308 --- Q200610130003
Scientific Notebook No. 735: Calculation of Radionuclides in Groundwater (08/26/2005 through 10/09/2006)

LABORATORY NOTEBOOK

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NOTEBOOK NO. _____

CONTINUED FROM NOTEBOOK NO. _____ CONTINUED TO NOTEBOOK NO. _____

ASSIGNED TO:

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SIGNATURE David A. Farrell DATE 8/26/05

DATE ISSUED _____ BY _____

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NOTES:

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LABORATORY NOTEBOOK GUIDELINES†

LABORATORY NOTEBOOK INTRODUCTION

Using a Laboratory Notebook to record ideas, inventions, experimentation records, observations and all work details is a vital part of any laboratory process. Careful attention to how you keep your Laboratory Notebook can have a positive impact on the patent outcome of a pending discovery or invention.

Following are some overall recommendations to help you keep more efficient and accurate Laboratory Notebook entries. Remember, however, that these are simply a suggested set of guidelines. Only your attorney can supply the exact guidelines she would like you to follow to satisfy specific legal requirements. That is why we recommend that you consult your legal counsel.

RECORDING DATA

Your Laboratory Notebook is a vital record of your work whether it is for patent purposes, legal records or documenting drug research under FDA guidelines. The Laboratory Notebook can help you prove:

a. Exact details and dates of conception
b. Details and dates of reduction to practice
c. Diligence in reducing your invention to practice
d. Details regarding the structure and operation of your invention
e. Experimentation observations and results
f. A chronological record of your work
g. Other work details

Follow a few simple rules of thumb

1. Always record entries legibly, neatly and in permanent ink.
2. Immediately enter into your notebook and date all original concepts, data and observations, using separate headings to differentiate each.
3. Record all concepts, results, references and other information in a systematic and orderly manner. (Language, charts and numbering systems should be maintained consistently throughout.)
4. It is acceptable to make your entries brief. Always, however, include enough details for someone else to successfully duplicate the work you have recorded.
5. Label all figures and calculations.
6. Never, under any circumstances, remove pages from your notebook.

Remember to treat your Laboratory Notebook as a legal document: It records the chronological history of your activities. The following guidelines should help you maintain the consistent and accurate entries needed for future legal purposes.

1. Start entries at the top of the first page, and always make successive, dated entries, working your way to the bottom of the last page.
2. After completing a page, sign it before continuing to the next page.
3. Make sure that you record the date of each entry clearly and unambiguously.
4. Never let anyone other than yourself write in your Notebook (excluding witness signatures, discussed later).
5. Never leave blank spaces, and never erase or remove material you have added. Simply draw lines through any blank spaces at the same time you are making your entries.
6. Do not erase errors. Just draw a single line through any erroneous entry, then add your initials. Enter the correct entry nearby.
7. You can supplement your entries with supporting material (e.g., test-result printouts and other documentation). But you must permanently affix the material onto a page in its proper chronological location.
8. Never rely solely on any supplemental attachment. Always include your own entry describing the attachment and add any conclusions that you might draw from its substance.
9. Occasionally, secondary sources might be too large or inappropriate to attach directly to your notebook. In this case, you can add all secondary sources to an ancillary record maintained precisely for this purpose. However, always remember to write a description of these secondary sources, clearly and unambiguously, in your notebook.

DOCUMENTING PATENT ACTIVITIES

A primary purpose of a Laboratory Notebook is the support of documenting work that may be patentable. To support patent activities, it is necessary to provide clear, concise, chronological entries with specific dates. To rely on these dates, you must have at least one non-inventor corroborate that the events actually happened and that he or she understood your invention by signing and dating the "Disclosed to and Understood by" signature blocks.

Your Laboratory Notebook should help you document and prove:

1. *Conception Date*—The date that you knew your invention would solve the problem.
2. *Date of reduction to practice*—The moment that you made a working embodiment of your invention.
3. *Diligence in reducing your invention to practice*—Diligence refers to your intent and conscious effort to make a working embodiment. You are not required to rush, or even to take the most efficient development strategy. But your Notebook must include details relating to your diligent activities. These are dates and facts that show what activities you have conducted to reduce the invention to practice, and when such activities were conducted. Since you may still be diligent despite periods of not working on reducing your invention to practice, always remember to provide reasonable excuses for these periods of inactivity by supplying facts relating to why there was no activity during the period in question. (e.g., unavailability of test conditions or equipment).
4. *How to make and use your invention*—provide documentation details sufficient to teach a colleague how to make and use your invention.
5. *The best mode of practicing your invention*—document the best way to practice your invention.

A non-inventor colleague should corroborate each of these events/facts by signing the "Disclosed to and Understood by" on the relevant pages.

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1 **OBJECTIVES** — 8/26/05

2 This notebook documents work performed on project # 06002.01.282
3 Concentration of Radionuclides in Groundwater. In particular, the notebook
4 documents work performed to support the evaluation of potential plume sizes
5 that may occur at the 18km regulatory compliance boundary after 10,000 years
6 following a release from the repository. The simulations were performed using the
7 groundwater flow model for the region previously developed by J. Winterle, and
8 documented in Winterle et al. (2002) and Winterle (2003), and the MT3DMS
9 computer code. MT3DMS is a solute transport code capable of simulating
10 the transport of solutes that may be conservative or that are undergoing
11 radioactive decay and sorption. For the purposes of this work it is assumed
12 that solutes emanating from the location of the repository are conservative,
13 that is, the solutes do not undergo radioactive decay (D.A.T. 8/26/05) or sorption, or any other
14 form of chemical alteration. As a result, plumes simulated in the model will
15 ~~more than likely represent the~~ (D.A.T. 8/26/05) may over predict, in terms of size, plumes of radionuclide (D.A.T 8/26/05)
16 expected at the compliance boundary during the 10,000 year regulatory compliance
17 boundary. More representative plumes will be simulated in future work. The
18 models also ~~assume that~~ (D.A.T 8/26/05) consider transport only in the saturated zone.
19 Transport in the unsaturated zone is currently ignored. This notebook is
20 an extension of CNWRA Scientific Notebook 728E currently assigned to
21 V. Brieno Rankin. This notebook documents simulations performed by D. Farrell
22 that are not included in SN 728E. The simulations documented in this notebook
23 will be used to support the CNWRA deliverable 06002.01.282.531.
24
25
26 **Summary of the Solute Transport Model**
27 Solute transport modeling was performed using MT3DMS version 4.5 developed
28 by Zheng and Wang (1999). As noted the model represents solute transport
29 in the saturated zone. Solutes are assumed to be conservative. The simulation
30 grid used to support the simulation is similar to that used by Winterle et al. (2002) and
31 Winterle (2003), that is, $\Delta X = \Delta Y = 300$ m and ΔZ variable such that
32 $50\text{m} \leq \Delta Z \leq 200\text{m}$. At the watertable $\Delta Z = 50$ m and near the base of the

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model $\Delta z = 200$ m. Grid cells above the watertable were not considered in the numerical procedure. However, only a subset of the grid used for the MODFLOW simulations were used for the transport simulations. The region used for the transport simulations was focused on the region through which the plume was expected to migrate. This reduction in the size of the domain increased the computational efficiency of the simulations. Figure 1 shows a comparison between the computational flow and transport simulation grids. The two grids are readily displayed by clicking on the MODFLOW or MT3DMS tabs in GMS (D.AT 8/26/05) the Groundwater Modeling System (GMS v.5.1) (D.AT 8/26/05) graphical user interface. Note that GMS input files exist for all simulations prepared under this project. These are included on the CD's contained in this notebook and notebook 728E.

In this analysis, the repository footprint is projected to the watertable. Grid simulation cells within the repository footprint were considered potential source cells for the numerical simulation. Potential source cells are shown in Figure 2. Note that because the watertable slopes in the vicinity of the Yucca Mountain (D.AT. 8/26/05) ~~source~~ potential source cells are assigned over several layers of the model. (The potential D.AT. 8/26/05) Potential source concentrations in each cell was 10 mg/L.

Transport was simulated using MT3DMS version 4.5 (Zheng and Wang, 1999). The transport solution used was the HMOC ... Hybrid Method of Characteristics which combines the MOC (Method of Characteristics) with the MMOC (Modified Method of Characteristics). The HMOC formulation essentially draws on the relative advantages of each method to overcome their individual weaknesses. In particular, the HMOC method is described as being stable at extremely high grid peclet numbers and efficient in its ~~use of~~ (D.AT. 8/26/05) particle tracking scheme. More information on the HMOC method is contained in Zheng and Wang (1999 ... 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 ... prepared for the U.S. Army Corp of Engineers. ~~Note that the groun~~ (D.AT 8/26/05)

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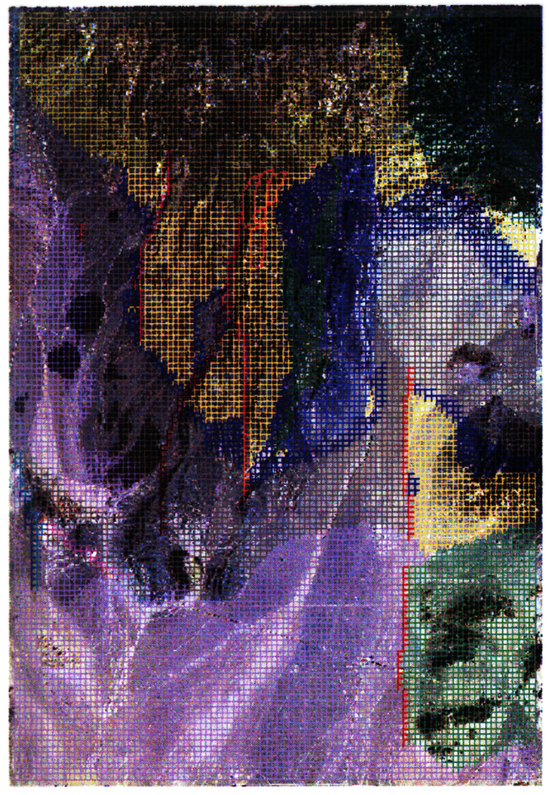

Flow simulation grid

Figure 1a

The groundwater velocities required to support the simulations were based on the steady-state groundwater model developed by Wilson et al. (2002) and Wilson (2003) for the region.

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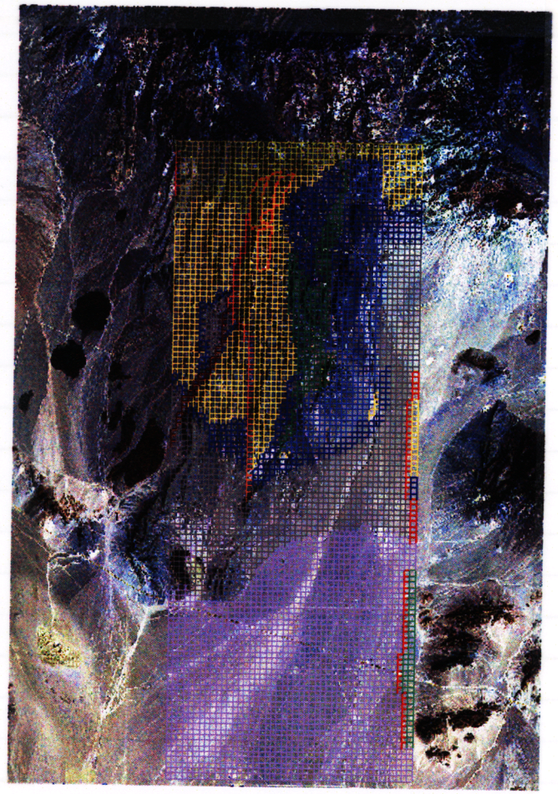

Transport simulation grid

Figure 1b

Winterle, J., "Evaluation of Alternative Concepts for Saturated Zone Flow: Effects of Recharge and Watertable Rise on Flow Paths and Travel Times at Yucca Mountain", CNWRA.2003

Winterle, J., M. Hill, and C. Manepally. "Concepts of Saturated Zone Modeling for Development of a Site-Scale Groundwater Flow Model for Yucca Mountain. CNWRA. 2002.

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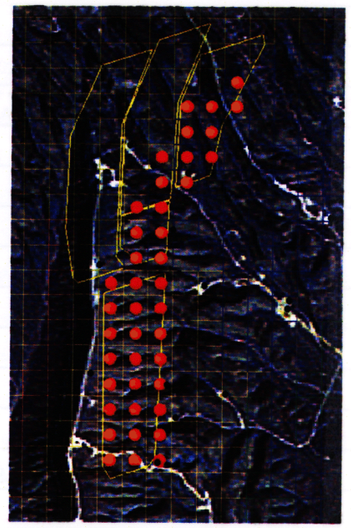
1 PAGE

Source cells in layer 3

Source cells in layer 4

Source cells in layer 5



Source cells in layer 6

Revised (D.A.T. 8/29/05)
Figure 2: Source cells in each layer of the model

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Summary of Simulations Contained in this Scientific Notebook

The following simulations are included in this scientific notebook. Note that molecular diffusion is not included in the current models.

→ S6-run2-modified_alt_rep_All_ps_disp300_10k.gpr
- simulation assumes tuff and alluvium both have a longitudinal dispersivity of 300 m
- $\alpha_L/\alpha_{TH} = 10$ $\alpha_L/\alpha_{TV} = 100$ } common dispersivity ratios
- all potential source locations within the repository footprint are active

→ S6-run2-modified_alt_rep_All_PS_DOE_disp300_10k.gpr
- Simulation assumes tuff and alluvium both have a longitudinal dispersivity of 300 m
- $\alpha_L/\alpha_{TH} = 200$ $\alpha_L/\alpha_{TV} = 20,000$ } DOE dispersivity ratios
- all potential source locations within the repository footprint are active

→ S6-run2-modified_alt_rep_All_PS_disp1_10k.gpr
- Simulations assume tuff and alluvium both have a longitudinal dispersivity of 1 m
- $\alpha_L/\alpha_{TH} = 10$ $\alpha_L/\alpha_{TV} = 100$ } common dispersivity ratios
- all potential source locations within the repository footprint are active

→ S6-run2-modified_alt_rep_All_PS_DOE_disp1_10k.gpr
- simulations assume tuff and alluvium both have a longitudinal dispersivity of 1 m
- $\alpha_L/\alpha_{TH} = 200$ $\alpha_L/\alpha_{TV} = 20,000$ } DOE dispersivity ratios
- all potential source locations within the repository footprint are active

S6-run2-modified_alt_rep_All_PS_disp150_10k.gpr
→ ~~S6-run2-modified_alt_rep_All_ps_disp150.gpr_10k~~ (D.AT. 8/24/05)
- Simulations assume tuff and alluvium both have a longitudinal dispersivity of 150 m
- $\alpha_L/\alpha_{TH} = \frac{10}{200}$ $\alpha_L/\alpha_{TV} = \frac{100}{20,000}$ (D.AT 8/26/05)
- all potential source locations within the repository footprint are active

→ S6-run2-modified_alt_rep_All_PS_DOE_disp150_10k.gpr
- Simulation assumes tuff and alluvium both have a longitudinal dispersivity of 150 m
- $\alpha_L/\alpha_{TH} = 200$ $\alpha_L/\alpha_{TV} = 20,000$
- all potential source locations (D.AT. 8/24/05) are active within the repository are active

→ S6-run2-modified_All_PS_alt_disp135_alluvium450_10k.gpr
- Simulation assumes tuff and alluvium have different longitudinal dispersivities
  $\alpha_{L\,tuff} = 135$ m $\alpha_{L\,alluv.} = 450$ m
- $\alpha_L/\alpha_{TH} = 10$ $\alpha_L/\alpha_{TV} = 100$
- all sources within the repository footprint are active

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→ S6-run2-modified_All_PS_alt_disp135_alluvium450_DOE_10k.gpr
- tuff and alluvium have differing longitudinal dispersivities: $\alpha_{L\,tuff} = 135$ m $\alpha_{L\,alluv.} = 450$ m
- $\alpha_L/\alpha_{TH} = 200$ $\alpha_L/\alpha_{TV} = 20,000$
- all sources are active.

→ S6-run2-modified_All_PS_alt_disp170_alluvium100_10k.gpr
- tuff dispersivity = 170 m alluvium dispersivity = 100 m
- $\alpha_L/\alpha_{TH} = \frac{200}{10}$ (D.AT. 8/25/05) $\alpha_L/\alpha_{TV} = \frac{20,000}{100}$ (D.AT. 8/24/05)
- all sources are active

→ S6-run2-modified_All_PS_alt_disp170_alluvium100_DOE_10k.gpr
- tuff and alluvium have differing dispersivities: $\alpha_{L\,tuff} = 170$ m $\alpha_{L\,alluv.} = 100$ m
- $\alpha_L/\alpha_{TH} = 200$ m $\alpha_L/\alpha_{TV} = 20,000$
- all sources are active

→ S6-run2-modified_All_PS_alt_disp150_alluvium275_10k.gpr
- tuff and alluvium have differing dispersivities: $\alpha_{L\,tuff} = 150$ m $\alpha_{L\,alluv.} = 275$ m
- $\alpha_L/\alpha_{TH} = 10$ $\alpha_L/\alpha_{TV} = 100$
- all sources are active

→ S6-run2-modified_All_PS_alt_disp150_alluvium275_DOE_10k.gpr
- tuff and alluvium have differing dispersivities: $\alpha_{L\,tuff} = 150$ m $\alpha_{L\,alluv.} = 275$ m
- $\alpha_L/\alpha_{TH} = 200$ $\alpha_L/\alpha_{TV} = 20,000$
- all sources are active

→ S6-run2-modified_alt_rep_west_PS_disp10_10k.gpr
- all materials have same dispersivity: $\alpha_L = 10$ m
- source located ~~to the~~ in the (D.AT. 8/26/05) western portion of the repository
- $\alpha_L/\alpha_{TH} = 10$ $\alpha_L/\alpha_{TV} = 100$

→ S6-run2-modified_alt_rep_west_PS_DOE_disp10_10k.gpr
- all materials have the same dispersivity: $\alpha_L = 10$ m
- $\alpha_L/\alpha_{TH} = 200$ $\alpha_L/\alpha_{TV} = 20,000$
- source located in the western portion of the repository (single source cell)

→ S6-run2-modified_alt_rep_west_PS_disp1_10k.gpr
- all materials have the same dispersivity $\alpha_L = 1$ m
- source located in the western portion of the repository (single source cell)
- $\alpha_L/\alpha_{TH} = 10$ $\alpha_L/\alpha_{TV} = 100$

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→ S6-run2-modified_alt_rep_west_PS_DOE_disp1_10k.gpr
- Tuff and alluvium have the same dispersivity: $\alpha_L = 1m$
- $\alpha_L/\alpha_{TH} = 200$ $\alpha_L/\alpha_{TV} = 20,000$
- Source located in the western portion of the repository

→ S6-run2-modified_alt_rep_east_west_ps_disp1_10k.gpr
- tuff and alluvium have the same dispersivity : $\alpha_L = 1m$
- $\alpha_L/\alpha_{TH} = 10$ $\alpha_L/\alpha_{TV} = 100$
- one source in the western portion of the repository, one source in the eastern portion of the repository

→ S6-run2-modified_alt_rep_east_west_PS_DOE_disp1_10k.gpr
- tuff and alluvium have the same dispersivity : $\alpha_L = 1m$
- $\alpha_L/\alpha_{TH} = 200$ $\alpha_L/\alpha_{TV} = 20,000$
- one source in the western portion of the repository, one source in the eastern portion of the repository

→

NOTE THAT ALL OF THE SIMULATIONS LISTED ABOVE ARE STORED ON:
BEMORE in folder d:\vrankin\GMS Data\Selected Point Sources\S6-run2_modified_repository

- files related to all point sources being ~~turned~~ D.A.F. 8/26/05 turned on during the simulation are stored in subfolder "ALL_PS"
- Similarly the ~~folder~~ D.A.F. 8/26/05 subfolder "East_PS" contains simulations based on a single point source in the eastern portion of the repository
- subfolder "West_PS" contains simulations based on a single point source in the western portion of the repository
- subfolder "north_PS" contains simulations based on a single point source in the northern portion of the repository
- subfolder "south_PS" contains simulations based on a single point source in the southern portion of the repository
- subfolder "east_west" contains simulations based on a single point source in the eastern and western portions of the repository
- subfolder "north_south" contains simulations based on a single point source in the northern and southern portions of the repository.

Accuracy of the simulations was not addressed in Scientific Notebook 728E. This subject is briefly discussed here. The matrix solution solution package used is the "GCG" package under MT3DMS version 4.5

... max # of outer iterations = 25
... max # of inner iterations = 50
... Preconditioner = Modified Incomplete Choleski
... Dispersion tensor = ~~lumped~~ (D.A.F. 8/26/05) lump all cross terms to RHS
... convergence criterion = 1×10^{-3}

The convergence criterion requires further discussion. Initially a convergence criterion of 1×10^{-6} was selected. However, this increased the computational effort as several iterations were required at each time step. To reduce this computational effort a more relaxed convergence criterion was selected (1×10^{-3}). The 1×10^{-3} criterio is lower than the 1×10^{-2} concentration that is used to delineate the boundary of the plume. With this said, it should be noted that the results of the simulations should be viewed in a relative sense as opposed to an absolute sense due to the somewhat relaxed convergence criterion. Future work, will consider using a more restrictive convergence criterion. However, given the uncertainties and assumptions inherent in the model it is not yet clear whether the greater accuracy is meaningful with respect to ~~true~~ real (D.A.F. 8/6/05) plumes that may evolve at the site.

8/30/05

The model was based on present day conditions. Future work should ~~evaluate~~ D.A.F. (8/30/05) evaluate plume sizes under future climatic conditions. For each plume simulated several parameters were determined including the cross-sectional dimensions of the plume at the regulatory compliance boundary and the annual groundwater flux through the plume. These are summarized in the following tables.

Table 1

Plume Parameters at the Compliance Boundary (ALL SOURCES TURNED ON)

	Long. (α_L) Disp (m)	Horz. Disp. Ratio	Vert. Disp. Ratio	Width (max) (m)	Depth (max) (m)	Flow (m^3/yr)	Flow (acre-ft/yr)
COM	300	$\alpha_L/10$	$\alpha_L/100$	4650	1150	1,739,772.5	1410.4
DOE	300	$\alpha_L/200$	$\alpha_L/20,000$	2450	900	919,253	745.2
COM	100	$\alpha_L/10$	$\alpha_L/100$	3150	940	1,378,960	1118
DOE	100	$\alpha_L/200$	$\alpha_L/20,000$	2250	860	923,793*	749
COM	10	$\alpha_L/10$	$\alpha_L/100$	2200	875	923,793*	749
DOE	10	$\alpha_L/200$	$\alpha_L/20,000$	2000	810	923,793*	749
COM	1	$\alpha_L/10$	$\alpha_L/100$	1800	750	671,965#	545
DOE	1	$\alpha_L/200$	$\alpha_L/20,000$	1800	750	671,965#	545

COM = Commonly used dispersivity ratios

DOE = DOE based dispersivity ratios

depth = vertical thickness

* = approximated due to minor differences in overall size

= approximated.

Table 2

Plume Parameters at the Compliance Boundary (north & south sources)

	Long. (α_L) Disp. (m)	Horz. Disp. Ratio	Vert. Disp. Ratio	Width (max) (m)	Depth (max) (m)	Flow (m^3/yr)	Flow (acre-ft/yr)
COM	100	$\alpha_L/10$	$\alpha_L/100$	2200	800	923,778	749
DOE	100	$\alpha_L/200$	$\alpha_L/20,000$	1850	500	715,451	580
COM	10	$\alpha_L/10$	$\alpha_L/100$	1700	500	715,451	580
DOE	10	$\alpha_L/200$	$\alpha_L/20,000$	1750	460	715,451	580
COM	1	$\alpha_L/10$	$\alpha_L/100$	1500	450	393,433	318
DOE	1	$\alpha_L/200$	$\alpha_L/20,000$	1500	450	393,433	318

(D.AT 8/30/05) See symbols for * & † Table 1

depth = vertical thickness

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Table 3

Plume Parameters at the Compliance Boundary (East & West Sources)

	Long. (α_L) Disp (m)	Horz. Disp. Ratio	Vert. Disp. Ratio	Width (max) (m)	Depth (max) (m)	Flow (m^3/yr)	Flow (acre-ft/yr)
COM	100	$\alpha_L/10$	$\alpha_L/100$	(D.AT 8/30/05) 678 1800	675	687,876	558
DOE	100	$\alpha_L/200$	$\alpha_L/20,000$	(D.AT 8/30/05) ~~525~~ 1350	525	658,647	534
						~~5~~ (D.AT 8/30/05)	
COM	10	$\alpha_L/10$	$\alpha_L/100$	(D.AT 8/30/05) ~~500~~ 1075	500	508,785	412.5
DOE	10	$\alpha_L/200$	$\alpha_L/20,000$	(D.AT 8/30/05) ~~480~~ 1150	480	508,785	412.5
COM	1	$\alpha_L/10$	$\alpha_L/100$	(D.AT 8/30/05) ~~450~~ 900	450	281,415	228.1
DOE	1	$\alpha_L/200$	$\alpha_L/20,000$	(D.AT 8/30/05) ~~450~~ 900	450	303,680	246.2

depth = vertical thickness

Table 4 Plume Parameters at Compliance Boundary (west source)

	Long. (α_L) Disp (m)	Horz. Disp. Ratio	Vert. Disp. Ratio	Width (max) (m)	Depth (max) (m)	Flow (m^3/yr)	Flow (acre-ft/yr)
COM	100	$\alpha_L/10$	$\alpha_L/100$	1350	525	397,741	322.4
DOE	100	$\alpha_L/200$	$\alpha_L/20,000$	1200	525	338,464	274.4
COM	10	$\alpha_L/10$	$\alpha_L/100$	1000	450	271,670	220.2
DOE	10	$\alpha_L/200$	$\alpha_L/20,000$	1000	450	271,670	220.2
COM	1	$\alpha_L/10$	$\alpha_L/100$	900	425	205093	166.3
DOE	1	$\alpha_L/200$	$\alpha_L/20,000$	900	425	205093	166.3

depth = vertical thickness

D.AT 8/30/05

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Table 5

Plume Parameters at the Compliance Boundary

(all sources turned on; different longitudinal dispersivities used for the tuff and alluvium ... ~~parameter based~~ dispersivities based on TPA code version 5.0)

	Long. (K) Disp. (m)	Horz. Disp. (m)	Vert. Disp. (m)	Width (max) (m)	depth (max) (m)	Flow (m³/yr)	Flow (acre-ft/yr)
CCM	$\alpha_{L,TUFF}$ = 170 $\alpha_{L,alluv}$ = 100	$\alpha_L/10$	$\alpha_L/200$	3300	1025	1,233,299	1000
DOE	"	$\alpha_L/200$	$\alpha_L/20,000$	2000	900	827,199	670.6
CCM	$\alpha_{L,TUFF}$ = 135 $\alpha_{L,alluv}$ = 450	$\alpha_L/10$	$\alpha_L/100$	4500	940	1,650,768	1338.4
DOE	"	$\alpha_L/200$	$\alpha_L/20,000$	2400	900	910,055	737.8

D.AF 8/30/05 Corr DOE

- first model assumes a travel distance in the tuff of approximately 17 Km and a travel distance in the alluvium of approximately ~~from~~ 1.0 Km (D.AF 8/30/05)

- second model assumes a travel distance of 13.5 Km in the tuff and approximately 4.5 Km in the alluvium.

Assumptions Implicit in Modeling

① constant concentration source.

- Assumes a constant mass flux arriving at the watertable
- mass well mixed in source cells
- constant mass flux at the watertable assumes that ~~in each grid cell~~ (D.AF 8/30/05) waste packages in the footprint of each grid release mass (D.AF 8/30/05) ~~limit~~ at a rate that when combined with the groundwater flux produces a constant mass flux at the watertable. Hence all of the waste packages are not required to release mass simultaneously

② Molecular diffusion is currently ignored as it is small compared to hydrodynamic dispersion.

Figures in the Report

Figures contained in the report are contain in the CD attached to the scientific notebook. The figures can also be reconstructed using the file:

Computer: Bemore

folder: d:\vrankin\GMS data\

8/27/05

The following summarizes some statistics from the simulations performed in CNWRA SN 727E. ~~The Comparisons of analytic~~ 8/27/05 The calculations of RMS error between the analytical and numerical solutions were performed by A. Sun.

Test 1 : computed RMS error = 0.00282

Test 2 : " " " = 0.0310

Test 3 : " " " = 0.0195

Test 4 : 4 source model → RMS error = 0.0491

9 source model → RMS error = 0.0147

16 source model → RMS error = 0.009

computed by D. Farrell

Test 6 : MOC comparison → RMS error = 0.015
Ultimate comparison → RMS error = 0.018
Upstream FD → RMS error = 0.027

} data used is contained in A. Boseman's folder in the file: "advection package comparison.xls"

see d:\mt3d\advection package comparison-rms-error.xls or MEDUSA for an example calculation.

Tests : MOC comparison → RMS error = very small less than 0.01
Ultimate comparison → RMS error = 0.058
Upstream FD → RMS error = 0.107

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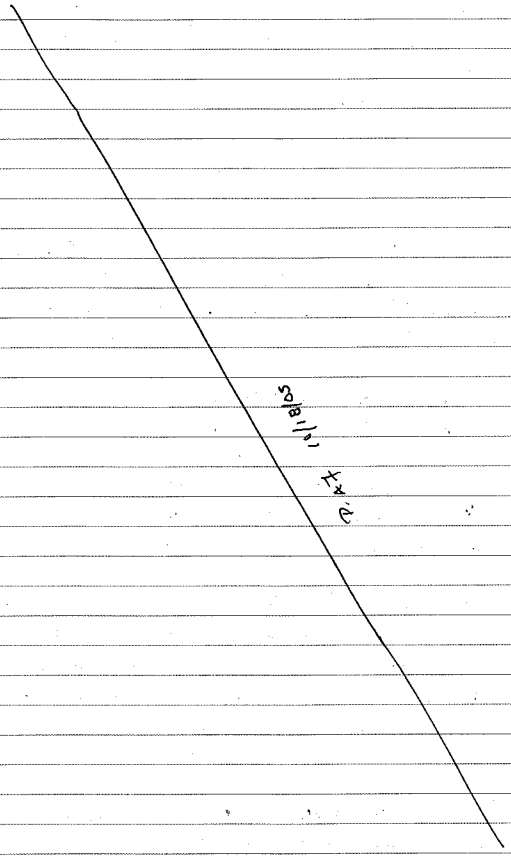
D.A7 10/18/05



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11 PAGE

D.A7 10/18/05

Initial preparation for simulating radioactive solutes in MT3DMS 4.5. As a start technecium (D.A7 10/18/05) transport will be simulated. Other radionuclides will be simulated later

Tc^{99} half life = 211,100 years = 77,051500 days

∴ the rate constant for Tc^{99} as defined by MT3DMS 4.5 is

$$\lambda_{Tc} = \frac{\ln 2}{t_{1/2}} = \frac{\ln 2}{77051500} = 8.99589 \times 10^{-9} \text{ days}^{-1}$$

EPA estimate for half life of Tc^{99} = 212,000 years = ~~8.9577 x10⁻⁹ days⁻¹~~ (D.A7 10/18/05)

= 77380000 days

$$\lambda_{Tc} = \frac{\ln 2}{t_{1/2}} = \frac{\ln 2}{77380000} = 8.9577 \times 10^{-9} \text{ days}^{-1}$$

For iodine I^{129}

I^{-129} half life = 15.7×10^6 years = 5.7305×10^9 days

$$\lambda_I = \frac{\ln 2}{t_{1/2}} = \frac{\ln 2}{5.7305 \times 10^9} = 1.2096 \times 10^{-10}$$

Impact of decay on source concentration of Tc^{99} ... over 10,000 yr period

$C = C_0 e^{-\lambda t}$

assume $C_0 = 10$

then after 10,000 yrs $C = 10\, e^{-(8.9577 \times 10^{-9})t}$

Using EPA estimate (D.A7 10/18/05) to calculate λ

$C = 10\, e^{-(8.9577 \times 10^{-9}) \times 3650000} = 9.68$

∴ ΔC over 10,000 yr time period = 10 − 9.68 = 0.32

or 3.2% change in concentration

∴ for 10,000 year simulations use of a constant source concentration is ok.

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Over 1,000,000 years

$C = 10\, e^{-(8.9577 \times 10^{-9}) \times 365 \times 10^6} = 0.38$

therefore variable source concentration source must be used in simulations for 1,000,000 years. D.AT 10/18/05

ΔC over 1,000,000 years $= 10 - 0.38 = 9.62$

percent change = 96.2

Impact of decay on source concentration of I^{129}

1,000,000 yr time frame

$C = 10\, e^{-(1.209 \times 10^{-10}) \times 365 \times 10^6} = 9.568$

$\therefore \Delta C = 10 - 9.568 = 0.432$

$\approx 4\%$ of the source concentration ... hence using a constant source concentration to simulate I^{129} source concentration over 1,000,000 yrs should be reasonable.

(DAT 2/2/06)

Analysis of Source Decay on the Evolution of Radionuclide Solute Plumes

The aim of this analysis is to evaluate radionuclide plume evolution when the source strength is decaying [i.e., the source concentration is a function of time $C_0(t) = C_0' e^{-\lambda t}$, where $C_0' = C_0(t=0)$]. It is expected that this condition will be observed at the Yucca Mtn site if the half life of the radionuclide solute is much smaller than the period of performance.

To explore (D.AT 2/2/06) examine this phenomenon, two dimensional models were constructed and simulations were performed using (DAT 2/2/06) the modified codes based on (D.AT 2/2/06) the TDAST.for (Groundwater Transport: Handbook of Mathematical Models by Javandel, Doughty and Tsang ... published by American Geophysical Union – Water Resources Monograph 10). Note that the code listing is given on p.161 of the referenced book. A slightly modified version of the code with a number of the format statements removed is presented in the following (also note that the function DOIBAF in Subroutine conc has been replaced with the

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function A@NG distributed with the Lahey95 compiler. D01BAF is distributed as part of the NAG Library [Numerical Algorithms Group (NAG), 1981].

d:\tdaot\tdast-1.for

```
      PROGRAM TDAST_DAF
c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c     This program evaluates the two dimensional analytical solute    c
c     transport solution considering convection, dispersion, decay,   c
c     and adsorption.                                                 c
c                                                                     c
c  Source: Appendix D, Groundwater Transport                          c
c          Handbook of Mathematical Models                            c
c          Javendel, Doughty, and Tsang                               c
c                                                                     c
c  Modified by: David Farrell                                         c
c               CNWRA, SwRI                                           c
c               6220 Culebra Rd                                       c
c               San Antonio                                           c
c               TX 78238                                              c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

Information potentially subject to copyright protection was redacted from this location. The redacted material is from the code listed above.

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Information potentially subject to copyright protection was redacted from this location. The redacted material is from the code listed on page 13 of this scientific notebook.

Compile command:
lf95 tdast-1.for -lib "c:\program files\lf9556\lib\ssl2.lib"

D.AT
2/2/06

The installation test case file is given in "d:\tdast\infile.dat". Note that the parameters in this file are identical to the parameters on p.134 (Appendix C... Groundwater Transport: Handbook of Mathematical Models). A listing of "infile.dat" is as follows:

```
16 12 1 1        NUMX, NUMY, NUMT, NNS
10.0 15.0 20.0 25.0 30.0 35.0 40.0 45.0 50.0 60.0 75.0 100.0 125.0 150.0 175.0 200.0   X(i)
0.0   5.0 10.0 20.0 30.0 40.0 45.0 50.0 55.0 60.0 70.0 80.0   Y(i)
100.0   T(i)
1.0 0.1 0.1 50.0   DL, DT, V, A
1E-20 1.0 1E-20    ALAM, R, ALFA
1 NS(i)
```

The output file generated by TDAST-1. for based on infile.dat is contained in outfile.dat. This is summarized in the following listing (compare to the listing given on p.134 (Appendix C... Groundwater Transport: Handbook of Mathematical Models):

```
Simulation time =  100.0000000000000  days
0.100D+02  0.000D+00  0.714D+00
0.100D+02  0.500D+01  0.714D+00
0.100D+02  0.100D+02  0.714D+00
0.100D+02  0.200D+02  0.714D+00
0.100D+02  0.300D+02  0.714D+00
0.100D+02  0.400D+02  0.713D+00
0.100D+02  0.450D+02  0.685D+00
0.100D+02  0.500D+02  0.357D+00
0.100D+02  0.550D+02  0.291D-01
0.100D+02  0.600D+02  0.108D-02
0.100D+02  0.700D+02  0.100D-06
0.100D+02  0.800D+02  0.118D-12
0.150D+02  0.000D+00  0.535D+00
0.150D+02  0.500D+01  0.535D+00
0.150D+02  0.100D+02  0.535D+00
0.150D+02  0.200D+02  0.535D+00
0.150D+02  0.300D+02  0.535D+00
0.150D+02  0.400D+02  0.533D+00
0.150D+02  0.450D+02  0.502D+00
0.150D+02  0.500D+02  0.267D+00
0.150D+02  0.550D+02  0.325D-01
0.150D+02  0.600D+02  0.139D-02
0.150D+02  0.700D+02  0.137D-06
0.150D+02  0.800D+02  0.165D-12
0.200D+02  0.000D+00  0.365D+00
0.200D+02  0.500D+01  0.365D+00
0.200D+02  0.100D+02  0.365D+00
0.200D+02  0.200D+02  0.365D+00
0.200D+02  0.300D+02  0.365D+00
0.200D+02  0.400D+02  0.364D+00
0.200D+02  0.450D+02  0.337D+00
0.200D+02  0.500D+02  0.182D+00
0.200D+02  0.550D+02  0.280D-01
0.200D+02  0.600D+02  0.137D-02
0.200D+02  0.700D+02  0.146D-06
0.200D+02  0.800D+02  0.179D-12
0.250D+02  0.000D+00  0.226D+00
```

d:\tdast\outfile.dat

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```
0.250D+02  0.500D+01  0.226D+00
0.250D+02  0.100D+02  0.226D+00
0.250D+02  0.200D+02  0.226D+00
0.250D+02  0.300D+02  0.226D+00
0.250D+02  0.400D+02  0.225D+00
0.250D+02  0.450D+02  0.206D+00
0.250D+02  0.500D+02  0.113D+00
0.250D+02  0.550D+02  0.200D-01
0.250D+02  0.600D+02  0.110D-02
0.250D+02  0.700D+02  0.127D-06
0.250D+02  0.800D+02  0.160D-12
0.300D+02  0.000D+00  0.126D+00
0.300D+02  0.500D+01  0.126D+00
0.300D+02  0.100D+02  0.126D+00
0.300D+02  0.200D+02  0.126D+00
0.300D+02  0.300D+02  0.126D+00
0.300D+02  0.400D+02  0.125D+00
0.300D+02  0.450D+02  0.113D+00
0.300D+02  0.500D+02  0.628D-01
0.300D+02  0.550D+02  0.123D-01
0.300D+02  0.600D+02  0.740D-03
0.300D+02  0.700D+02  0.932D-07
0.300D+02  0.800D+02  0.120D-12
0.350D+02  0.000D+00  0.628D-01
0.350D+02  0.500D+01  0.628D-01
0.350D+02  0.100D+02  0.628D-01
0.350D+02  0.200D+02  0.628D-01
0.350D+02  0.300D+02  0.628D-01
0.350D+02  0.400D+02  0.623D-01
0.350D+02  0.450D+02  0.562D-01
0.350D+02  0.500D+02  0.314D-01
0.350D+02  0.550D+02  0.654D-02
0.350D+02  0.600D+02  0.426D-03
0.350D+02  0.700D+02  0.583D-07
0.350D+02  0.800D+02  0.776D-13
0.400D+02  0.000D+00  0.281D-01
0.400D+02  0.500D+01  0.281D-01
0.400D+02  0.100D+02  0.281D-01
0.400D+02  0.200D+02  0.281D-01
0.400D+02  0.300D+02  0.281D-01
0.400D+02  0.400D+02  0.278D-01
0.400D+02  0.450D+02  0.250D-01
0.400D+02  0.500D+02  0.140D-01
0.400D+02  0.550D+02  0.306D-02
0.400D+02  0.600D+02  0.212D-03
0.400D+02  0.700D+02  0.314D-07
0.400D+02  0.800D+02  0.431D-13
0.450D+02  0.000D+00  0.112D-01
0.450D+02  0.500D+01  0.112D-01
0.450D+02  0.100D+02  0.112D-01
0.450D+02  0.200D+02  0.112D-01
0.450D+02  0.300D+02  0.112D-01
0.450D+02  0.400D+02  0.111D-01
0.450D+02  0.450D+02  0.993D-02
0.450D+02  0.500D+02  0.560D-02
0.450D+02  0.550D+02  0.126D-02
0.450D+02  0.600D+02  0.922D-04
0.450D+02  0.700D+02  0.146D-07
0.450D+02  0.800D+02  0.207D-13
0.500D+02  0.000D+00  0.398D-02
0.500D+02  0.500D+01  0.398D-02
0.500D+02  0.100D+02  0.398D-02
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0.500D+02  0.300D+02  0.398D-02
0.500D+02  0.400D+02  0.394D-02
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0.500D+02  0.500D+02  0.199D-02
0.500D+02  0.550D+02  0.461D-03
0.500D+02  0.600D+02  0.350D-04
0.500D+02  0.700D+02  0.591D-08
0.500D+02  0.800D+02  0.864D-14
0.600D+02  0.000D+00  0.353D-03
0.600D+02  0.500D+01  0.353D-03
0.600D+02  0.100D+02  0.353D-03
0.600D+02  0.200D+02  0.353D-03
0.600D+02  0.300D+02  0.353D-03
```

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0.600D+02	0.400D+02	0.350D-03
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0.600D+02	0.500D+02	0.177D-03
0.600D+02	0.550D+02	0.425D-04
0.600D+02	0.600D+02	0.342D-05
0.600D+02	0.700D+02	0.643D-09
0.600D+02	0.800D+02	0.999D-15
0.750D+02	0.000D+00	0.382D-05
0.750D+02	0.500D+01	0.382D-05
0.750D+02	0.100D+02	0.382D-05
0.750D+02	0.200D+02	0.382D-05
0.750D+02	0.300D+02	0.382D-05
0.750D+02	0.400D+02	0.378D-05
0.750D+02	0.450D+02	0.335D-05
0.750D+02	0.500D+02	0.191D-05
0.750D+02	0.550D+02	0.474D-06
0.750D+02	0.600D+02	0.404D-07
0.750D+02	0.700D+02	0.856D-11
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0.125D+03	0.700D+02	0.121D-20
0.125D+03	0.800D+02	0.249D-26
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0.150D+03	0.100D+02	0.397D-22
0.150D+03	0.200D+02	0.397D-22
0.150D+03	0.300D+02	0.397D-22
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0.175D+03	0.300D+02	0.188D-30
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0.175D+03	0.600D+02	0.232D-32
0.175D+03	0.700D+02	0.665D-36
0.175D+03	0.800D+02	0.157D-41
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0.200D+03	0.300D+02	0.419D-40
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0.200D+03	0.450D+02	0.364D-40
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0.200D+03	0.550D+02	0.550D-41
0.200D+03	0.600D+02	0.524D-42
0.200D+03	0.700D+02	0.155D-45
0.200D+03	0.800D+02	0.379D-51

↑ x ↑ y ↑ conc.

Illustration of the Behavior of the Concentration along the Center Line of A plume for the case where the Solute Undergoes Radionuclide Decay And the Strength of the Source Also Decreases Due to Decay: (input files for this problem are listed in:

d:\tdast\infile2.dat ⇒ $T_{1/2}$ = 2000 yrs

d:\tdast\infile3.dat ⇒ no decay

d:\tdast\infile4.dat ⇒ ~~$T_{1/2}$ = 2000 yrs~~ (D.AT 2/2/06) $T_{1/2}$ = 1000 yrs

d:\tdast\infile5.dat ⇒ $T_{1/2}$ = 4000 yrs

Output files for the simulations are summarized in

d:\tdast\outfile2.out

d:\tdast\outfile3.out

d:\tdast\outfile4.out

d:\tdast\outfile5.out

Note the groundwater velocity for this simulation is 0.0022 m/d

Figure 3 shows a plot of the results: (location is approximately 18.5 km downstream)

The figure shows that if the half life of the solute is much shorter than the period of performance ~~that~~ (D.AT 2/2/06) (ie, the simulation period) then a significant decrease in concentration can be expected. Note that a peak concentration is reached prior to the subsequent decline.

Figure 4 shows the case where the groundwater velocity is increased to 0.021 m/d... approximately ×10 in the previous case. Note the higher centerline concentrations in Figure 4 relative to Figure 3 reflect the earlier arrival times that result from the higher velocity.

input files for Figure 4

d:\tdast\upper bnd\infile2.dat ⇒ $T_{1/2}$ = 2000 yrs

d:\tdast\upper bnd\infile3.dat ⇒ $T_{1/2}$ = no decay

d:\tdast\upper bnd\infile4.dat ⇒ $T_{1/2}$ = 1000 yrs

d:\tdast\upper bnd\infile5.dat ⇒ $T_{1/2}$ = 4000 yrs

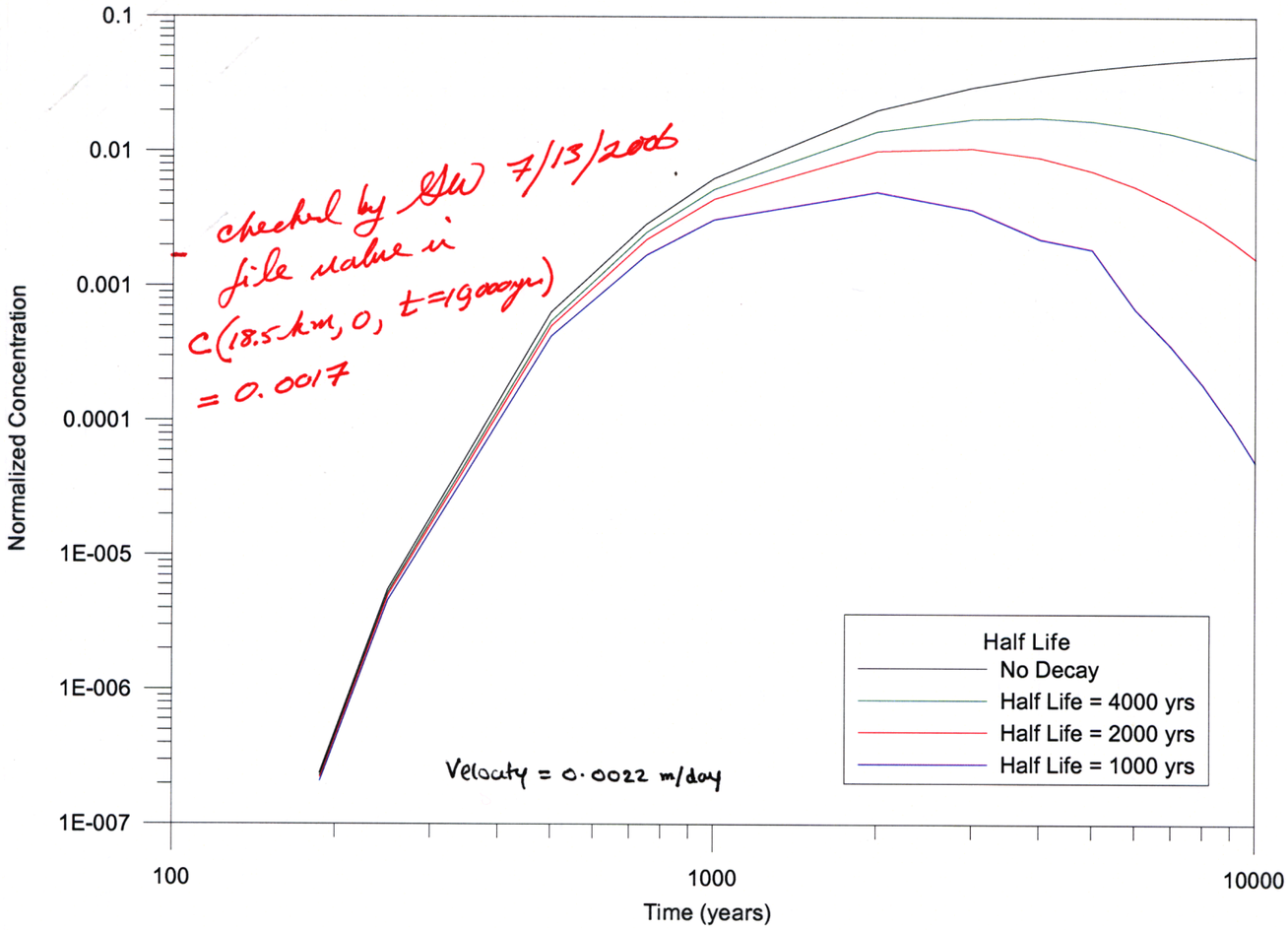

Figure 3: plume centerline concentration 18.5 km downstream

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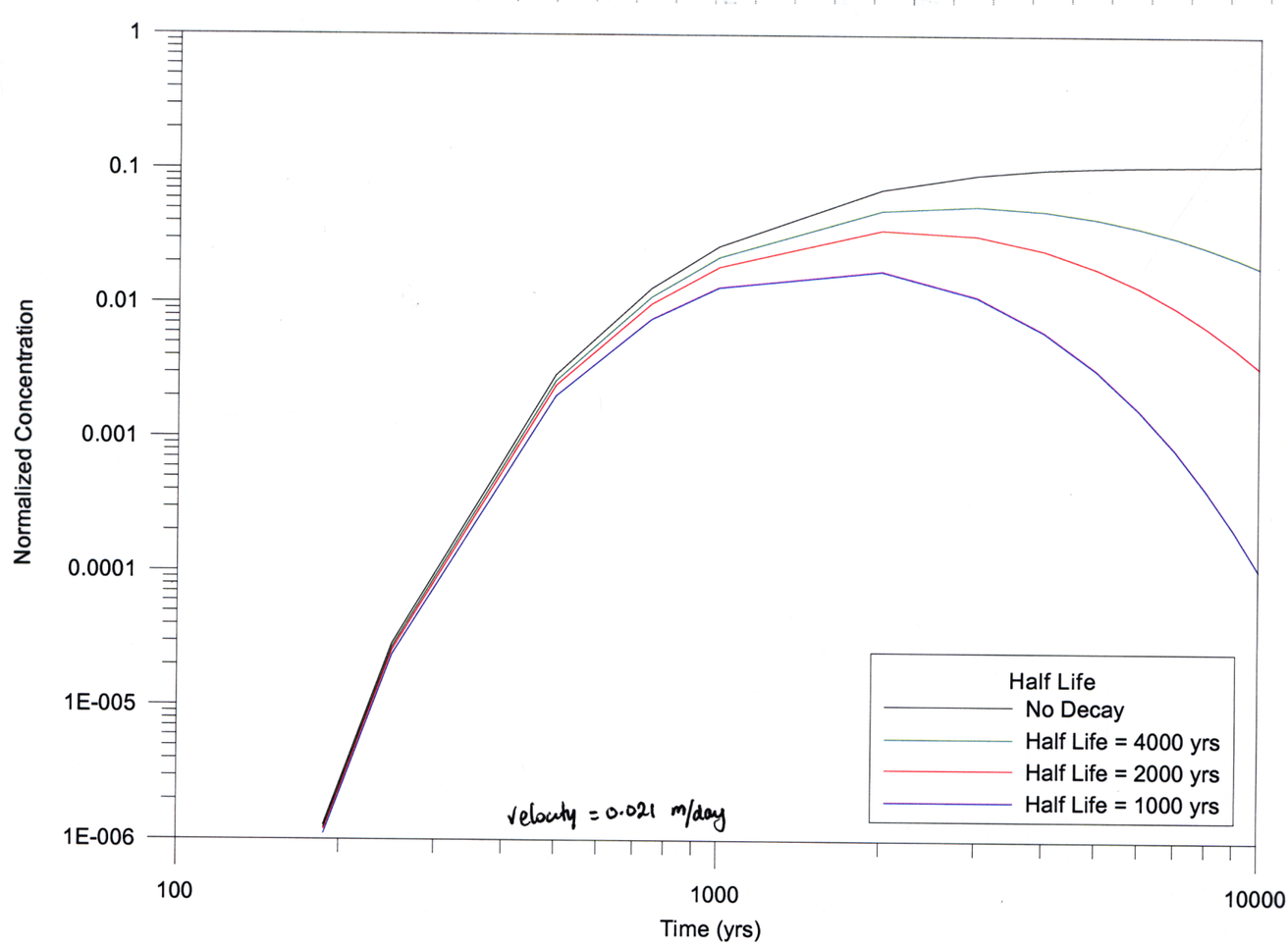

Figure 4: plume centerline concentration 18.5 km downstream

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Associated output files are :

d:\tdast\upper bnd\outfile2.out
d:\tdast\upper bnd\outfile3.out
d:\tdast\upper bnd\outfile4.out
d:\tdast\upper bnd\outfile5.out

D.AT 2/10/06

Comparison Of the Arrival times of Peak Plume Concentration and Peak Plume Width

The following examines whether the arrival times for the peak plume concentration along a plane downstream is in phase with the peak plume width along the plane; that is, whether the peak concentration arrives at the same time as the peak plume width. This can be important for evaluating/ review DOE approach for demonstrating compliance with applicable regulatory standards.

Input and output files for this analysis are located in d:\tdast\TC99. Note that the simulations were performed using the code Tdast-2.exe which is a variant of tdast-1.exe. The source code is d:\tdast\tdast-2.for

Figure 5 and 6 show that for the high velocity simulations that the peak concentration arrives at the plane earlier than the peak plume width.

Simulations to better understand this behavior were performed by Veronica Rankin Brieno using tdast-2.exe. The simulations are contained in :

d:\tdast\veronica\files1
d:\tdast\veronica\files2
d:\tdast\veronica\files3
d:\tdast\veronica\files4

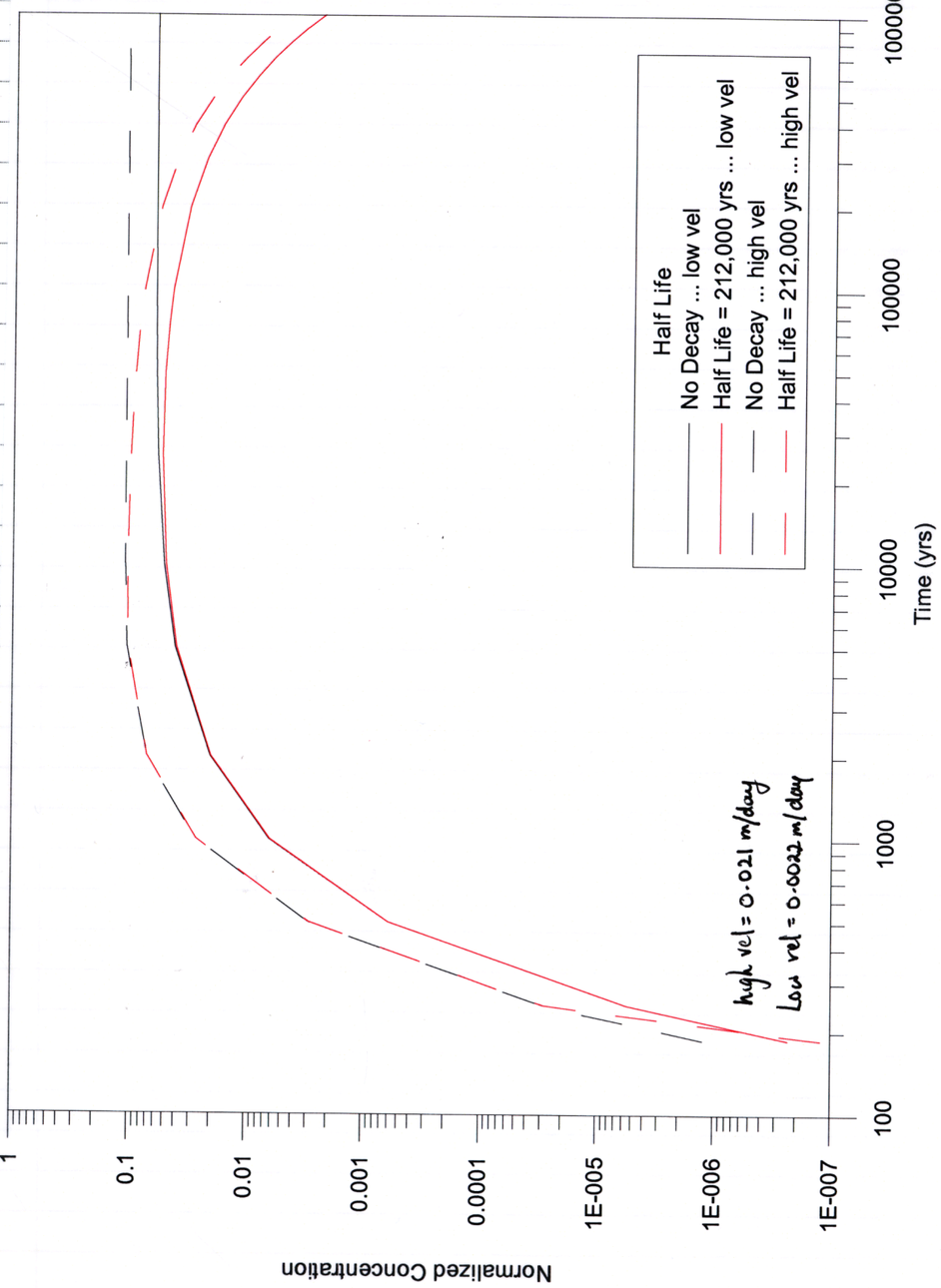

Figure 5: Centerline plume concentration at 18.5km downstream

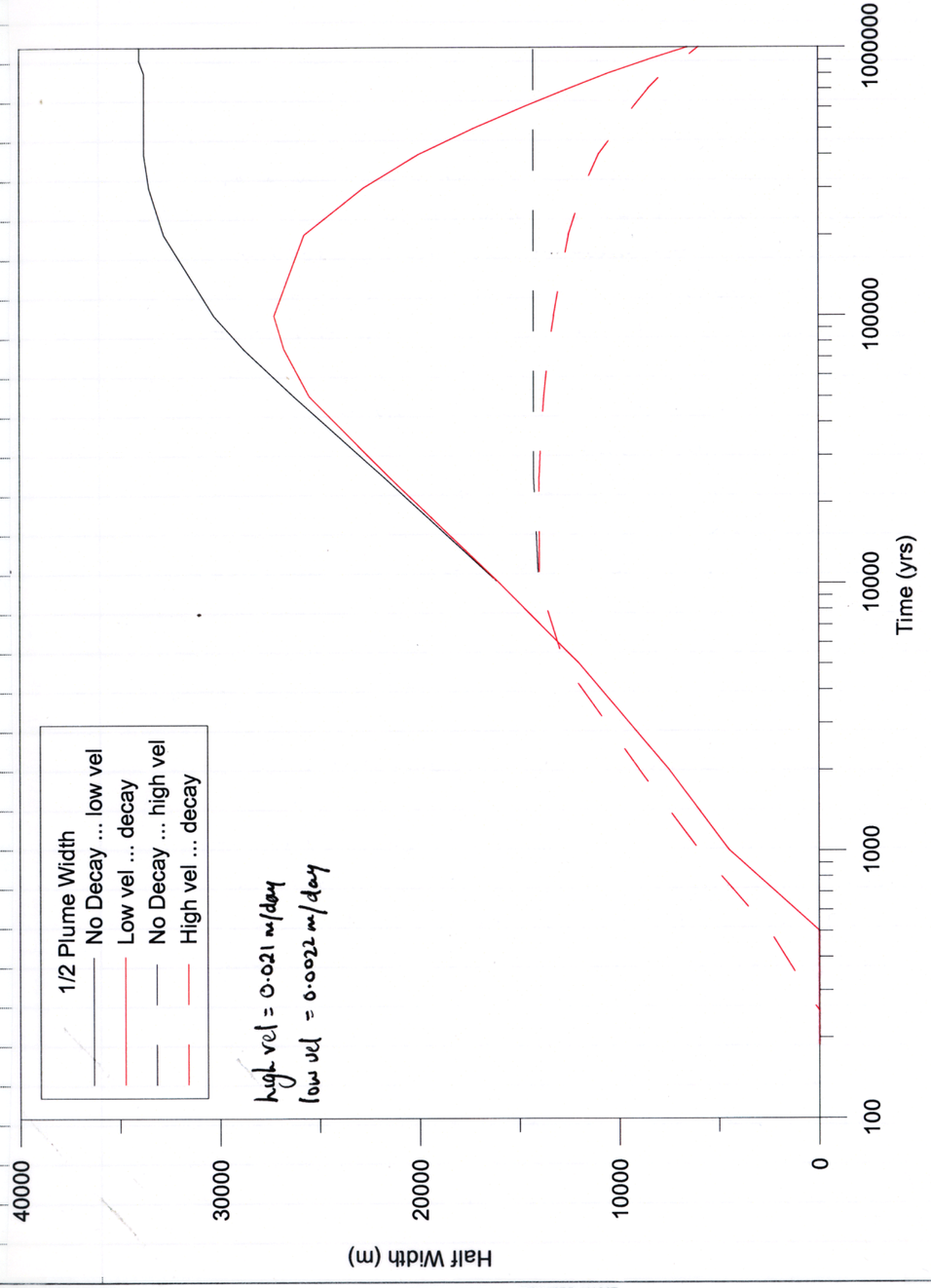

Figure 6: Plume half-width at 18.5 km downstream

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D.AT 2/15/06

Simulation of Solute Transport from YM Under Future Climates & Long Timeframes

The aim of this work is to extend the previous work on the simulation of radionuclide migration through the saturated zone to consider: (i) simulation times of 1,000,000 years; (ii) future climate; ~~and~~ (iii) radionuclide decay; and (iii) source strength decay. (D.AT 2/15/06) (D.AT 2/15/06) Initial runs runs using HHT3 the HMOC algorithm in MT3DMS version 4 (D.AT 2/15/06), with a simulation time of 1,000,000 years, indicated run times would be on the order of weeks if stability criteria were to be honored. Using the finite difference scheme in MT3DMS version 4 indicated that run times on the order of days to a week were achievable if stability criteria were violated. However, preliminary runs for 10,000 – 100,000 year time frames produced unacceptable levels of numerical diffusion which produced plume dimensions at the compliance boundary that were significantly larger than those previously documented in the 2005 report by Farrell et al. ~~EPA~~ (D.AT 2/15/06). To attempt to reduce run time (D.AT 2/15/06) ~~were est.~~ we are experimenting with particle tracking methods.

The SLIM code by Andy Thomson (developed originally at MIT and later at LLNL) is being evaluated due to its capabilities, previous CNWRA experience with the code (see Bagtzoglou et al.'s development and implementation of SUFLAT), and source code availability. Unlike the previous approaches briefly described above, excessive time stepping may not be a concern; however, the number of particles required to achieve a stable/acceptable solution may be a limitation for our application. Because SLIM does not compute the velocity field but rather relies on an imported velocity field several steps are required to implement SLIM for our application:

- the velocity field from Modflow need to be imported into SLIM
- the variable porosity field from Modflow needs to be imported into SLIM
- SLIM must be modified to handle a variable porosity field ... it was only designed for a single porosity
- the dispersion formulation in SLIM needs to be expanded to allow a more flexible form of the dispersion tensor that caters for the definition of dispersivity in the 3-component directions (i.e., α_L, α_{TH}, α_{TV}) ... the current formulation only accounts for α_L and α_T.

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Modifications to SLIM Computer Code

The modifications to the SLIM computer code were performed using a 3 stage approach. The following summarizes these stages.

- Implementation of the variable porosity model:

  The variable porosity model was implemented in SLIM3Z-por.for in \Slim-por. Note that ~~this version of the~~ original version of SLIM3.FOR was given to the Center by Andy Thomson (LLNL) the code's developer. Modifications ~~to~~ to the original code are documented in SLIM3Z-por.for. These modifications include: (D.Aff 4/14/06) (Superceded by SLIM3Z-por-update.for D.Aff 4/14/06)

  (i) adding a read statement to read in the new file containing the porosity data file — (D.Aff 4/14/06) these modifications to

  (a) input 1 (porosity no longer read when the dispersivity values are read)

  (b) (D.Aff 4/14/06) input main program

  (ii) adding statements to calculate the velocity based on the variable porosity file

  (iii) computing concentrations based on the variable porosity field.

  Note that to implement the variable porosity a preprocessor prestim.for was developed to read in the porosity data contained in the MT3DMS4 input files *.btn. Note that the portion of the *.btn file containing the porosity data must be copied and pasted into a new file before execution of prestim.for.

- Also implemented in SLIM3Z-por.for is an (DAff 4/14/06) modified additional source particle placement option. The new option is controlled by the parameter iplace read in from the input file rxn.1.dat. Under the new option particles remaining in the source cell after a time step are (D.Aff 4/14/06) ~~maintained~~ used in the next timestep. The alternative is to replace all particles remaining in the source cell

with new particles. The modifications made to support this option are in

- subroutine place
- ~~subroutine update~~ (D.Aff 4/14/06) subroutine book

- Implementation of the modified dispersivity framework:

  The original version of SLIM3.FOR only supported defining α_L and α_T and did not allow for independent treatment of α_{TH} and α_{TV} (ie, the dispersivities in the horizontal transverse and vertical transverse directions. (D.Aff 4/14/06) ~~This support~~ MT3DMS4 supports the latter formulation, and therefore maintain consistency with the previous work performed it is necessary that this formulation be implemented in (D.Aff 4/14/06) ~~MT3D~~ SLIM. The dispersion model in MT3DMS4 is based on Burnett and Frind (WRR 23(4) p. 695-705, 1987).

$$D_{xx} = \alpha_L \frac{V_x^2}{|V|} + \alpha_{TH} \frac{V_y^2}{|V|} + \alpha_{TV} \frac{V_z^2}{|V|} + D^*$$

$$D_{yy} = \alpha_L \frac{V_y^2}{|V|} + \alpha_{TH} \frac{V_x^2}{|V|} + \alpha_{TV} \frac{V_z^2}{|V|} + D^*$$

$$D_{zz} = \alpha_L \frac{V_z^2}{|V|} + \alpha_{TH} \frac{V_x^2}{|V|} + \alpha_{TV} \frac{V_y^2}{|V|} + D^*$$

$$D_{xy} = D_{yx} = (\alpha_L - \alpha_{TH}) \frac{V_x V_y}{|V|}$$

$$D_{xz} = D_{zx} = (\alpha_L - \alpha_{TV}) \frac{V_x V_z}{|V|}$$

$$D_{yz} = D_{zy} = (\alpha_L - \alpha_{TV}) \frac{V_y V_z}{|V|}$$

The modified formulation is implemented in:
- (D.A7 4/14/06) subroutine displa1
- subroutine displa2

note that to implement this model requires a change to subroutine input1 to read the dispersivity in the 3-component directions.

Note that the modified code \disperse\slim3z-por-disp.for accounts for these new changes as well as other previous changes.

The changes made to the software require testing for accuracy before use.

Post-processing

Concentration outputs from SLIM are stored in the binary file plotc.dat. To access this file use the program SLIM2TEC-3D.for. This program generates and (D.A7 4/14/06) x, y, z, conc file that can be loaded into TECPLOT for contouring and visualization.

To visualize particle locations open the file plotp.capture in a text editor and select the time period required. Note that the file has the following format

(D.A7 4/14/06)

time 1
x_1, y_1, z_1
x_2, y_2, z_2
⋮
x_n, y_n, z_n

time 2
x_1, y_1, z_1
⋮
x_n, y_n, z_n

D.A7 4/14/06

Simply copy the particle locations for the required time period, copy them into a new text file and save the file. The location file can be loaded into TECPLOT and viewed using the "scatter" option.

Additional Preprocessing Step

The GMS program generates a volumetric flow file from the MODFLOW (D.A7 4/14/06) output (D.A7 4/14/06) ~~[Qx (m³~~ [Q_x (L^3/t), Q_y (L^3/t), and Q_z (L^3/t)]. To compute DarcyFluxes ~~that~~ can be (D.A7 4/14/06) ~~implem~~ imported into SLIM the programs
\slim-por\calc-flux-slim-mod.for
~~was developed. The program reads Qx~~ (D.A7 4/14/06)
\slim-por\velocity interp.m

Velocity interp.m (matlab file) ⇒ developed by Alex Sun performs a bilinear interpolation on Q_x, Q_y, and Q_z as output from GMS. Because the grid spacing in the vertical direction on Winterle's YM groundwater flow model is irregular interpolation is required to produce Q_x', Q_y', and Q_z' on a regular grid.

calc-flux-slim-mod.for ⇒ reads the output from velocityinterp.m, computes the Darcy flux, and writes the output in a form and orientation that is consistent with SLIM.

No new entries will be made to this scientific notebook
David A. Farnell 4/14/06

This SN complies with QAP-001.
Gordon Wittmeyer 10/9/2006

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