CHEMFLUX™

2D / 3D Contaminant Transport Modeling Software

Verification Manual

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1 INTRODUCTION

The word “Verification”, when used in connection with computer software can be defined as “the ability of the computer code to provide a solution consistent with the physics defined by the governing partial differential equation, PDE”. There are also other factors such as initial conditions, boundary conditions, and control variables that also affect the accuracy of the code to perform as stated.

“Verification” is generally achieved by solving a series of so-called “benchmark” problems. “Benchmark” problems are problems for which there is a closed-form solution or for which the solution has become “reasonably certain” as a result of long-hand calculations that have been performed. Publication of the “benchmark” solutions in research journals or textbooks also lends credibility to the solution. There are also example problems that have been solved and published in User Manual documentation associated with other comparable software packages. While these are valuables checks to perform, it must be realized that it is possible that errors can be transferred from one’s software solution to another. Consequently, care must be taken in performing the “verification” process on a particular software package. It must also be remembered there is never such a thing as complete software verification for “all” possible problems. Rather, it is an ongoing process that establishes credibility with time.

SoilVision Systems takes the process of “verification” most seriously and has undertaken a wide range of steps to ensure that the CHEMFLUX software will perform as intended according to the theory of saturated-unsaturated contaminant transport.

The following models represent comparisons made to textbook solutions, hand calculations, and other software packages. We at SoilVision Systems Ltd. are dedicated to providing our clients with reliable and tested software. While the following list of example models is comprehensive, it does not reflect the entirety of models, which may be posed to the CHEMFLUX software. It is our recommendation that mass balance checking be performed on all model runs prior to presentation of results. It is also our recommendation that the modeling process move from simple to complex models with simpler models being verified through the use of hand calculations or simple spreadsheet calculations.

2 ONE-DIMENSIONAL TRANSPORT

This chapter will compare CHEMFLUX to other software packages and published solutions. The scope of this comparison will be one-dimensional contaminant transport in a uniform flow field. This chapter will also present each software packages ability to cope with inherent problems encountered when solving contaminant transport including artificial oscillation and numerical dispersion.

2.1 1D COUPLED SOLUTION

The purpose of the following examples is to test the fully coupled solutions in SVFLUX / CHEMFLUX against the textbook finite difference examples and closed form analytical solutions. The textbook solutions are presented by Fetter (1999).

A set of EXCEL spreadsheets, are available free from SoilVision Systems Ltd. (CONTAM.zip). These spreadsheets provide finite-difference and closed-form solutions to the contaminant transport processes. This verification example compares the results of a 1D CHEMFLUX model against the spreadsheet FDadvdis.xls. Three cases are considered:

Case 1: Diffusion Only
Case 2: Diffusion and Advection
Case 3: Diffusion, Advection, and Dispersion

The CONTAM.zip spreadsheet can be downloaded here.

Project: Columns
Model: FDDiffOnly, FDDiffAdv, FDDiffAdvDis

2.1.1 Model Description: Case 1 - Diffusion Only

In this model the process of diffusion is examined in isolation. A vertical model is set in stagnant flow conditions. A constant diffusion coefficient is used to allow reasonable diffusions rates. The spreadsheet values are then compared to the results of the CHEMFLUX analysis. This analysis is considered a stepping-stone analysis to the ore complicated coupled analysis.

Project: Columns
Model: FDDiffOnly

The following simulates the material properties, geometry and boundary conditions that are used for the setup of the numerical model.

Simulation time (t) = 946,707,780s (30 years)

- **Material Properties**

Groundwater seepage velocity (ν) = 0.2 mm/s

Case 1: Diffusion Only
Groundwater seepage velocity (n) = 0.00 m/s
Diffusion Constant (D^*) = 1.00E-11 m^2/s
Longitudinal Dispersivity = 0.00 m

- **Geometry/Boundary Conditions**
  The model is a 1D vertical column that is 0.4m deep. Nodes exist every 0.1m. A concentration of 1g/m^3 is specified on the top boundary. A Zero Flux (no flow) boundary is applied to the bottom.

2.1.2 Results and Discussions: Case 1

The following figure displays the comparison between CHEMFLUX and the finite-difference solution calculated in CONTAM.zip FDadvdis.xls for the diffusion only scenario. There is agreement between results.

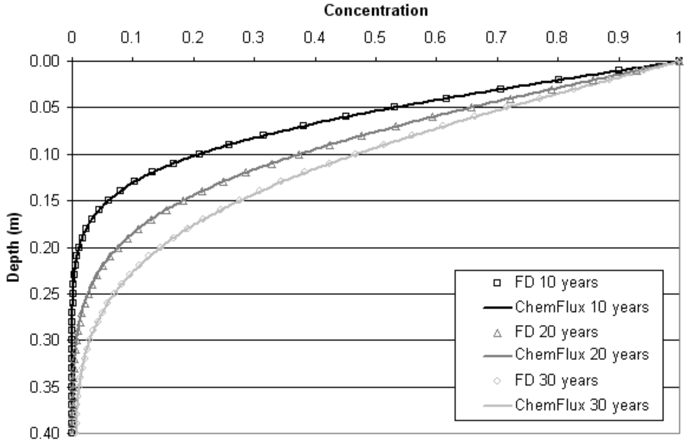

Figure 1 1D CHEMFLUX versus CONTAM.zip - Diffusion Only

2.1.3 Model Description: Case 2 - Diffusion and Advection

In this model the combined influences of diffusion and advection are compared between the spreadsheet and the SVOFFICE (CHEMFLUX) solution.

Project: Columns
Model: FDDiffAdv

The following simulates the material properties, geometry and boundary conditions that are used for the setup of the numerical model.

Simulation time (*t*) = 946,707,780s (30 years)

- **Material Properties**
  Groundwater seepage velocity (ν) = 0.2 mm/s

Case 2: Diffusion, Advection
Groundwater seepage velocity (n) = 2.00E-10 m/s
Diffusion Constant (D^*) = 5.00E-12 m^2/s
Longitudinal Dispersivity = 0.00 m

- **Geometry/Boundary Conditions**
  The model is a 1D vertical column that is 0.4m deep. Nodes exist every 0.1m. A concentration of $1g/m^3$ is specified on the top boundary. A Zero Flux (no flow) boundary is applied to the bottom.

2.1.4 Results and Discussions: Case 2

The following figure displays the comparison between CHEMFLUX and the finite-difference solution calculated in CONTAM.zip FDadvdis.xls for the diffusion and advection scenario. There is agreement between results.

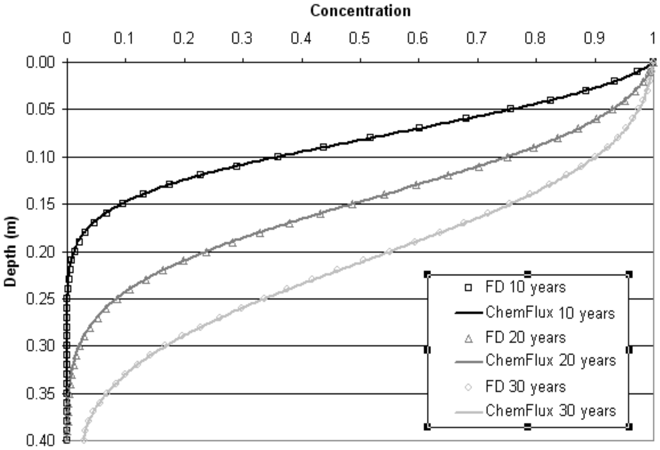

Figure 2 1D CHEMFLUX versus CONTAM.zip - Diffusion and Advection

2.1.5 Model Description: Case 3 - Diffusion, Advection and Dispersion

This model represents the increased complexity of including the processes of diffusion, advection and dispersion. The results between the spreadsheet and SVOFFICE (CHEMFLUX) are compared**.**

Project:	Columns
Model:	FDDiffAdvDis

The following simulates the material properties, geometry and boundary conditions that are used for the setup of the numerical model.

Simulation time (*t*) = 946,707,780s (30 years)

- **Material Properties**
  Groundwater seepage velocity (ν) = 0.2 mm/s

Case 3: Diffusion, Advection, Dispersion
Groundwater seepage velocity (*n*) = 2.00E-10 m/s
Diffusion Constant ($D*$) = 5.00E-14 m^2/s
Longitudinal Dispersivity = 0.01 m

- **Geometry/Boundary Conditions**
  The model is a 1D vertical column that is 0.4m deep. Nodes exist every 0.1m. A concentration of $1g/m^3$ is specified on the top boundary. A Zero Flux (no flow) boundary is applied to the bottom.

2.1.6 Results and Discussions: Case 3

The following figure displays the comparison between CHEMFLUX and the finite-difference solution calculated in CONTAM.zip FDadvdis.xls for the diffusion, advection, and dispersion scenario. There is agreement between results.

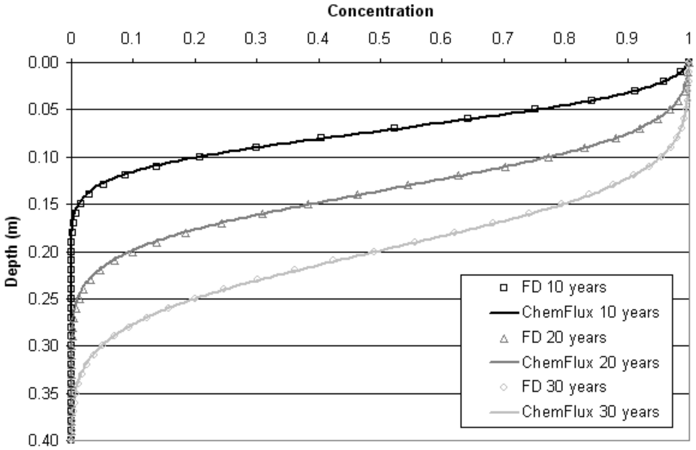

Figure 3 1D CHEMFLUX versus CONTAM.zip - Diffusion, Advection, and Dispersion

2.2 MT3DMS

A set of one-dimensional benchmark models are presented in the MT3DMS user documentation to test the ability of MT3DMS to model contaminant transport processes including advection, dispersion, adsorption, and decay with a uniform flow field. The MT3DMS code implements three mathematical methods to obtain accurate results to transport models dominated by one of the above processes. The mathematical methods include method of characteristics (MOC), modified method of characteristics (MMOC), and total-variation-diminishing (TVD) method. CHEMFLUX will be tested against the MT3DMS code to illustrate its ability to use the finite element (FEM) method, to give accurate results to the advection only transport model.

A classic and difficult model to solve with the fate and transport partial differential equations is the "advection only" model. In this model, diffusion is set equal to zero and the contaminant is carried by a water gradient only. A perfect theoretical solution is a step function. However, if this model is posed to many software packages the result is what looks like some dispersion results, but is actually the result of truncation errors. The purpose of this example is to evaluate the CHEMFLUX software in light of solving this difficult model.

The model is a simple rectangle that is 1000m long and 1m high. The seepage solution was prepared in SVFLUX. Constant head boundary conditions were chosen in SVFLUX to obtain the required groundwater seepage velocity. A concentration of $1g/m^3$ is specified along the left boundary; a concentration of $0g/m^3$ is specified along the right boundary, while a concentration gradient of zero is specified for the top and bottom boundaries of the rectangle.

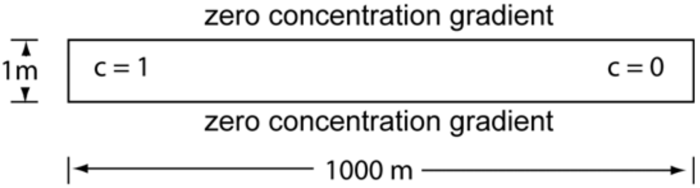

Figure 4

2.2.1 Model Description: Case 1a

In this example the CHEMFLUX model is tested against the TVD and FD methods implemented is MT3D.

Project: VerifyCHEMFLUX
Model: MT3DMS_Case1a

The material properties used for the model were as follows:

Groundwater seepage velocity (ν) = 0.24 m/day
Porosity (θ) = 0.25
Simulation time (t) = 2,000 days

Longitudinal Dispersivity, α = 0
Distribution Coefficient, (also K_d) R = 0
Dissolved Half-Life, λ = 0

Advection process is considered.

2.2.2 Results and Discussions: Case 1a

Case 1a is pure advection. CHEMFLUX is compared to the MT3DMS total-variation-diminishing (TVD) method. It should be noted that the method of characteristics (MOC) implemented in the MT3DMS model is free of numerical dispersion. However, the MOC technique can also lead to large mass balance discrepancies under certain situations because the discrete nature of the particle-tracking-based mixed Eulerian-Lagrangian solution techniques does not guarantee local mass conservation at a particular time-step (Zheng and Wang, 1999). Therefore, CHEMFLUX is compared to the third-order TVD method available in MT3DMS. This third-order ULTIMATE scheme is mass conservative, without excessive numerical dispersion, and essentially oscillation-free (Zheng and Wang, 1999). The ULTIMATE scheme was significantly superior to some popular second-order TVD schemes (Leonard, 1988) and was considered to be possibly the most accurate practical method available (Roache, 1992).

For advection-dominated models that exist under many field conditions, a Eulaerian method may be susceptible to excessive numerical dispersion or artificial oscillation. To overcome these models, restrictively small grid spacing and time-steps may be required (Zheng and Wang, 1999). CHEMFLUX utilizes both automatic mesh refinement and automatic time step refinement giving CHEMFLUX the power to overcome artificial oscillation and numerical dispersion. The above results show that CHEMFLUX is just as accurate as the TVD scheme and far surpasses the results of the upstream finite difference scheme.

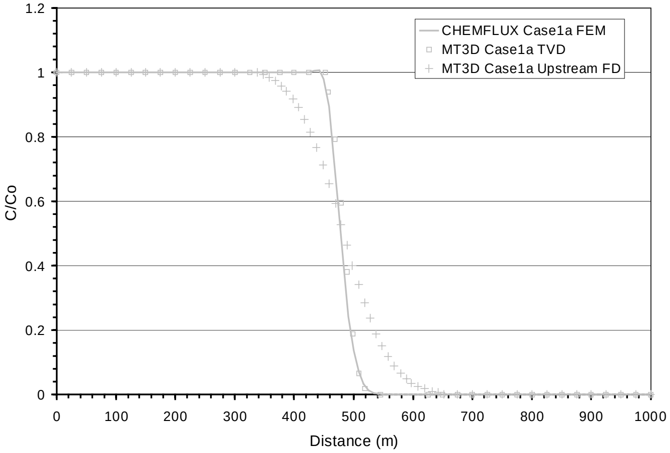

Figure 5 - CHEMFLUX versus MT3DMS for Case 1a

2.2.3 Model Description: Case 1b

In this example the results of MT3DMS are compared to CHEMFLUX. The model includes both advection and dispersion and therefore avoids the numerical difficulties associated with an "advection only" type problem.

Project:	VerifyCHEMFLUX
Model:	MT3DMS_Case1b

The material properties used for the model were as follows:

Groundwater seepage velocity (ν) = 0.24 m/day
Porosity (θ) = 0.25
Simulation time (*t*) = 2,000 days

Longitudinal Dispersivity, α = 10m
Distribution Coefficient, (also K_d) *R* = 0
Dissolved Half-Life, λ = 0

Advection and dispersion processes are considered.

2.2.4 Results and Discussions: Case 1b

Case 1b models the affects of advection and dispersion. In this case the front is no longer abrupt due to the inclusion of dispersion. For this case CHEMFLUX is compared to the MOC scheme, as the results from the TVD scheme were not available. The CHEMFLUX software matches the solution of the MOC scheme and provides added assurance that the solution is mass conservative. The results of this comparison between MT3D and CHEMFLUX may be seen in Figure 6.

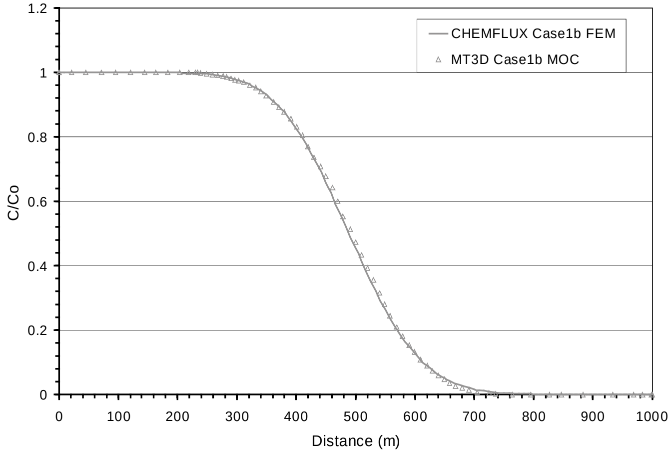

Figure 6 - CHEMFLUX versus MT3DMS for Case 1b

2.2.5 Model Description: Case 1c

This example model includes the effects of advection, dispersion and adsorption. The differences between MT3DMS and CHEMFLUX are compared.

Project:	VerifyCHEMFLUX
Model:	MT3DMS_Case1c

The material properties used for the model were as follows:

Groundwater seepage velocity (ν) = 0.24 m/day
Porosity (θ) = 0.25
Simulation time (t) = 2,000 days

Longitudinal Dispersivity, α = 10m
Distribution Coefficient, (also K_d) R = 5
Dissolved Half-Life, λ = 0

Advection, dispersion, and adsorption processes are considered.

2.2.6 Results and Discussions: Case 1c

Case 1c models the affect of advection, dispersion, and adsorption. In this case the front does not move as far as the pure advection case or the advection dispersion case due to chemical adsorbing to material particles. CHEMFLUX is compared to the modified method of characteristics (MMOC). This method is used only when the model will is not dominated by advection. The MMOC technique introduces considerable numerical dispersion, especially for sharp front models (Zheng and Wang, 1999). The MMOC technique is normally faster than the MOC technique, requires much less memory, and is also free of artificial oscillations. CHEMFLUX results are just as reliable as those obtained with the MMOC and also provide the same benefits over the MOC in time-savings, computer memory requirements, and numerical oscillations.

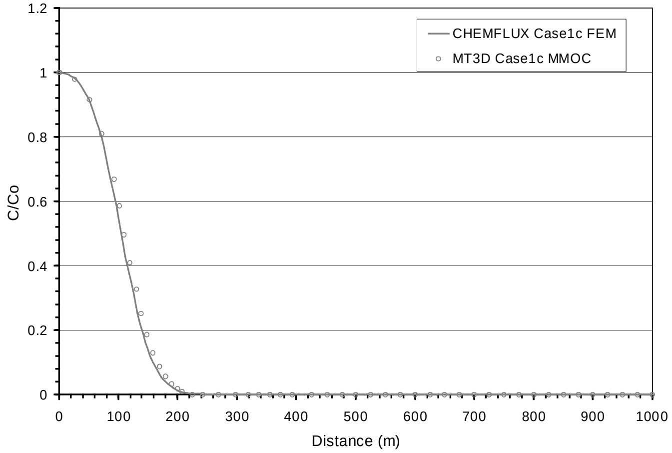

Figure 7 - CHEMFLUX versus MT3DMS for Case 1c

2.2.7 Model Description: Case 1d

This example further enhances the comparison in that the process of decay is included. Results between MT3DMS and CHEMFLUX are compared.

Project: VerifyCHEMFLUX
Model: MT3DMS_Case1d

The material properties used for the model were as follows:

Groundwater seepage velocity (ν) = 0.24 m/day
Porosity (θ) = 0.25
Simulation time (t) = 2,000 days

Longitudinal Dispersivity, α = 10m
Distribution Coefficient, (also K_d) R = 5
Dissolved Half-Life, λ = 0

Advection, dispersion, adsorption, and decay processes are considered.

2.2.8 Results and Discussions: Case 1d

Case 1d models the affect of advection, dispersion, adsorption, and decay. This case illustrates the affect decay has on the transport process causing the front to move even slower across the model. CHEMFLUX is again compared against the MMOC and it again provides the same reliable results.

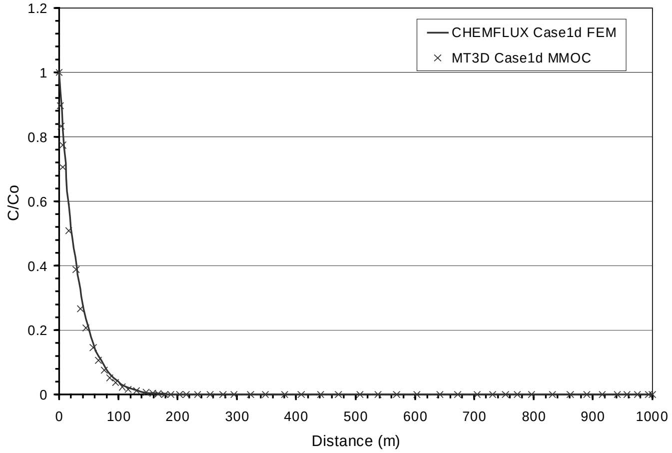

Figure 8 - CHEMFLUX versus MT3DMS

2.3 1D CTRAN/W

The following one-dimensional benchmark provides a comparison to the CTRAN/W software. The models presented will always include advection and dispersion with varying scenarios of adsorption and decay. CTRAN/W Solve cannot be used to analyze the advective component of contaminant transport in the absence of any dispersion (CTRAN/W user's guide 1991-2001), and as such does not provide any examples to test its abilities against those of CHEMFLUX to mitigate against such models as artificial oscillation or numerical dispersion.

The model is a simple rectangle that is 3m long and 0.1m high. The seepage solution was prepared in SVFLUX. Arbitrary constant head boundary conditions were chosen in SVFLUX to obtain the required groundwater seepage velocity. The CHEMFLUX model uses both the Dirichlet boundary condition and the Neuman boundary condition. The Dirichlet boundary condition specifies a concentration along a boundary for the duration of the solution, while the Neuman boundary condition specifies a concentration gradient. A concentration of 1g/m^3 is specified along the left boundary; a concentration of 0g/m^3 is specified along the right boundary, while a concentration gradient of zero is specified for the top and bottom boundaries of the rectangle.

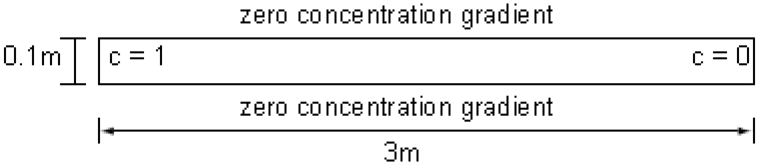

Figure 9

2.3.1 Model Description: Case 1

This model only compares the process of diffusion.

Project: VerifyCHEMFLUX
Model: CTranCase1

A description of the material properties, geometry, and boundary conditions used in the numerical model is as follows:

Groundwater seepage velocity (v) = 0.2 mm/s
Porosity (θ) = 0.5
Simulation time (t) = 6,000 seconds

Longitudinal Dispersivity, α = 0
Distribution Coefficient, (also K_d) R = 0
Dissolved Half-Life, λ = 0

No adsorption and no decay processes are considered.

2.3.2 Results and Discussions: Case 1

Figure 10 displays the comparison between CHEMFLUX and CTRAN/W. There is agreement between results.

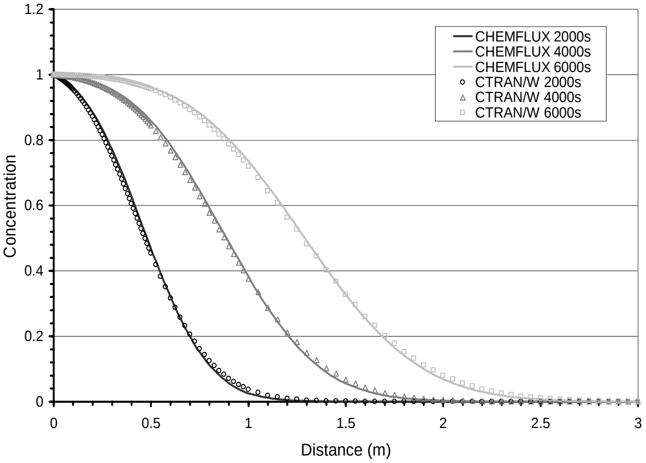

Figure 10 - No adsorption no decay

2.3.3 Model Description: Case 2

This example model includes the effect of adsorption.

Project:	VerifyCHEMFLUX
Model:	CTranCase2

A description of the material properties, geometry, and boundary conditions used in the numerical model is as follows:

Groundwater seepage velocity (v) = 0.2 mm/s
Porosity (θ) = 0.5
Simulation time (t) = 6,000 seconds

Longitudinal Dispersivity, α = 100m
Distribution Coefficient, (also K_d) R = 2
Dissolved Half-Life, λ = 0

With adsorption process considered.

2.3.4 Results and Discussions: Case 2

Figure 11 displays the results between the two software packages for the case of adsorption and no decay. The results show agreement between the two software packages.

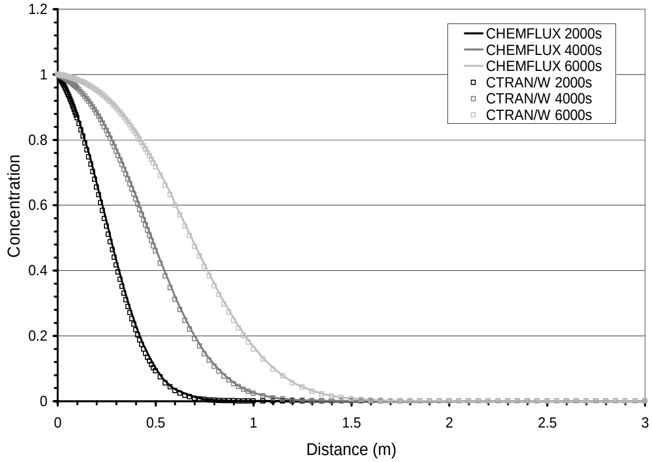

Figure 11 - Adsorption no decay

2.3.5 Model Description: Case 3

This example model includes the effect of decay.

Project: VerifyCHEMFLUX
Model: CTranCase3

A description of the material properties, geometry, and boundary conditions used in the numerical model is as follows:

Groundwater seepage velocity (v) = 0.2 mm/s
Porosity (θ) = 0.5
Simulation time (t) = 6,000 seconds

Longitudinal Dispersivity, α = 100m
Distribution Coefficient, (also K_d) R = 0
Dissolved Half-Life, λ = $1.0e^{-04}$

With decay process considered.

2.3.6 Results and Discussions: Case 3

Figure 12 displays the results from the two software packages modeling the affect of decay. There is again agreement between results.

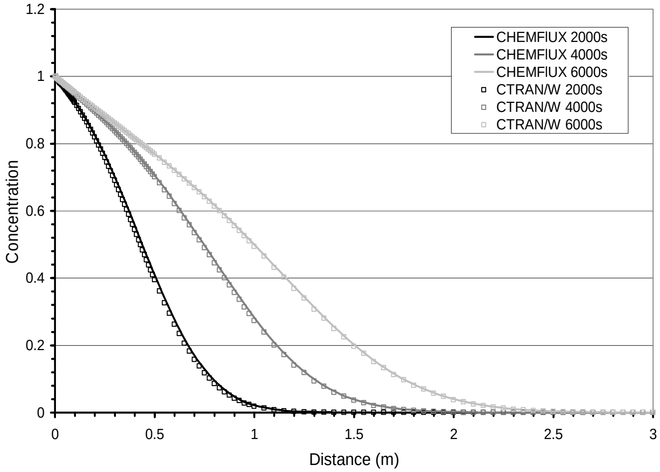

Figure 12 - With decay

2.3.7 Model Description: Case 4

This example includes the effect of both adsorption and decay.

Project: VerifyCHEMFLUX
Model: CTranCase4

A description of the material properties, geometry, and boundary conditions used in the numerical model is as follows:

Groundwater seepage velocity (ν) = 0.2 mm/s
Porosity (θ) = 0.5
Simulation time (*t*) = 6,000 seconds

Longitudinal Dispersivity, α =100m
Distribution Coefficient, (also K_d) *R* =2
Dissolved Half-Life, λ =1.0e^{-04}

With adsorption and decay processes considered.

2.3.8 Results and Discussions: Case 4

Figure 13 displays the results from the two software packages for the case of adsorption and decay. This graph illustrates agreement between results.

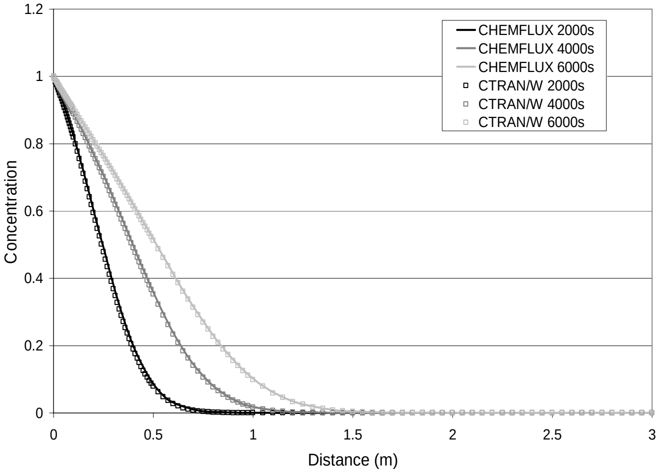

Figure 13 - With adsorption and decay

3 TWO-DIMENSIONAL TRANSPORT

This Chapter will compare CHEMFLUX to CTRAN/W and MT3DMS. The scope of this comparison will be two-dimensional contaminant transport.

3.1 2D CTRAN/W

This section will compare CHEMFLUX to CTRAN/W using a two-dimensional contaminant transport model presented in the CTRAN/W User's Manual. From this comparison you will find that not only does CHEMFLUX give reliable results, but in most cases the results are improved by the automatic mesh refinement provided in CHEMFLUX.

Project:	Ponds
Model:	T2DBank, 2DBank

3.1.1 Model Geometry and Material Properties

A description of the material properties, geometry, and boundary conditions used in the numerical model is as follows:

Groundwater seepage velocity (ν) = Obtained from SVFLUX
Longitudinal Dispersivity (α) = 2
Transverse Dispersivity (α) = 1

The model is an earth embankment consisting of a reservoir on the left and a river at elevation 4m on the right. The seepage solution was prepared in SVFLUX. A constant head boundary condition of 10.25m was set along the bottom the reservoir while a constant head boundary condition of 4m was set along the 4m portion on the right hand side of the model to simulate the river. The CHEMFLUX analysis used a constant concentration boundary condition along the reservoir floor of 10 g/m^3. The model is run over a time of 2750 days.

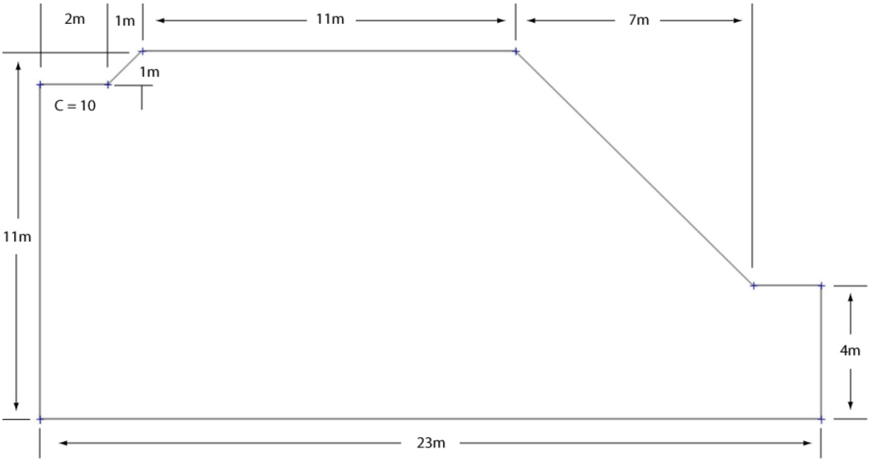

Figure 14

3.1.2 Results and Discussions

From the below figures it can be seen that the results obtained from CHEMFLUX are a close match to those obtained with CTRAN/W. The main difference in the results occurs in the unsaturated area of the model. CHEMFLUX's ability to refine the mesh while the model solves allows for a much more accurate solution especially in unsaturated zones. Plots of the solution mesh from both programs

are provided to highlight differences. The CHEMFLUX solution mesh higher has resolution in the unsaturated zone locate throughout the upper portion of the model.

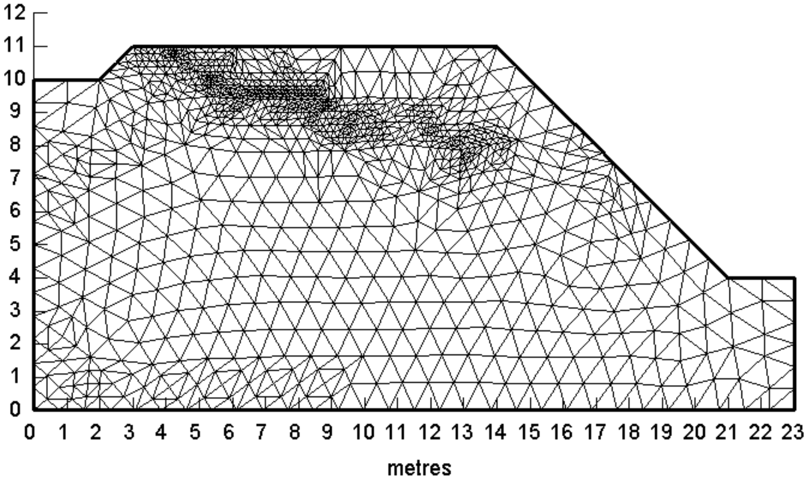

Figure 15 - CHEMFLUX solution mesh

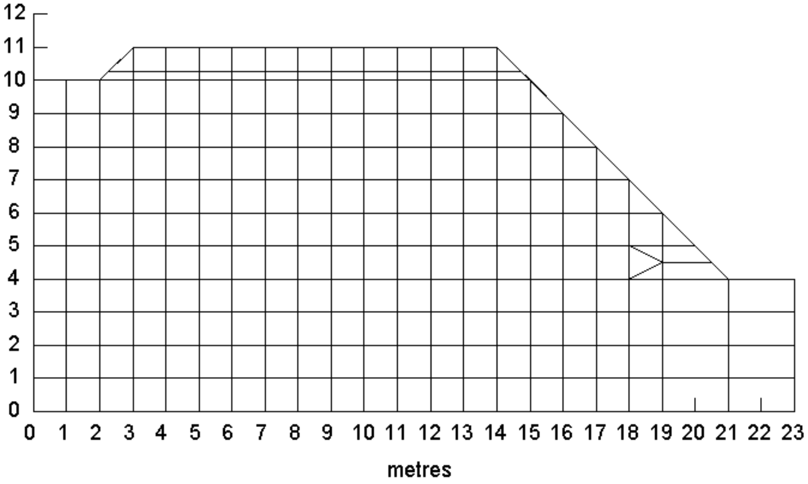

Figure 16 - CTran/W solution mesh

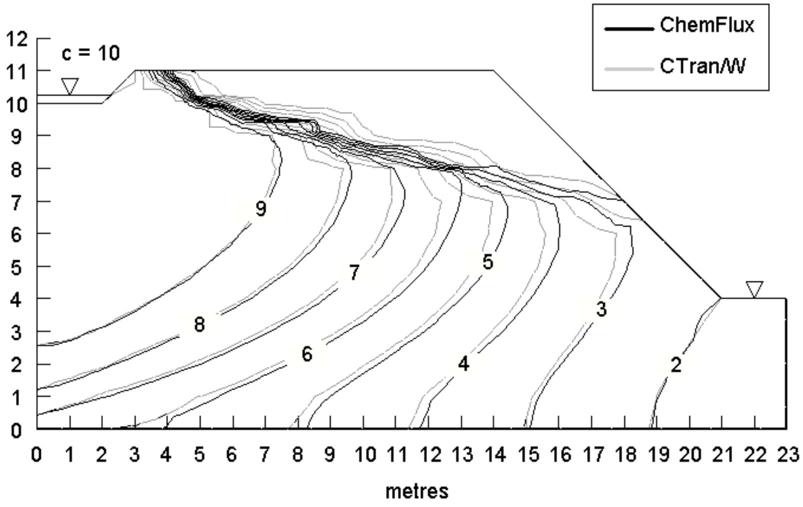

Figure 17 - Concentration Contours

3.2 2D MT3DMS

This section will compare CHEMFLUX to MT3DMS using a two-dimensional contaminant transport model presented in Zheng and Wang (1999). The model considers flow and solute transport in a highly irregular flow field, dispersion parameters that are small compared with the spatial discretization, and a large contrast between longitudinal and transverse dispersivities Zheng and Wang (1999). Van der Heijde (1995) presents this model as an example of “Level 2” testing, in which the objectives are to test the potentially problematic parameter combinations and to determine a code’s applicability to typical real-work models Zheng and Wang (1999).

3.2.1 Model Geometry and Boundary Conditions

Project:	ContaminantPlumes
Model:	VanderHeijdeSS, VanderHeijde

The model geometry, boundary conditions, and material properties are described as follows:

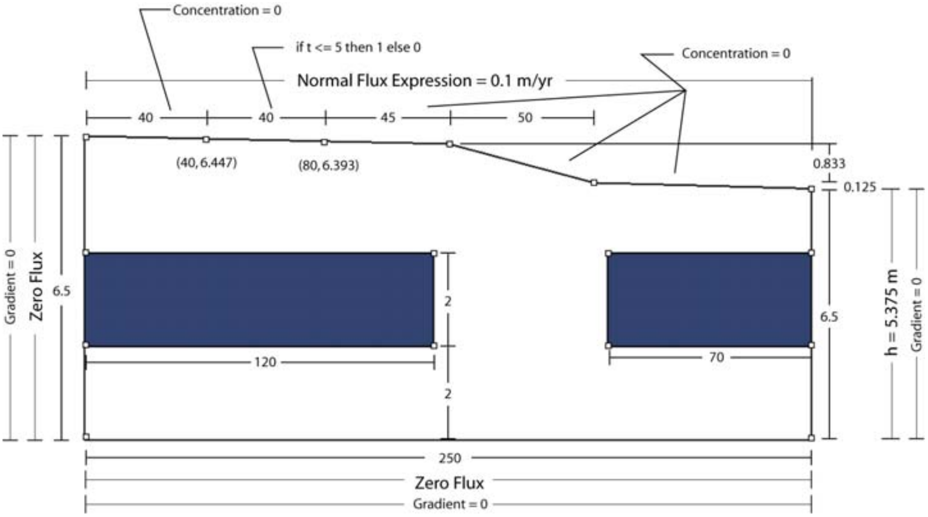

Figure 18 - 2D MT3DMS Geometry, Boundary Conditions, and Material Properties

🟦 Ksat = 10^{-2} cm/s

⬜ Ksat = $5x10^{-04}$ cm/s

The flow system is solved under steady state conditions. The boundary conditions include a constant head along the right side of the model of 5.375m and a uniform recharge of 0.1m/yr along the top boundary. The remaining two boundaries are set to Zero Flux.

Longitudinal Dispersivity (α_L) = .5m

Transverse Dispersivity (α_T) = .005m

Diffusion (D^*) = $1.34x10^{-05}$ cm^2/s

The contaminant transport boundary conditions are set as shown in the above diagram. The concentration boundary condition between the points (40,6.44) and (80,6.39) changes with time. For the first five years the concentration is set to one, for the remaining fifteen years the concentration is set to zero.

3.2.2 Results and Discussions

From the below figures it can be seen that the results obtained from CHEMFLUX are a close match to those obtained with MT3DMS. For each of the reported times, CHEMFLUX shows good agreement for both the location of the plume and the maximum concentration within the plume.

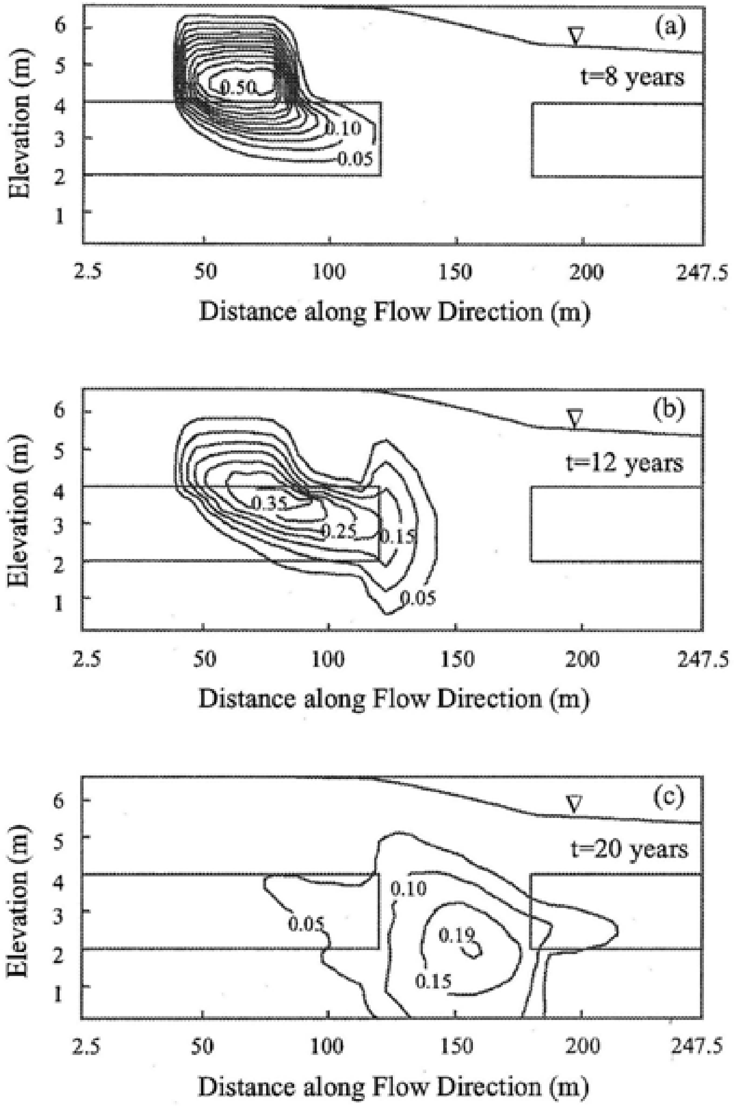

Figure 19 - MT3DMS Concentration Contours

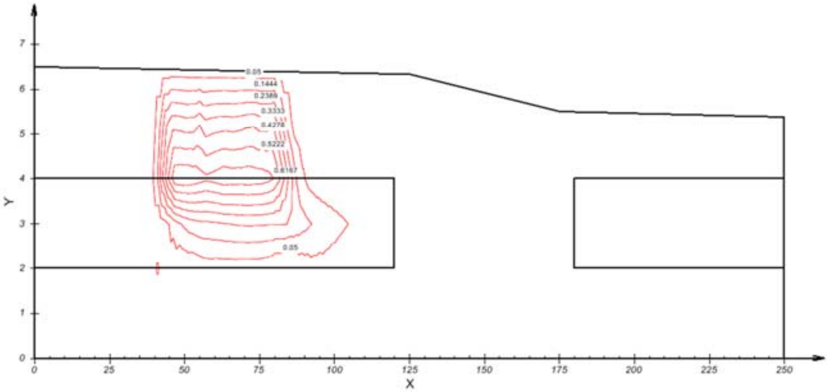

Figure 20 - CHEMFLUX 8 Year Concentration Contours

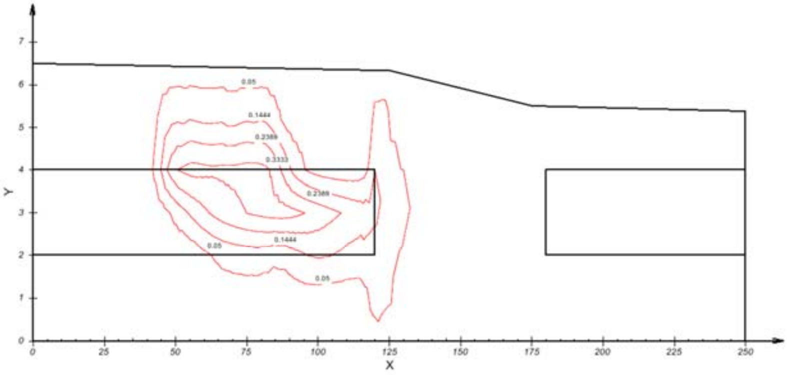

Figure 21 - CHEMFLUX 12 Year Concentration Contours

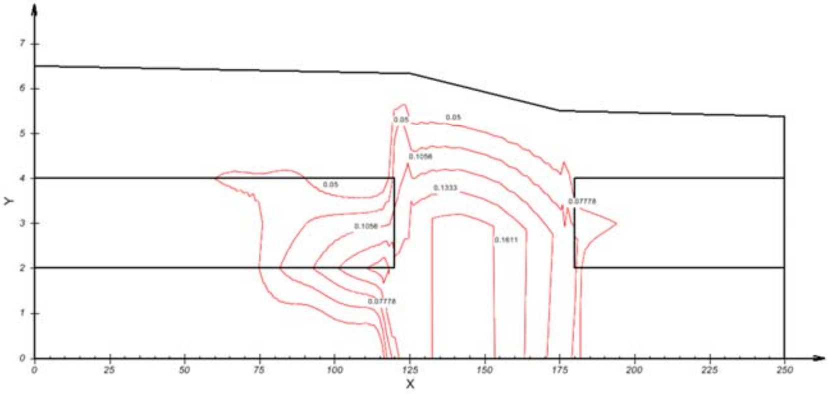

Figure 22 - CHEMFLUX 20 Year Concentration Contours

4 THREE-DIMENSIONAL TRANSPORT

The following models benchmark the reliability of CHEMFLUX as benchmarked against 3D examples.

4.1 PARALELLEPIPEDAL SOLUTE SOURCE PROBLEM

SoilVision Systems Ltd. would like to thank Nader Ebrahimi, M.Sc. at the University of Saskatchewan, Saskatoon, SK. for contributing this benchmark model. This model is presented in Segol (1994).

Project: VerifyCHEMFLUX
Model: Leij1991

4.1.1 Model Geometry and Boundary Conditions

Figure 23 shows the schematic of the model. The solute is initially distributed uniformly in a bounded region of the material (i.e., a paralellepipedal). Fresh water flows in *z* direction with the velocity equal to *v*. In initial time, $t=0$, the concentration of the solute within the box is $c_{0..}$ The task is simulating the movement of the contaminant plume in three-dimensions at different times.

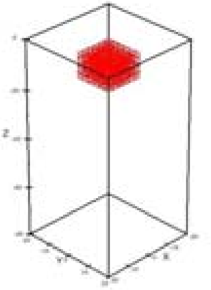

Figure 23 - Schematic of the paralellepipedal solute source model

The set of material properties for which the published analytical solutions for Equation (1) are available, are presented in Table 1.

Table 1 - Material properties used in solving the paralellepipedal contaminant source model

Material Properties	Value
Dx (m^2/day)	20
Dy (m^2/day)	10
m (1/day)= l(gr/m^3/day)	0
R	1
vx , *vy* (m/day)	0
vz	50

Boundary and initial conditions for the model can be written as follows:

No contaminant transport boundary condition may be assumed for the bounded area of porous media far enough from solution domain.

$$\frac{\partial c}{\partial x} = 0$$ on the planes x=20 and x=-20

$$\frac{\partial c}{\partial z} = 0$$ on the planes y=20 and y=-20

$$\frac{\partial c}{\partial y} = 0$$ on the planes z=0 and z = -80

The following initial conditions are also defined:

At t = 0 for

$-7.5 < x < 7.5$ m ,
$-7.5 < y < 7.5$ m , and
$-5 < z < -15$ m ,
$c = c_0 = 1$

4.1.2 Results and Discussions

Leij et al. (1991) solved the paralellepipedal solute source model with boundary and initial conditions as given in section 4.1 and provided the results on the plane x=0.

The model has been solved numerically using the CHEMFLUX software with the same boundary and initial conditions and the same material properties. Figure 24 shows the solute concentrations versus depth below the material surface *(Z)* and transverse direction (*Y*) for different times *(t*=0.5 and *t*=1 hour).

Available analytical solutions and solutions obtained using CHEMFLUX for the paralellepipedal solute source model is plotted on the same scale (Figure 24).

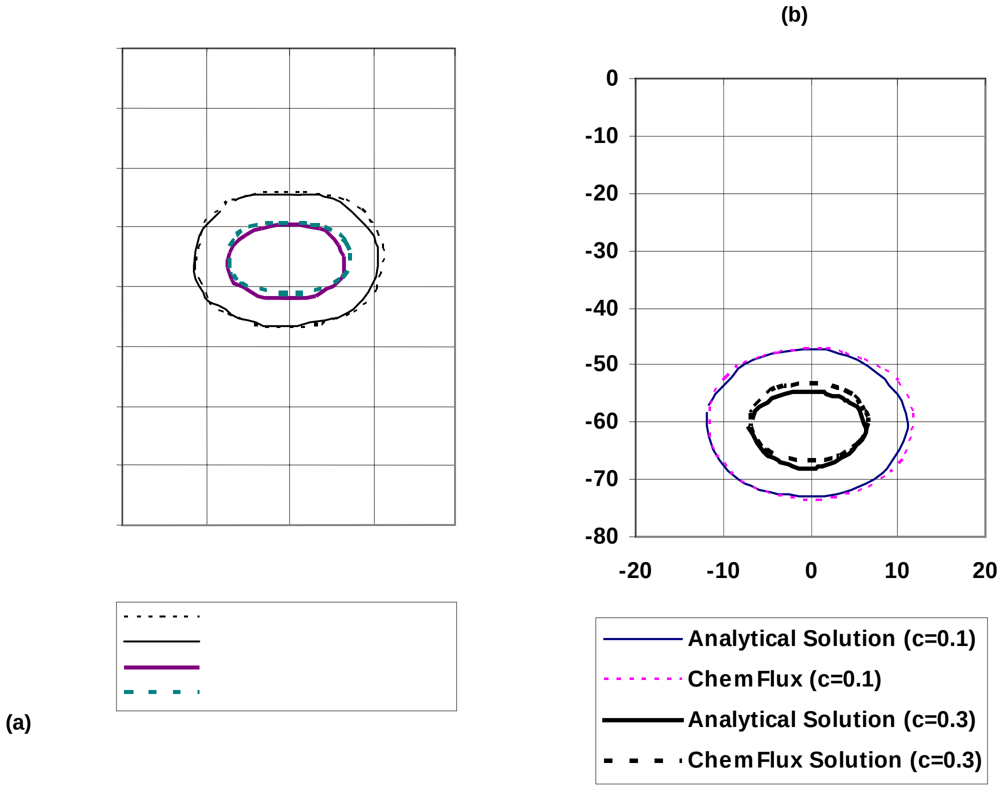

Figure 24 - Comparison of the simulated contaminant transport using CHEMFLUX and analytical solutions for the contours 0.1 and 0.3 at a) t=0.5 and b) t=1 hours

The reliability of CHEMFLUX software in simulating non-reactive tracer movement from a box solute source buried in a saturated porous media has been evaluated. The solutions simulated using CHEMFLUX software is compared with available analytical solutions. The simulated data obtained using CHEMFLUX were shown to obtain good agreement with available analytical solutions.

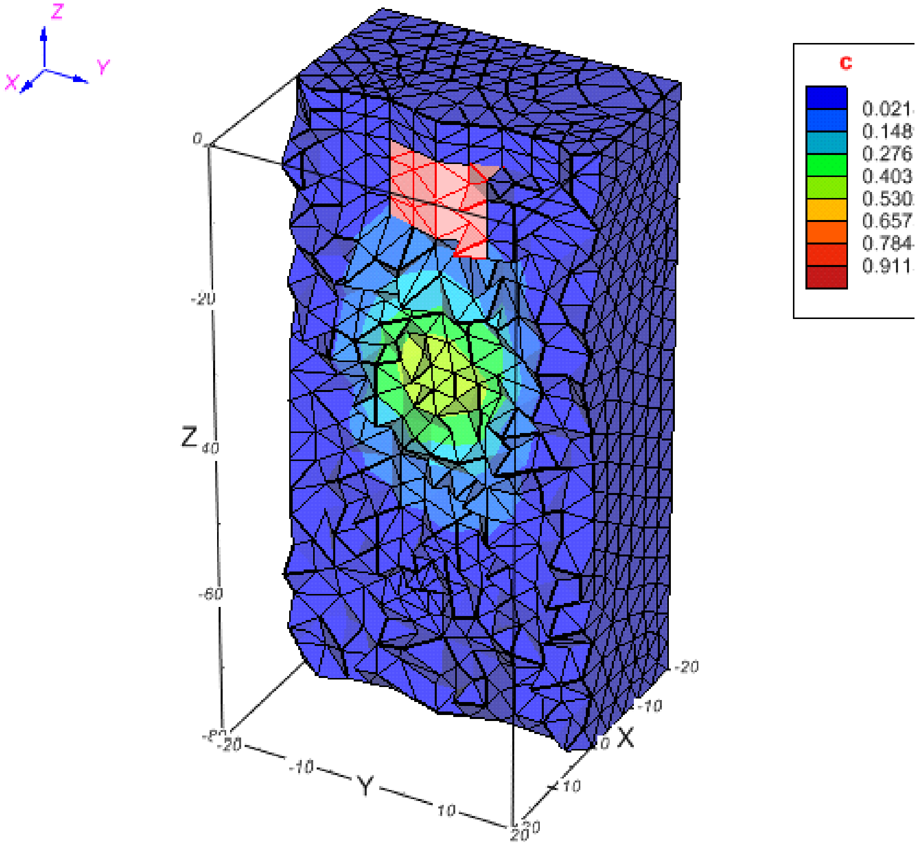
Z
Y
X
c
0.021
0.148
0.276
0.403
0.530
0.657
0.784
0.911
0
-20
Z
40
-60
-20
-10
Y
10
20
20
10
0
X
-10
-20

Figure 25

5 REFERENCES

CTRAN/W User's Guide, (1991-2001). GEO-SLOPE International Ltd., Calgary, Alberta, Canada.

Fetter, C.W. (1999). "Contaminant Hydrogeology," Precntice Hall, NJ, USA.

Leonard, B.P. (1988). "Universal Limiter for transient interpolation modeling of the advective transport equations: The Ultimate conservative difference scheme," NASA Technical Memorandum 1009161COMP-88-11, Washington, DC., U.S.A.

Roache, P.J. (1992). "A flux-based modified method of characteristics," Int. J. Numerical Methods in Fluids 15, 1259-75.

Segol, Genevieve, 1994, "Classic Groundwater Simulations: Proving and Improving Numerical Models", PTR Prentice Hall, Englewood Cliffs, New Jersey.

Van Genuchten, M. Th., and Alves, W.J. (1982). "Analytical solutions of the one-dimensional convective-dispersive solute transport equation," U.S. Department of Agriculture Technical Bulletin No. 1661

Van der Heijde (1995)

Zheng, Chunmiao, and Wang, P. Patrick. (1999), MT3DMS, "A modular three-dimensional multi-species transport model for simulation of advection, dispersion and chemical reactions of contaminants in groundwater systems"; documentation and user's guide, U.S. Army Engineer Research and Development Center Contract Report SERDP-99-1, Vicksburg, MS, 202 p.

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