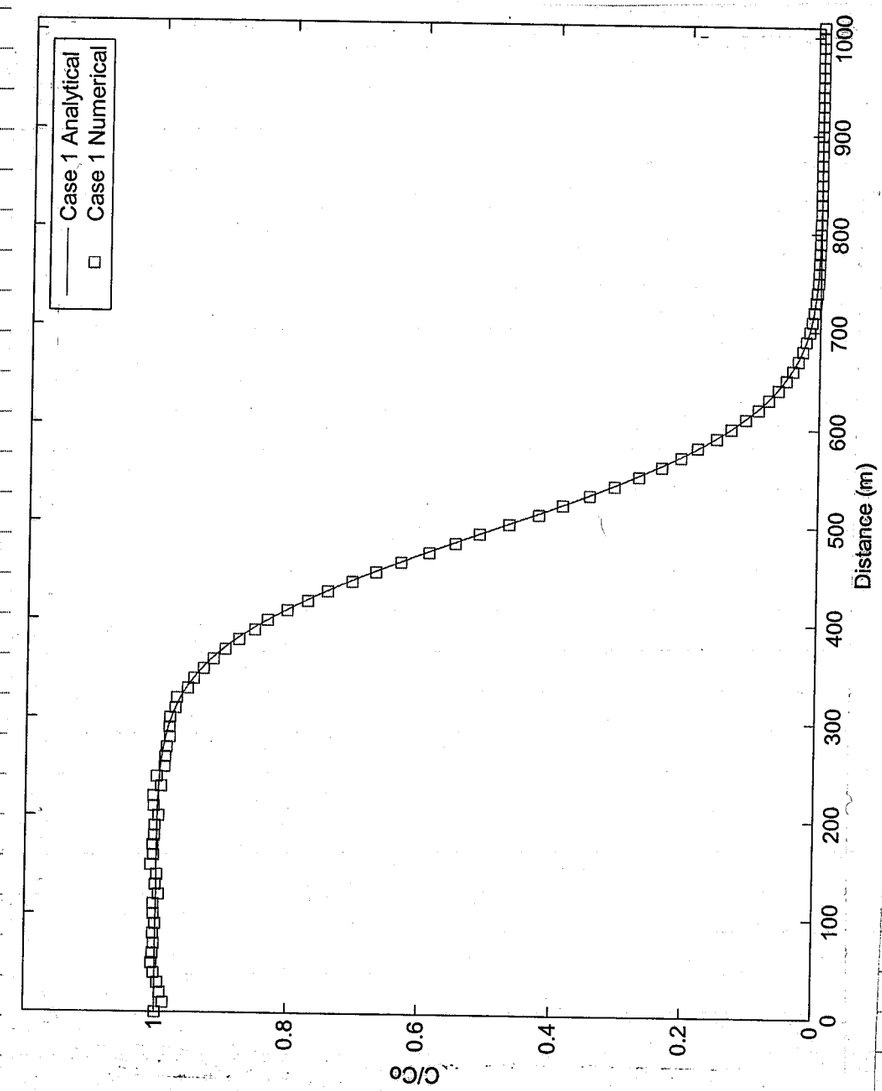


Figure 1: Comparisons of Analytical Solutions and Numerical Solution for 1-d Transport w/ Advection & Longitudinal Dispersion

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ABW

from: Software Validation-SLIM\Code\1d run\Final Results\decay\analytical solution_1d.MATLAB

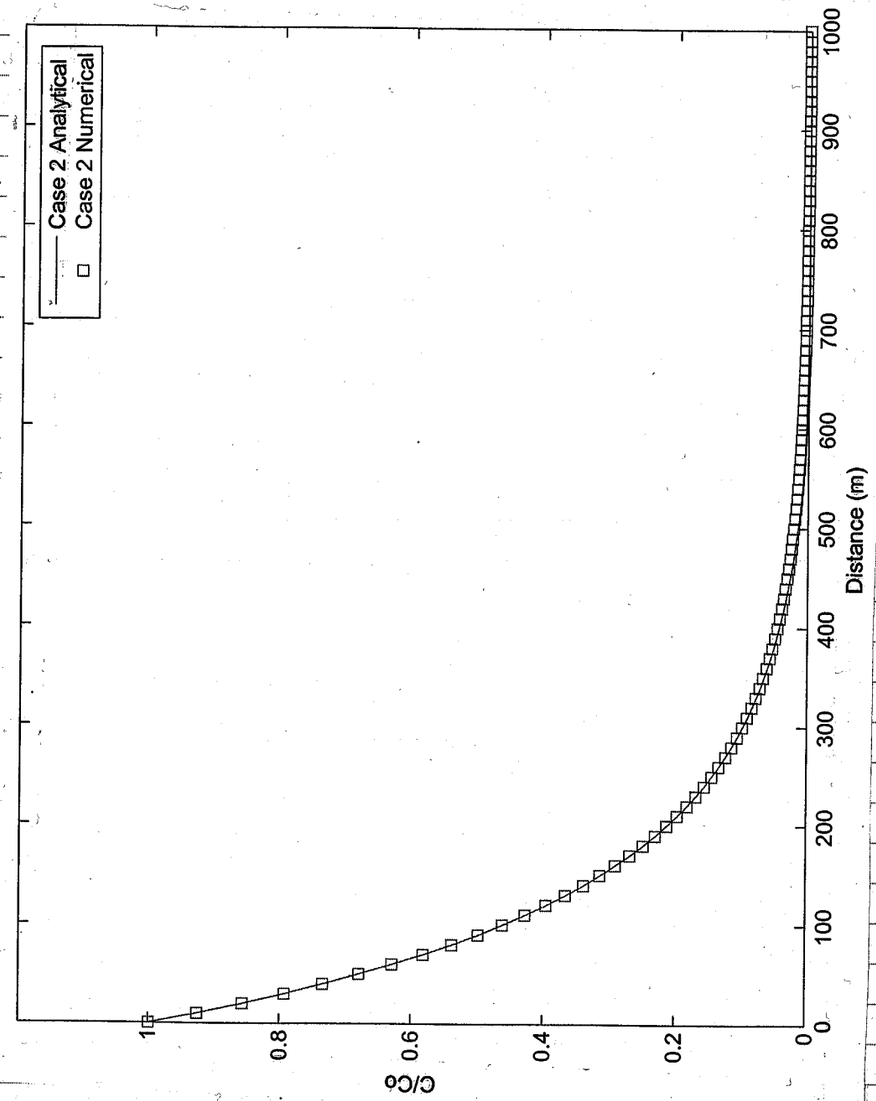


Figure 2: Comparison of the analytical solution and numerical solution for 1-d transport w/ advection, longitudinal dispersion, & decay





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7.10.06
ABW

## Three-Dimensional Transport in a Uniform Flow Field: Procedure

The 3d procedure was very similar to that of the 1d test cases. SLIM will be used to simulate a 3-d transport w/ advection & dispersion. The transport will be a slightly modified version of Example 17.6 provided by Domenico & Schwartz (1990). No decay is present. ABW 7.10.06

The parameters are as follows:

| | |
|---|---|
| $\alpha_x = 1.0$ m | $t = 5470$ days |
| $\alpha_y = 0.1$ m | $Y = 15$ m (source size y-direction) |
| $\alpha_z = 0.01$ m | $Z = 10$ m (source size z-direction) |
| $\theta = 0.300$ | $V = 0.05$ m/days |

7.18.06
ABW

The slightly modified version of the analytical solution performed for the validation of MT3D in MATLAB is found below.

```
% This program was written by Anna Buseman-Williams to solve a variation of example 17.6
in Domenico and Schwartz
% on pg. 653. It demonstrates three dimensional spreading of a plume in a one-dimensional
velocity
% field (y=0 and z=0) with no retardation.

%Define Constants

v=0.05; % groundwater velocity (m/day)
alfx=1.0; % dispersivity (m)
alfy=0.10; % dispersivity (m)
alfz=0.01; % dispersivity (m)
Y=15; %source size (m)
Z=10; %source size (m)
x=[0:10:600]; %distance intervals in x-distance (m)
t=5470; % time (days)
```

Software Validation-SLIM\Code\3d run\David\3d Results\threed.m

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```
% The analytical solution was found in "Physical and Chemical Hydrogeology"
% by Domenico and Schwartz on pg. 647.

a=erfc((x-(v*t))/(2*sqrt(alfx*v*t)));
aa=double(a); %double precision
b=erf((Y)./(4*sqrt(x.*alfy)));
bb=double(b); %double precision
c=erf((Z)./(4*sqrt(x.*alfz)));
cc=double(c); %double precision
Co=(1/2).*aa.*bb.*cc; % where C is relative concentration
xo=[5:10:605;] %adjust the distance to account for SLIM calculating conc at midpt. of
cells
plot(xo,Co) %plots analytical solution
xlim([0 700]); %sets the x-axis scale to 0 to 700 meters
ylim([0 1]); %sets the y-axis scale to 0 to 1.0
xlabel('Distance (m)')
ylabel('C/Co')
hold on
```

It is important to note that when plotting the analytical solution the x-distances need to be at the midpoints in order to agree w/ the SLIM solution. If not, the graphs will be slightly off. This correction was needed when I found my numerical solution to be off.

• Three-dimensional Transport: Results.

Several runs of the numerical solution were completed. Run 1 consisted of nx, ny, nz values of 72, 10 and 8 respectively and dx, dy, dz values of 10, 15, and 10 in order to correspond to the source size values of 15 and 10 meters in the analytical solution. The cell in which initial particles were inputted was calculated to be located at i=10, j=5 and K=4 (x=90m, y=60m & z=30m)





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using the equation: source cell = (mx * my) * (iz-1) + mx(iy-1) + ix
where ix, iy & iz are the cell index and mx, my, mz are the number of cells in the respective direction (or nx-1, ny-1, nz-1)

This equation resulted in 20,000 particles being inputted into cell # 2211. It was also ensured that the "poros" file was adjusted to the number of lines needed to cover the whole grid, and the slim2tec file was corrected so the discretization corresponded to the parameters in the rxn.1.dat file. It is important to note that when entering these values in the slim2tec file mx, my & mz should be inputted, not nx, ny & nz. Figure 3 displays the result of a comparison of the first run w/ the analytical solution.

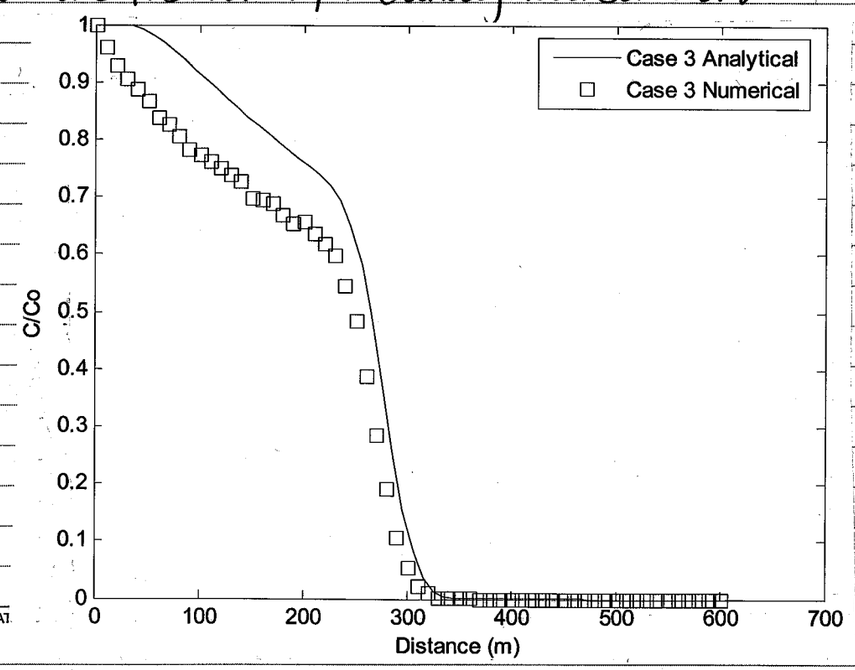


Figure 3: comparison of Run 1 (numerical solution) and the analytical solution for 3-d transport (from threed.m)

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As shown by Figure 3, the numerical and analytical are significantly off. Some possible solutions to this error are to decrease dy & dx to ensure enough particles are put in the source cell downstream and to continue to use a large amount of particles. Also to ensure that the data from the plotc OUT file is selected for the appropriate source cell.
The table below documents each run and notes on the results. The information in the table represents the significant changes made in each file.

| file name | rxn.1.dat (nx,ny,nz dx,dy,dz) | rxn.2.dat (starting cell, # of part.) | starting source cell | slum2tec_... | poros file (# of lines) |
|---|---|---|---|---|---|
| Run 1 | 72,10,8 10,15,10 | 2211, 20,000 | i=10 j=~~13~~ 6 k=~~7~~ 1 abw 7.18 | 71,9,7 10,15,10 | 448 |
| plotc1 | 72,10,8 ~~10,15,10~~ 10,5,5 abw 7.18 | abw 7.18 ~~2211, 20,000~~ 12364 12435 12506 14281 14352 14423 1,000 | i=10 j=13 k=7 (6) | 71,27,17 10,5,5 | ~~448~~ 2684 abw 7.18 *a lot of oscillating occur |
| plotc2 | " | " 10,000 | " | " | " *grid is smoother, but further refinement necessary |
| plotc3 | 72,46,36 10,3,2 | 49355... 62419 1,000 | i=10 j=21 k=16 (25) | 71,45,35 10,3,2 | 11,183 *a lot of oscillating/ noise occur for 1st 250 meters |
| plotc4 | " | " 10,000 | " | " | " *run not complete max # particles exceeded |
| plotc5 | " | " 5,000 | " | " | *matches better w/ analytical solution, noise still present |

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After increasing the max number of particles in rxn.1.dat file to 15,000,000 and increasing the htest value in the source code, two additional runs were completed to reduce noise in the numerical solution.

| filename | rxn.1.dat | rxn.2.dat | starting source cell | slum2tec_... | poros file |
|---|---|---|---|---|---|
| plotc6 | " | " 10,000 | " | " | " *noise still present |
| plotc7 | " | " 15,000 | " | " | " *only slightly off from 100-300 m |

Figure 4 displays a comparison of plotc7 and the analytical solution. It is slightly off @ the beginning distances, but it is expected that if the number of particles was increased, this noise would be reduced. The root mean square error value was calculated using Excel to be approximately 2 percent. It is important to note that while running plotc7, as well as the other runs w/ large amounts of sources &/or particles, a warning was given after compiling the source code. This warning stated that the total image size exceeds the maximum and that the image may not run, however this warning does not appear to affect the result. From the results, it can be concluded that SLIM is an accurate model for three-dimensional

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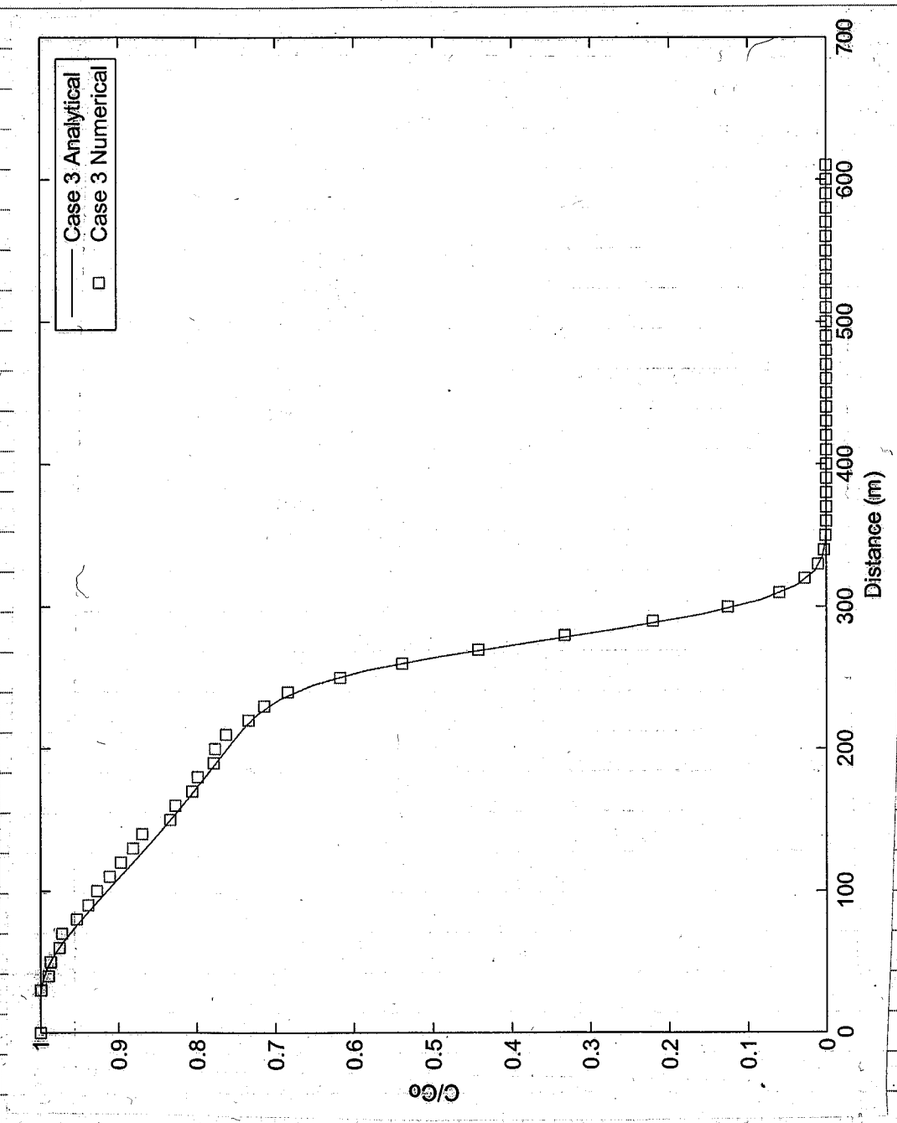


from: threed.m

Figure 4: Comparison of the analytical solution and numerical solution for 3-d transport w/ advection & dispersion

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transport with advection and dispersion.

8/10/06

D.A.T.

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NOTE THAT THE INFORMATION ON THIS PROJECT WAS TRANSCRIBED FROM THE AUTHOR'S NON-CNWRA NOTEBOOK AS THIS CNWRA SCIENTIFIC NOTEBOOK WAS NOT AVAILABLE. DOCUMENTS WORK PERFORMED BEFORE JULY 15, 2006.

DAT 8/10/06

The following summarized work contained deliverable "Development and Application of Models to Simulate Saturated Zone Transport Under Future Climates at Yucca Mountain". To support the report the following analyses were performed:

- 10,000 year simulations under a future climate scenario defined by J. Winterle in Winterle (2003)
- SLIM3 simulations to simulate solute (conservative) ~~under~~ DAT 8/10/06 over a 1,000,000 year period
- analytical simulations for decaying plumes with decaying sources over a 1,000,000 year period.

The results of the 10,000 year simulations performed under future climate conditions are useful for comparison with the results contained in Farrell et al (2005) that were performed under current climatic conditions. Note that both sets of simulations were performed using the computer code MT3DMS 4.5 contained in the GMS 5.0 package which is under control at CNWRA (i.e., TOP018).

* note: all electronic files are contained on supporting disks 2 & 3 (RSH 6/4/2007)

10,000 Year Simulations Under Future Climate

The 10,000 year simulations under future climate expanded on the previous model described in Farrell et al. (2005). As described in Farrell et al. (2005) the domain was 28.5 × 41.4 × 2.7 km and consisted of 95 columns, 138 rows, and 30 horizontal layers... $\Delta X = \Delta Y = 300$ m and $\Delta Z$ varied from 50 m near the water table to 200 m at depth. From a hydrogeologic perspective, the domain was divided into 19 hydrostratigraphic and structural units; these units were based on the hydrostratigraphic model constructed for the YM region by Sims et al. (1999) ... see Table 1... this is consistent with the description provided in Farrell et al. (2005)... see also Winterle (2003, Table 2-1). Figure 5 shows the distribution of hydrostratigraphic units at YM based on the model of Sims et al. (1999).

Material properties used in the model were based on Winterle (2003). These material properties were also used in Farrell et al. (2005). See Table 1 for a summary

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Table 1: Hydrostratigraphy & Material Properties Used in Numerical Model

| Material Type | Description | Hydraulic Conductivity (m/day)† | Porosity |
|---|---|---|---|
| PZ | Deep Paleozoic aquifer system | 0.05 | 0.01 |
| UVA | Uppermost volcanic aquifer | 0.5 | 0.001 |
| UVC | Upper volcanic confining unit | 0.15 | 0.1 |
| LVA | Lower volcanic aquifer | 0.15 | 0.001 |
| LVC | Lower volcanic confining unit | 0.0002 | 0.1 |
| Alluv | Valley-Fill alluvium | 3 | 0.1 |
| FMW | Fortymile Wash fault zone | 5 | 0.001 |
| BR–PBC | Bow Ridge–Paintbrush Canyon fault zone | 4 | 0.001 |
| Cald-pz | Caldera zone: altered Paleozoic rocks | 0.001 | 0.01 |
| Cald-vr | Caldera zone: altered volcanic rocks | 0.0003 | 0.01 |
| SC–IR | Solitario Canyon–Iron Ridge fault zone | 0.0005 | 0.01 |
| SC–West | Western splay of Solitario Canyon fault zone | 0.0005 | 0.01 |
| CF | Crater Flat fault zone | $5.0 \times 10^{-5}$ | 0.01 |
| VH1 | VH–1 fault zone | $5.0 \times 10^{-5}$ | 0.01 |
| BM | Bare Mountain fault zone | 0.05 | 0.01 |
| H95 | Highway 95 fault zone | 0.005 | 0.01 |
| Grav1 | Gravity fault zone #1 | 0.001 | 0.01 |
| Grav2 | Gravity fault zone #2 | 0.05 | 0.01 |
| CA | Central Amargosa fault zone | 0.5 | 0.01 |

of the material properties used. Calibration of the groundwater model (DAT 8/10/06) used to support the transport simulations was performed by Winterle (2003) ... the reader should refer to the reference for a detailed discussion. Note that the groundwater model was constructed for execution under MODFLOW-2000 using the Groundwater Modeling System (GMS) version 5.1 environment. GMS (DAT 8/10/06) was developed by Environmental Modeling Research Laboratory. (DAT 8/10/06).

Key aspects of Winterle (2003) wrt future climate simulation:

- future recharge is assumed to be 10 mm/yr (double present-day value)
- recharge was assumed to occur in the lower reaches of Fortymile Wash ... ≈ 200 mm/yr.
- Lateral boundaries were determined using an iterative process in which

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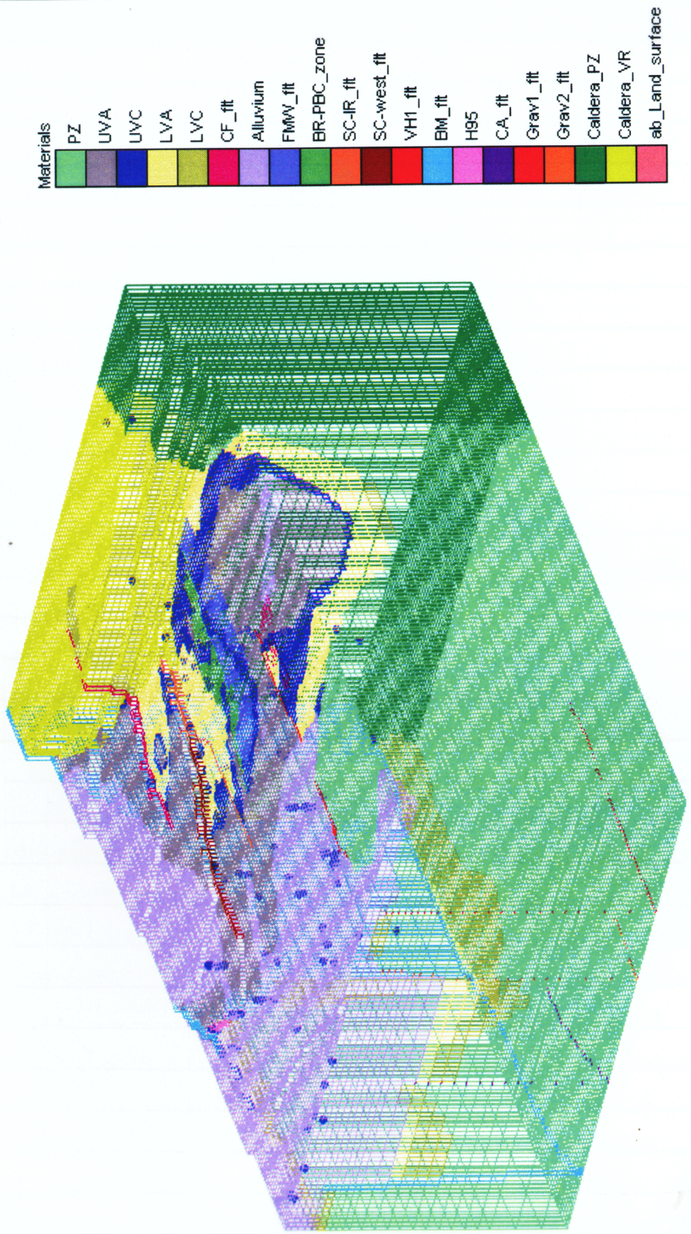
Figure 5: Hydrostratigraphic Model ~~ab~~ (DAT 8/10/06) at Yucca Mountain








the elevation of the water table along the lateral boundaries was systematically increased until discharge occurred at the paleo-spring deposits near Nye County Early Warning Drilling Program well NC-EWDP-9S. Boundary condition was 5% higher than present-day.

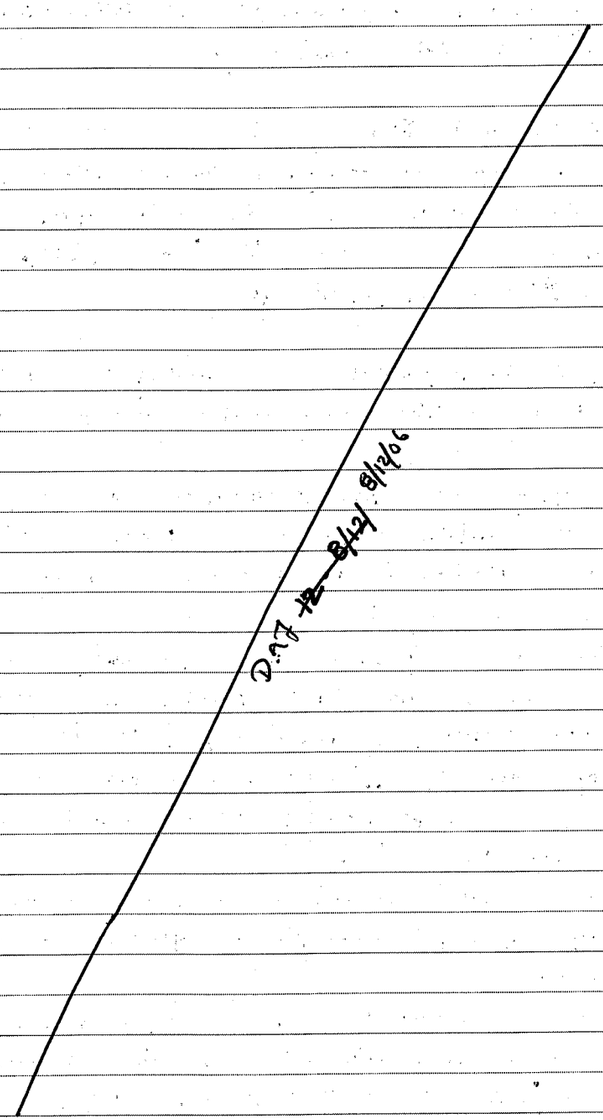
Figure 6 shows the hydrostratigraphic units at the water table. In addition the figure shows the repository footprint at the watertable. This footprint shows the potential source locations for the transport simulation. Note that for transport it is assumed that $C(x,y,z,t=0)=0$ and ~~C(x,y,z,t>0) ≠ 0~~ (DAT 8/10/06) $C(x,y,z,t>0) \geq 0$

As noted before, solute transport was simulated using MT3DMS Version 4.5 (MT3DMS ≡ Modular Three-Dimensional Multispecies Transport Model).

The following assumptions were made to maintain consistency with Farrell et al. (2005) and to facilitate comparison with results of that report:

- advection & hydrodynamic dispersion were the primary physical processes controlling plume evolution
- longitudinal dispersivity values used in the analysis were ~~assumed to~~ chosen to be consistent with Bechtel SAIC Company, LLC (2004) ["Saturated Zone Flow and Transport Model Abstraction"] and Mohanty et al. (2004) ["System-Level Performance Assessment of the Proposed Repository Footprint at Yucca Mountain Using the TPA Version 4.1 code"].
- Molecular diffusion is current assumed to be negligible relative to hydrodynamic dispersion ... this assumption will be verified at a later time.
- Dual domain formulation is not currently used but will be considered in future work due to potential importance of matrix diffusion (NRC, 2005 ... "NUREG-1762 – Integrated Issue Resolution Status Report").

Figure 6: Hydrostratigraphic Units at the Watertable & the Potential Repository footprint at the Water table



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- Porosities used in the model those identical to those in Winterle (2003) were within the distribution ranges for the alluvium valley-fill and volcanic units in Bechtel SAIC Company, LLC (2004 – Table 6-8).
- For some simulations tuff and alluvium can have identical longitudinal dispersivities as in Bechtel SAIC Company, LLC (2004).
- Two dispersivity ratios are once again considered — those based on the DOE model (0.5% and 0.005% for $\alpha_{TH}/\alpha_L$ and $\alpha_{TV}/\alpha_L$ respectively) and more traditional ratios (10% and 1% for $\alpha_{TH}/\alpha_L$ and $\alpha_{TV}/\alpha_L$ respectively).

## Scenario: Plume Size at Compliance Boundary

This simulation is similar to that performed in Farrell et al. (2005). It assumes that all potential sources (i.e., source cells) within the repository footprint are active ... this scenario correlates to the case where there are significant waste package failures across the repository footprint. All failures are assumed to occur almost simultaneously. Simulations performed under this Scenario are listed in Table 2.

Table 2: Simulations Performed

**Objective**

Determine the size of plumes that may cross the regulatory compliance boundary for selected values of longitudinal dispersivity sampled from the Bechtel SAIC Company, LLC (2004)* and the distributions in Mohanty, et al. (2004)†

**Source model**

All potential source grid cells within the repository footprint are active

**Model considerations**

- 10 mg/L constant concentration applied to all source cells
- Longitudinal dispersivity, $\alpha_L$ = 100, 10, and 1 m [330, 33, and 3.3 ft], respectively
  - Commonly used transverse dispersivity ratios
    - horizontal transverse dispersivity ($\alpha_{TH}$) ratio: $(\alpha_L/\alpha_{TH})$ = 10
    - vertical transverse dispersivity ($\alpha_{TV}$) ratio: $(\alpha_L/\alpha_{TV})$ = 100
  - Transverse dispersivity ratios in Bechtel SAIC Company, LLC (2004)*
    - horizontal transverse dispersivity ($\alpha_{TH}$) ratio: $(\alpha_L/\alpha_{TH})$ = 200
    - vertical transverse dispersivity ($\alpha_{TV}$) ratio: $(\alpha_L/\alpha_{TV})$ = 20,000

Dirichlet source strength in each source cell was 10 mg/L (D.A.T 8/10/06)

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Simulation models : (see accompanying DVD)

- All-Sources-Disp-1 : • Sources placed in all water table cells in repository footprint
  • longitudinal dispersivity $1\ m = \alpha_L$
  • common dispersivity ratios used

- All-Sources-Disp-10 : • Sources placed in all water table cells in repository footprint
  • longitudinal dispersivity $\alpha_L = 10\ m$
  • common dispersivity ratios used ~~to 5%~~ DAJ 8/10/06

- All-Sources-Disp-100 : • sources placed in all water table cells in repository footprint
  • longitudinal dispersivity $\alpha_L = 100\ m$
  • common dispersivity ratios used

- All-Sources-Disp-DOE-1 : • sources placed in all watertable cells in repository footprint
  • longitudinal dispersivity $\alpha_L = 1\ m$
  • DOE dispersivity ratios used (see p. 19)

- All-Sources-Disp-DOE-10 : • sources placed in all watertable cells in repository footprint
  • longitudinal dispersivity $\alpha_L = 10\ m$
  • DOE dispersivity ratios used (see p. 19)

- All-sources-Disp-DOE-100 : • sources placed in all watertable cells in repository footprint
  • longitudinal dispersivity $\alpha_L = 100\ m$
  • DOE dispersivity ratios used. (see p. 19)

SEE SAMPLE OUTPUT PLOTS ON PAGE 21

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red line represents approximate location of compliance boundary

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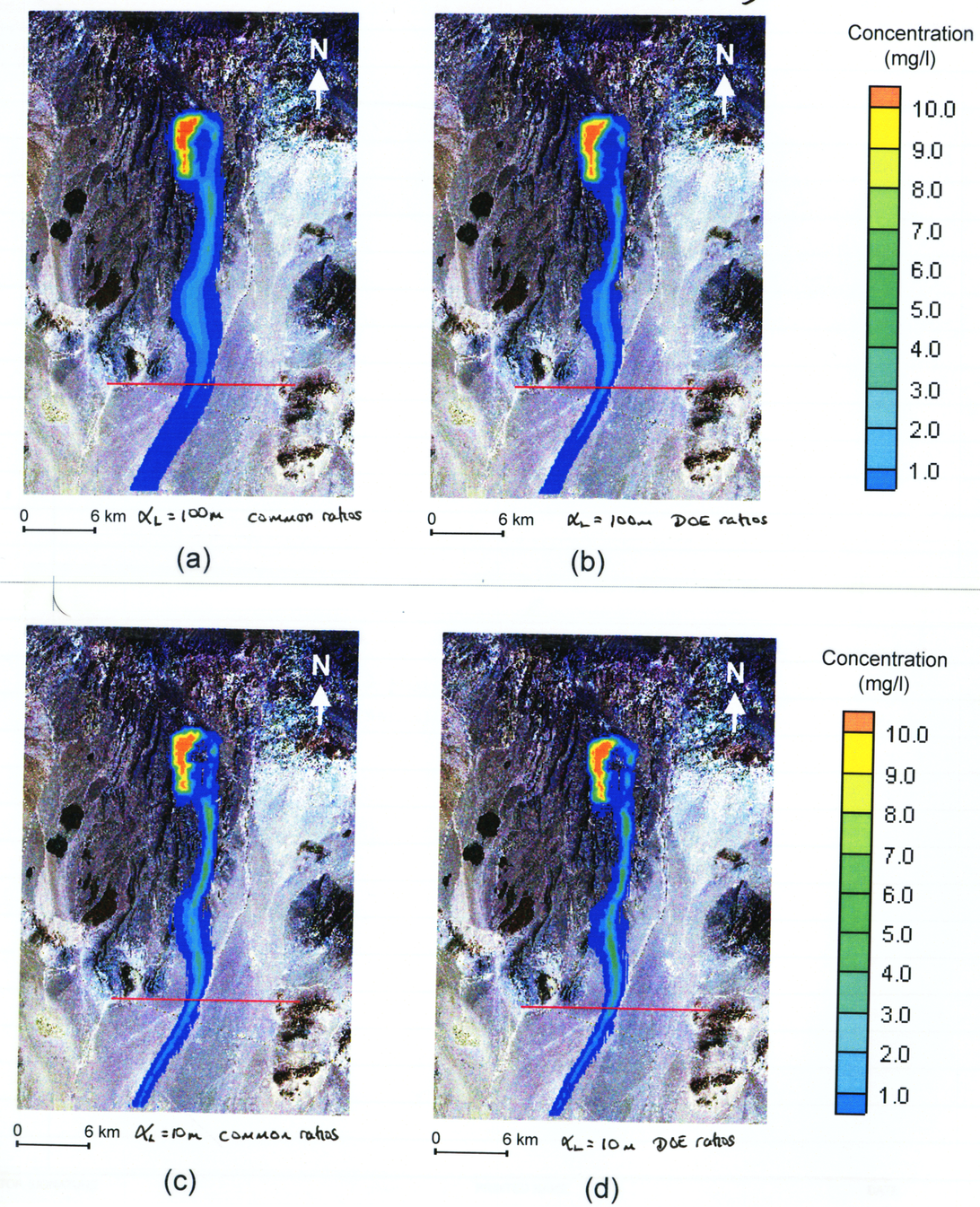
Figure 7: Plots Associated with Scenario All sources turned on (see p. 20)

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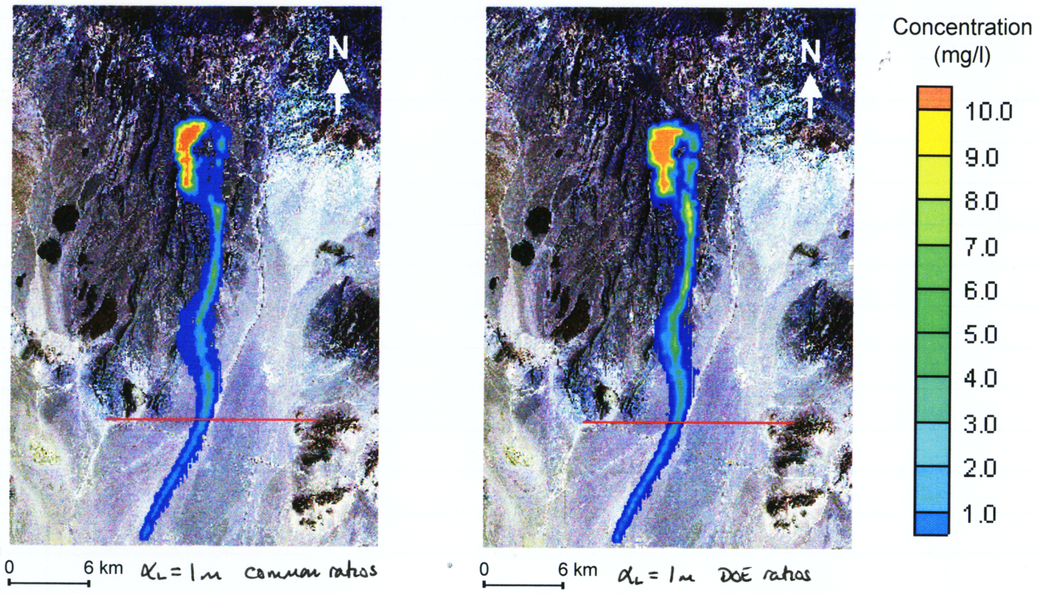
Relative Concentration Cutoff for plots = $10^{-3}$

red line represents approximate location of regulatory compliance boundary




(e) (f)

Table 3: Summary of Plume Dimensions for Simulations

| Longitudinal Dispersivity (m)† | Horizontal Transverse Dispersivity (m)† | Vertical Transverse Dispersivity (m)† | Maximum Plume Width (m)† | Maximum Plume Thickness (m)† |
|---|---|---|---|---|
| 100 | 10 | 1 | 3300 | 1200 |
| 100 | 0.5 | 0.005 | 2100 | 900 |
| 10 | 1 | 0.1 | 1900 | 950 |
| 10 | 0.05 | 0.0005 | 1800 | 900 |
| 1 | 0.1 | 0.01 | 1800 | 800 |
| 1 | 0.005 | 0.00005 | 1500 | 900 |

*Shaded rows represent data based on simulations conducted using the U.S. Department of Energy dispersivity ratios.

Scenarios described on p. 20





Table 4: Annual Groundwater Flow Through Plumes At the Regulatory Compliance Boundary ($10^{-3}$ relative Concentration Cutoff)

| Dispersivity (m) | | approximate plume width (m) | approximate vert. thickness (m) | approximate Flow through plume $m^3$/year | acre-ft/year |
|---|---|---|---|---|---|
| 1 | (DOE) | 1300 | 900 | 965425 | 783 |
| 1 | (common) | 1800 | 800 | 1,079,017 ~~1,079,016~~ (DAJ 8/10/06) | 875 |
| 10 | (DOE) | 1800 | 900 | 1,214,975.* | 985. |
| 10 | (common) | 1900 | 950 | 1,323,490 | 1073 |
| 100 | (DOE) | 2100 | 900 | 1,531,540 | 1242 |
| 100 | (common) | 3300 | 1200 | 2,223,945 | 1803.6 |

* Scenarios described on p. 20

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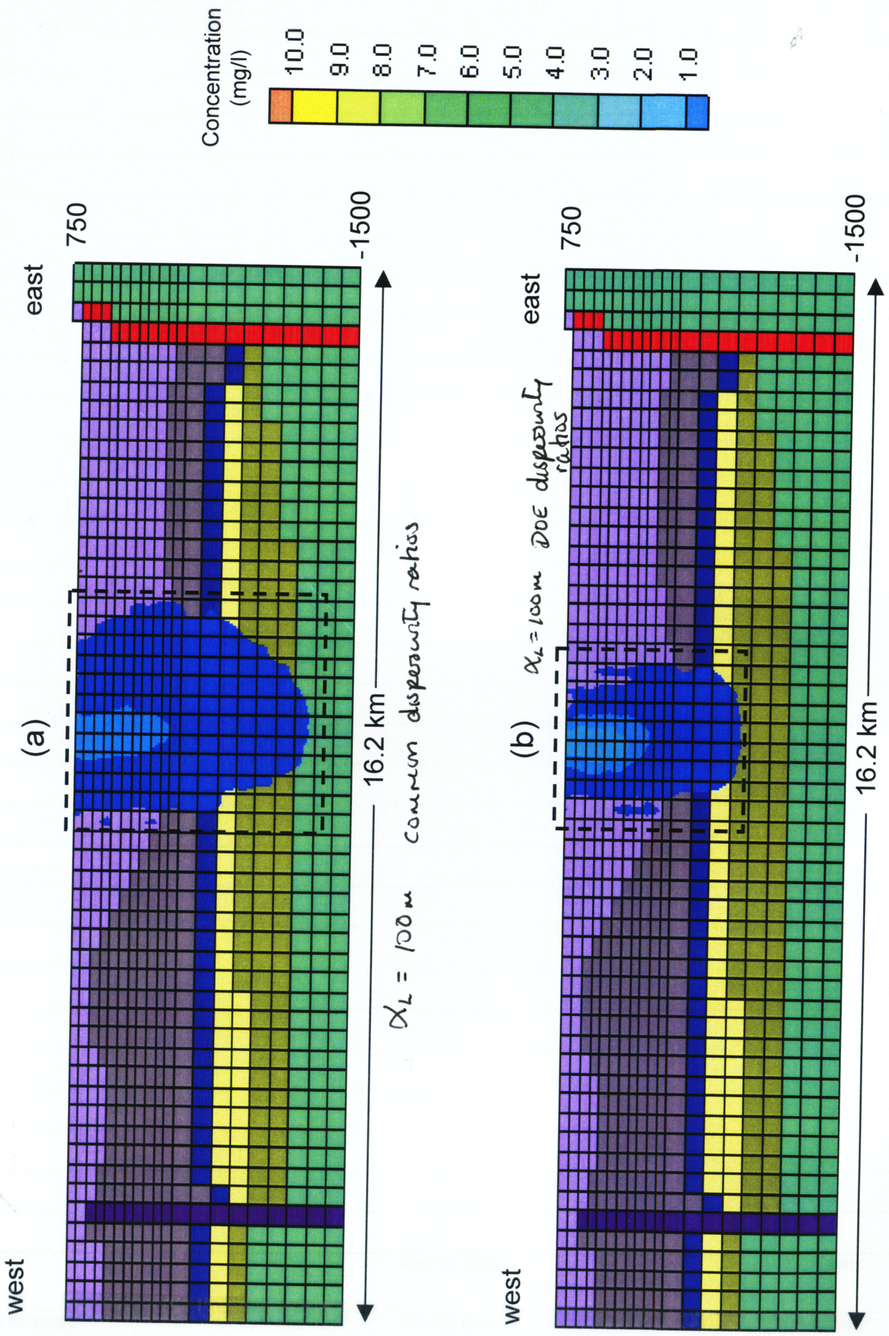
All sources Turned on

Figure 8: Vertical Cross-sections Through Plumes at the Regulatory Compliance Boundary




(Slice at row 107 of GWS model)

Geology summarized in Figure 10

Dotted box shows the region occupied by the plume (Slice at 107 row of grid)

Geology summarized in Figure 10 (Slice at row 107 of GWS model)

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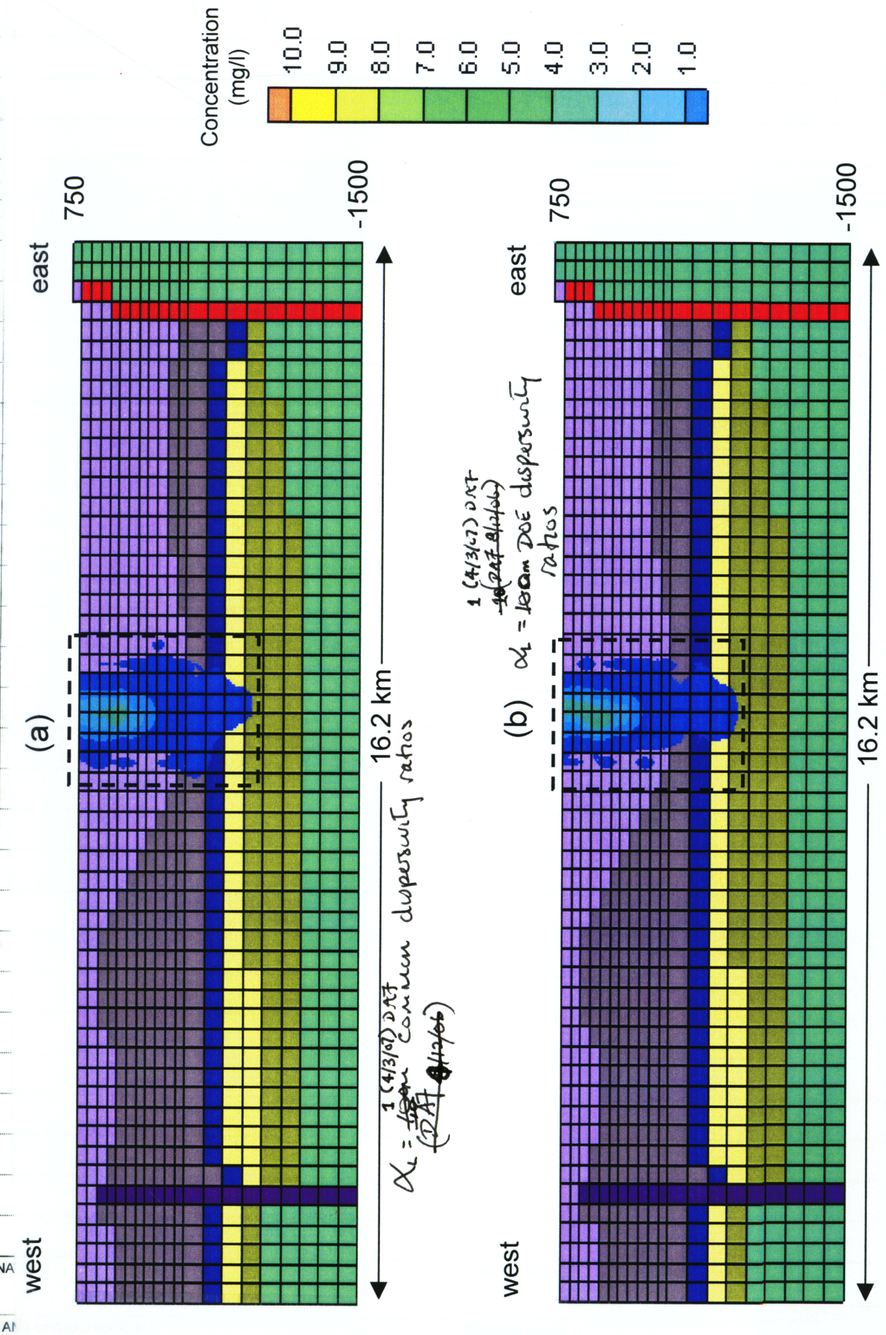
Figure 9: Vertical Cross-sections Through Plumes at the Regulatory Compliance Boundary




(Slice at 107 row of grid)

dotted Lines show region occupied by the plume

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Figure 10: Geology Present in Figures 8 & 9 and Subsequent Figures where Referenced

Abbreviations are explained in Table 1 of page 15.

CF_flt ← same as CF in Table 1
FMW_flt ← same as FMW in Table 1
BR-PBC_zone ← same as BR-PBC in Table 1
SC-IR_flt ← same as SC-IR in Table 1
SC-west_flt ← same as SC-west in Table 1
VH1_flt ← same as VH1 in Table 1
BM_flt ← same as BM in Table 1
CA_flt ← same as CA in Table 1
Grav1_flt ← same as Grav1 in Table 1 (DAJ 8/12/06)
Grav2_flt ← same as Grav1 in Table 1
Caldera_PZ ← same as Cald_pz in Table 1
Caldera_VR ← same as Cald_vr in Table 1
ab_Land_surface ← represents cells that are above ground level.

See figures 8 & 9 for concentration legends.

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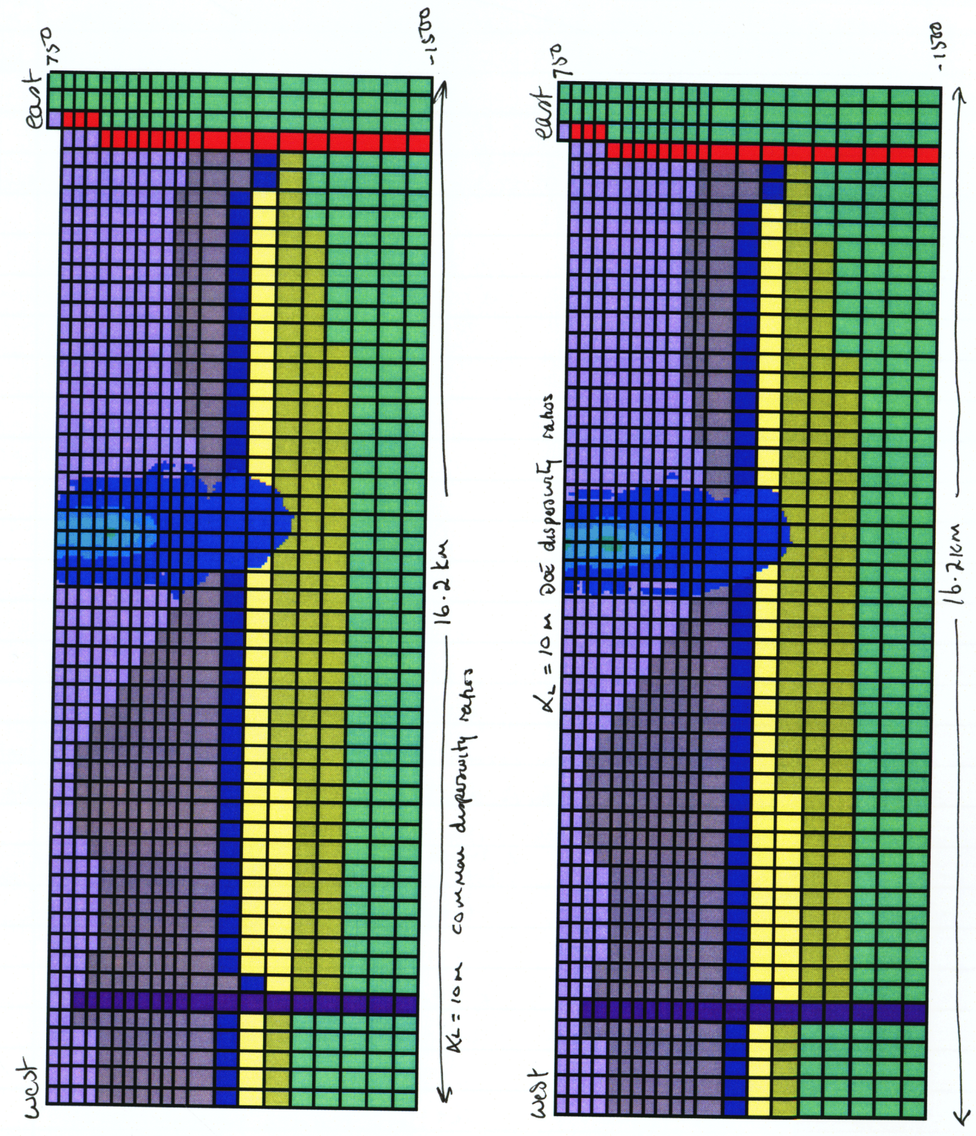
Figure 11: Vertical Cross-sections Through Plumes at the Regulatory Compliance Boundary

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## Formation of Multiple Independent Plumes

Farrell et al. (2005) showed small plumes migrating from opposite ends of the repository would eventually ~~coalesce~~ converge prior to reaching the regulatory compliance boundary. The following simulations were performed to see if this is still the case under the flow field that results from a future wetter ~~flow~~ climate at Yucca Mountain. The scenario is described in Table 5.

Table 5: Description of Scenario for Multiple Independent Plumes Analysis

**Objective**
Determine whether small, widely spaced plumes can cross the regulatory compliance boundary

**Source model**
Two source cells, one located in the northern portion of the repository and the other located in the southern portion of the repository

**Model considerations**
- 10 mg/L constant concentration applied to all source cells
- Longitudinal dispersivity, $\alpha_L$ = 100, 10, and 1 m [330, 33, and 3.3 ft]
  - Commonly used transverse dispersivity ratios
    - horizontal transverse dispersivity ($\alpha_{TH}$) ratio: ($\alpha_L/\alpha_{TH}$) = 10
    - vertical transverse dispersivity ($\alpha_{TV}$) ratio: ($\alpha_L/\alpha_{TV}$) = 100
  - U.S. Department of Energy transverse dispersivity ratios
    - horizontal transverse dispersivity ($\alpha_{TH}$) ratio: ($\alpha_L/\alpha_{TH}$) = 200
    - vertical transverse dispersivity ($\alpha_{TV}$) ratio: ($\alpha_L/\alpha_{TV}$) = 20,000

Sources were placed at the northern and southern ends of the repository footprint. In addition sources were placed at the eastern and western edges of the repository. The various simulations are summarized in simulation models:

On accompanying CD

- East-West Sources - Disp - 1 (longitudinal dispersivity $\alpha_L$ = 1m ; common dispersivity ratios)
- East-West Sources - Disp - 10 ($\alpha_L$ = 10m ; common dispersivity ratios)
- East-West Sources - Disp - 100 ($\alpha_L$ = 100m ; common dispersivity ratios)
- East-West Sources - Disp - DOE-1 ($\alpha_L$ = 1m ; DOE dispersivity ratios)
- East-West Sources - Disp - DOE-10 ($\alpha_L$ = 10m ; DOE dispersivity ratios)
- East-West Sources - Disp - DOE-100 ($\alpha_L$ = 100m ; DOE dispersivity ratios)
- North-South Sources - Disp - 1 ($\alpha_L$ = 1m ; common dispersivity ratios)

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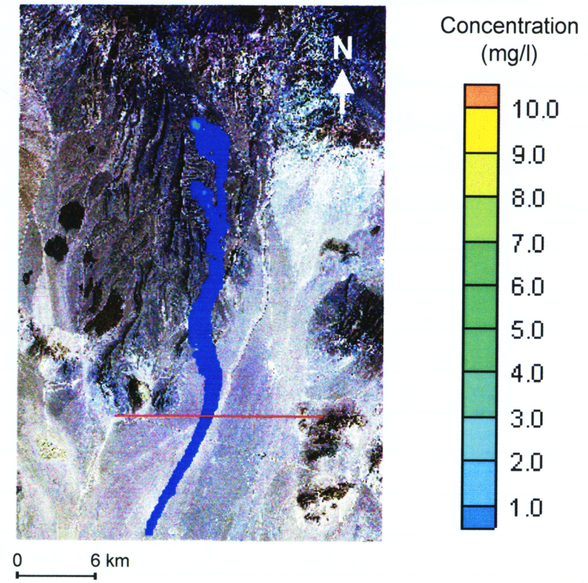
See simulation models on p. 28

Figure 12: North-South Simulation for $\alpha_L$ = 1m and Common Dispersivity ratios.




red line represents the compliance boundary

The simulation for North-South sources with $\alpha_L$ = 1m and DOE dispersivity ratios needs to be run for completeness but based on the results above and those in Farrell et al. (2005) it is very unlikely that ~~this~~ DAJ 8/12/06 such a simulation would result in results that are significantly different from those above.

Results show that plumes always converge prior to reaching the regulatory compliance boundary in Southern 40-mile Wash. This is mostly due to the convergent flow field in that part of the flow domain.

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