SVCHEM SVENVIRO
1D/2D/3D FINITE ELEMENT
CONTAMINANT TRANSPORT MODELING

Verification Manual

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Bentley Systems Incorporated

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.

Bentley Systems takes the process of "verification" most seriously and has undertaken a wide range of steps to ensure that the SVCHEM 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 Bentley Systems 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 SVCHEM 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 SVCHEM 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 / SVCHEM 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 Bentley Systems (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 SVCHEM 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 SVCHEM 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 (v)   = 0.2 mm/s

  Case 1:   Diffusion Only
               Groundwater seepage velocity (n)   = 0.00 m/s
               Diffusion Constant (D^*)   = 1.00×10^{-11} m^2/s
               Longitudinal Dispersivity   = 0.00 m

- **Geometry/Boundary Conditions**
  The model is a 1D vertical column that is 0.4 m deep. Nodes exist every 0.1 m. A concentration of 1 g/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

In Figure 1 it displays the comparison between SVCHEM and the finite-difference solution calculated in CONTAM.zip FDadvdis.xls for the diffusion only scenario. There is agreement between results.
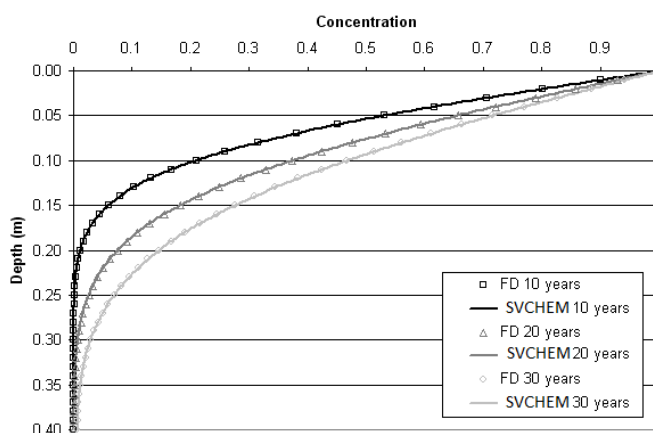
Figure 1 1D SVCHEM (formerly ChemFlux) versus CONTAM.zip - Diffusion Only

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 SVCHEM 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 (v)   = 0.2 mm/s

  Case 2:   Diffusion, Advection
                 Groundwater seepage velocity (n)   = 2.00×10^{-10} m/s
                 Diffusion Constant ($D*$)   = 5.00×10^{-12} m²/s
                 Longitudinal Dispersivity   = 0.00 m

- **Geometry/Boundary Conditions**
  The model is a 1D vertical column that is 0.4 m deep. Nodes exist every 0.1 m. A concentration of 1 g/m³ 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 SVCHEM and the finite-difference solution calculated in CONTAM.zip FDadvdis.xls for the diffusion and advection scenario. There is agreement between results.
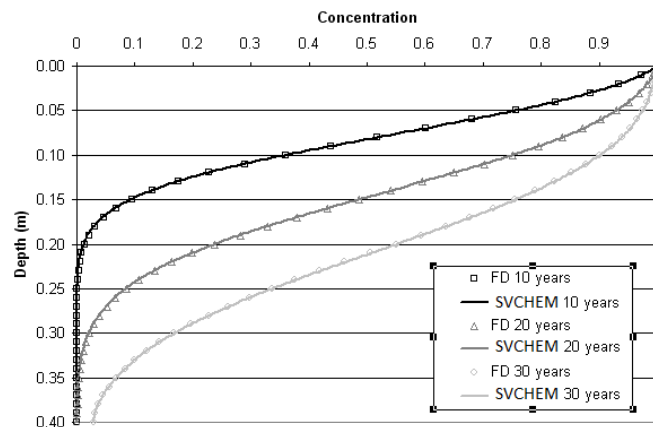

Figure 2 1D SVCHEM (formerly ChemFlux) versus CONTAM.zip - Diffusion and Advection

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 SVCHEM 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 (v)   = 0.2 mm/s
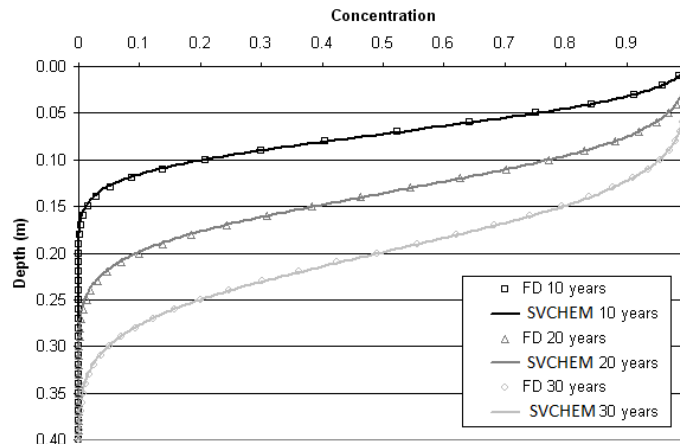
> Case 3:   Diffusion, Advection, and Dispersion
> Groundwater seepage velocity (n)   = 2.00×10^{-10} m/s
> Diffusion Constant (D^*)   = 5.00×10^{-14} m²/s
> Longitudinal Dispersivity   = 0.01 m

- **Geometry/Boundary Conditions**
> The model is a 1D vertical column that is 0.4 m deep. Nodes exist every 0.1 m. A concentration of 1 g/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

In Figure 3 it displays the comparison between SVCHEM 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 SVCHEM (formerly ChemFlux) versus CONTAM.zip Diffusion, Advection, and Dispersion

3 ONE-DIMENSIONAL GAS DIFFUSION

3.1 DOBCHUK CLOSED FORM BENCHMARK

A closed-form solution can be obtained for the gas diffusion governing equation in a simple case with a constant effective diffusion coefficient and a constant reaction rate of decay. The benchmarking was originally presented by Dobchuk (2002) to verify the numerical simulation of oxygen diffusion. Two cases are verified in this benchmark. One model includes gas decay, and another model does not. The same value of the effective diffusion coefficient is used in both models.

Project: GasDiffusion
Model: OxygenDiffusion_Dobchuk_NoDecay, OxygenDiffusion_Dobchuk_Decay

3.1.1 Model Description

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

Soil column height = 20 m
Saturation: = 40%
Porosity, n = 0.45
Volumetric water content, θ_w = 0.18
Volumetric air content, θ_a = 0.18
Equivalent porosity, n_{eq} = 0.2754
Simulation time (t) = 100 days

Effective diffusion coefficient D_e, = 0.032855 m^2/day
Gas reaction rate, k_r^* = 0.1480 1/day

Initial oxygen concentration = 0 g/m^3

Upper boundary condition = constant oxygen concentration, 280 g/m^3
Bottom boundary condition = zero flux

3.1.2 Results and Discussions

Figure 4 and Figure 5 are the comparison of the SVCHEM numerical results against the closed form solution for oxygen diffusion with and without consideration of gas decay. In both cases there is an excellent agreement between the numerical calculation by SVCHEM and the closed form solution.
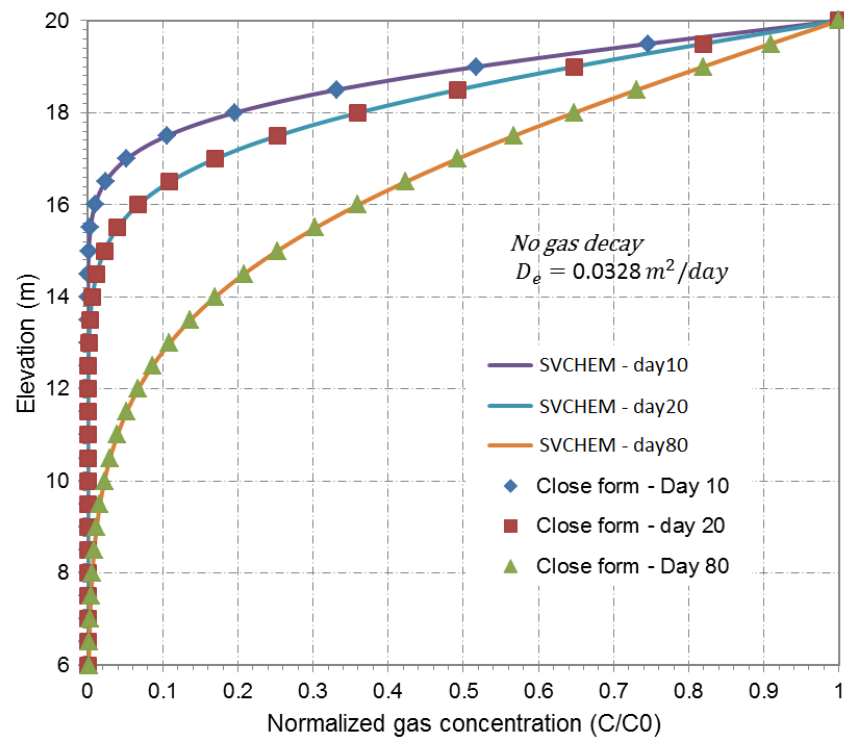
Figure 4 SVCHEM (formerly ChemFlux) versus Closed Form Solution - Oxygen diffusion without gas decay comparison
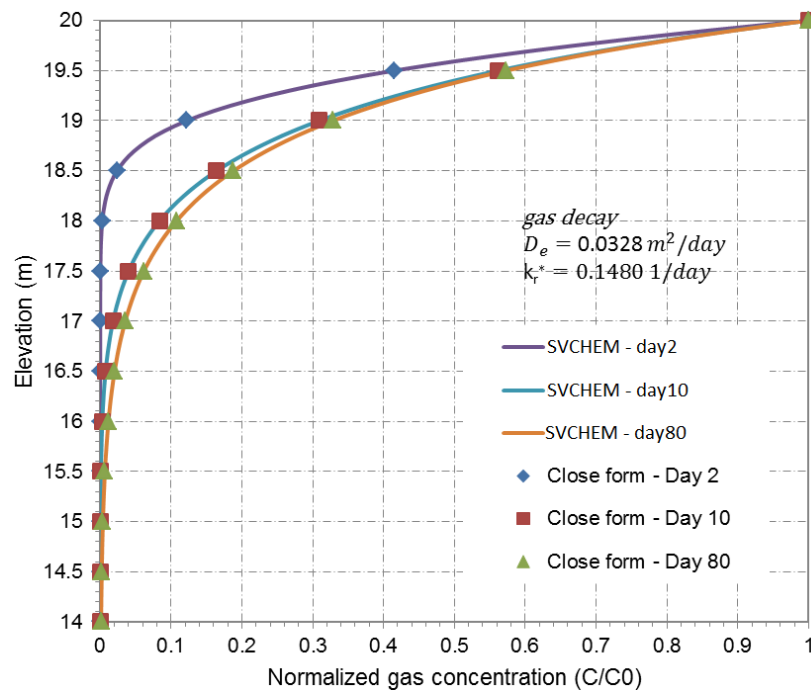

Figure 5 SVCHEM (formerly ChemFlux) versus Closed Form Solution - Oxygen diffusion with gas decay comparison

4 TWO-DIMENSIONAL TRANSPORT

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

4.1 2D CTRAN/W

This section will compare SVCHEM 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 SVCHEM give reliable results, but also in most cases the results are improved by the automatic mesh refinement provided in SVCHEM.

Project: Ponds
Model: T2DBank, 2DBank

4.1.1 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 (v)   = 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 4 m on the right. The seepage solution was prepared in SVFLUX. A constant head boundary condition of 10.25 m was set along the bottom the reservoir while a constant head boundary condition of 4 m was set along the 4 m portions on the right hand side of the model to simulate the river. The SVCHEM 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.
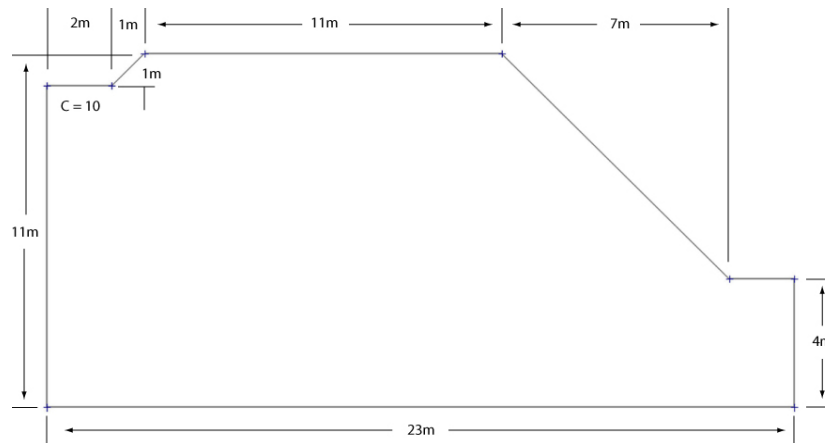

Figure 6

4.1.2 Results and Discussions

From the figures below it can be seen that the results obtained from SVCHEM are a close match to those obtained with CTRAN/W. The main difference in the results occurs in the unsaturated area of the model. SVCHEM'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 SVCHEM solution mesh higher has resolution in the unsaturated zone locate throughout the upper portion of the model.
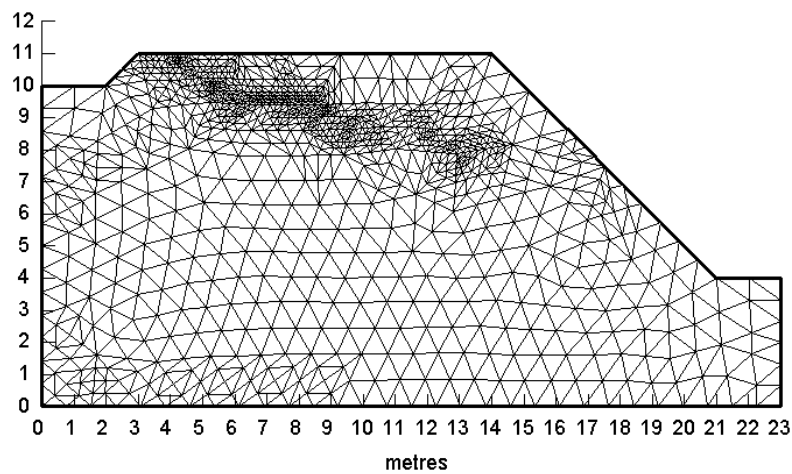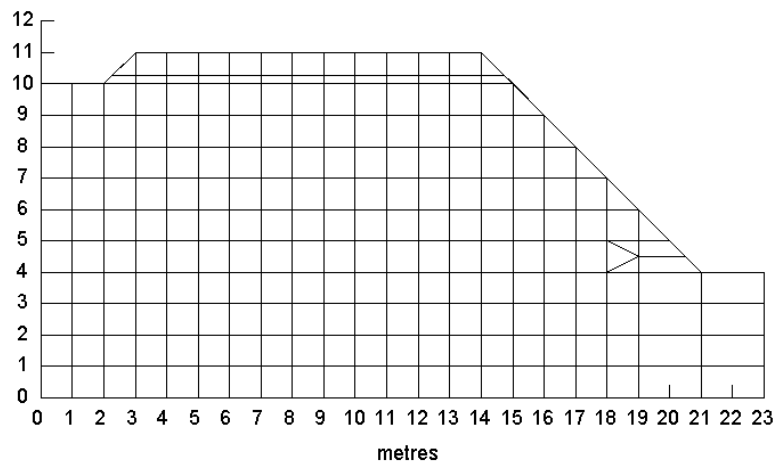
Figure 7 SVCHEM solution mesh

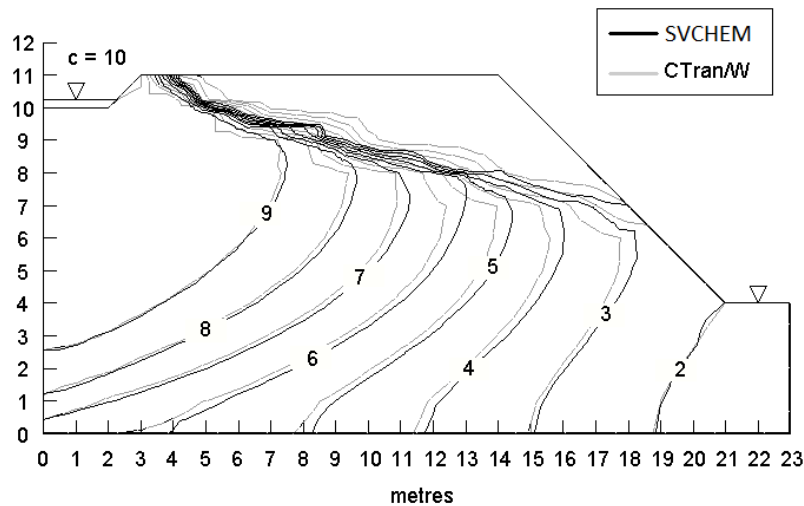**Figure 8 CTran/W solution mesh**

Figure 9 SVCHEM (formerly ChemFlux) versus CTran/W - Concentration Contours
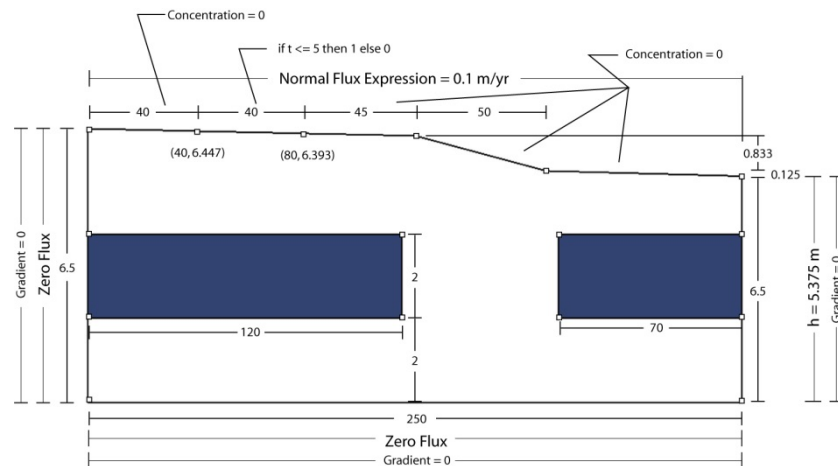
4.2 2D MT3DMS

This section will compare SVCHEM 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).

4.2.1   Model Geometry and Boundary Conditions

Project: ContaminantPlumes
Model: VanderHeijdeSS, VanderHeijde

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

Figure 10 2D MT3DMS Geometry, Boundary Conditions, and Material Properties

Ksat = 10^{-2} cm/s   Ksat = 5×10^{-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 5.375 m 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)   = 0.5 m
Transverse Dispersivity (α_T)   = 0.005 m
Diffusion (D^*)   = 1.34×10^{-5} 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.

4.2.2   Results and Discussions

From the following figures it can be seen that the results obtained from SVCHEM are a close match to those obtained with MT3DMS. For each of the reported times SVCHEM shows good agreement for both the location of the plume and the maximum concentration within the plume.
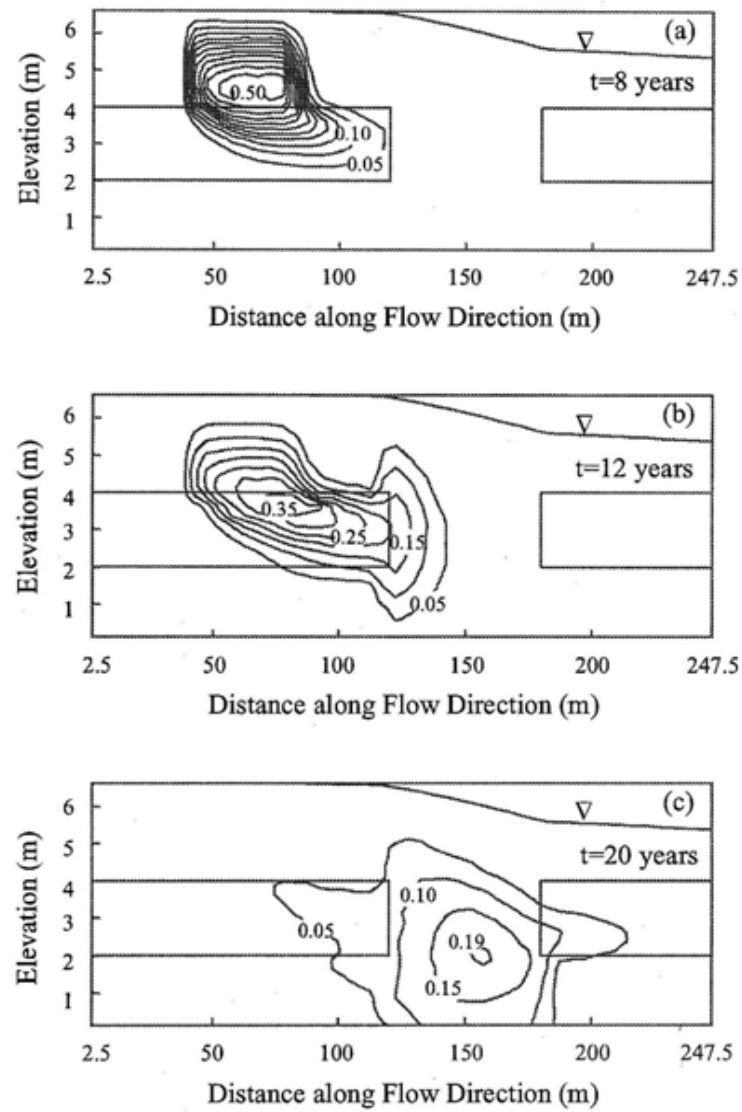
Figure 11 MT3DMS Concentration Contours
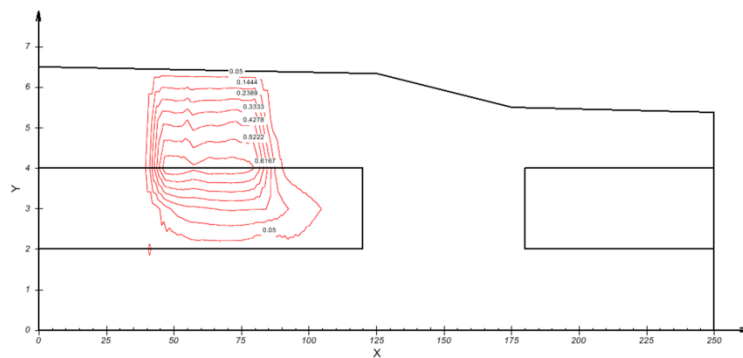
Figure 12 SVCHEM 8-Year Concentration Contours

Figure 13 SVCHEM 12-Year Concentration Contours

Figure 14 SVCHEM 20-Year Concentration Contours

4.3 HENRY PROBLEM (COUPLED WITH SVFLUX)

This benchmark illustrates the result simulated using SVCHEM coupled with SVFLUX for the Henry's problem, which has been widely used for the benchmark of density-dependent solute transport (SaltFlow 2002, Simpson et al. 2003, 2004, and Langevin and Guo 2002, 2006).

Project: SoluteTransport
Model: HenryModel, HenryModel_SimpsonModifed

4.3.1   Model Geometry and Boundary Conditions

The Henry's problem concerns the seawater intrusion to the fresh water aquifers. The model geometry is illustrated in Figure 15. It is a rectangle that is 2 *m* long in horizontal distance and 1 *m* in elevation. The fresh water flows at a constant rate of 6.6×10^{-5} *m/s* through a homogenous material from the left boundary to the right boundary. The sea water is intruded due to the salt concentrations applied on the right boundary. No water flow and solute transport occurs on the top and bottom. The boundary conditions for this model are depicted in Figure 15.
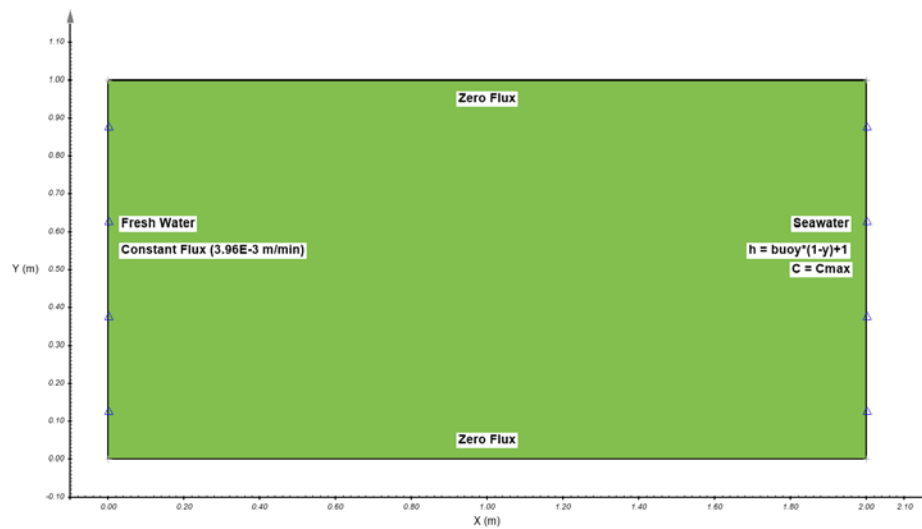
Figure 15 Model Geometry of Henry's problem

The symbols in the figure are defined as follows:

$$buoy = \frac{\rho_{mw} - \rho_w}{\rho_w}$$ [1]

where:

ρ_{mw}	= sea water density, kg/m^3,
ρ_w	= fresh water density, kg/m^3,
h	= water pressure head, m,
C	= the salt concentration, g/m^3, and
$Cmax$	= the maximum salt concentration, g/m^3.

NOTE:

1. The density-dependent option must be selected in the SVFLUX model settings dialog for this model. This will include the buoyant force in the seepage equation.

3. The buoy and Cmax are valid PDE variables in a SVCHEM density-dependent model.

Initial Conditions:
Initial head: 1 m,
Initial concentration: 0 g/m^3,

Material Properties:
The material properties used in this benchmark is listed in Table 1:

Table 1 Material properties used in Henry's problem

Symbol	Properties	value	unit
$Ksat$	Saturated hydraulic conductivity	0.01	m/s
$SatVWC$	Saturated water content	0.35	m^3/m^3
ρ_w	Fresh water density	1000	kg/m^3
ρ_{max}	The maximum seawater density	1025	kg/m^3
$Cmax$	The maximum solute concentration	35000	g/m^3
D	Dispersion coefficient	1.89×10^{-5}	m^2/s

4.3.2   Results and Discussions

The model is simulated in two cases. Case 1 is the original Henry's problem. Case 2 is the modified Henry's problem where the fresh water flow rate applied on the left side of model is reduced to half the value of the original Henry's problem.

Case 1: Simulation result with original Henry's problem

Figure 16 and Figure 17 shows the evolution of salt concentration, streamlines, head contours and velocity vectors at the time = 250 min that a steady-state condition is reached. Figure 18 is the comparison of SVCHEM simulation with semi-analytical results (Simpson 2004) at the isochlors of 25%, 50% and 75%. It can be seen from the figures that the SVCHEM simulation matches the semi-analytical result well (Simpson et al. 2004).

Case 2: Simulation result for the modified Henry's problem

In the modified Henry model, the flow rate of fresh water applied to the left side of the model is reduced to 3.3×10^{-5} *m/s*. The simulated results using SVCHEM coupled with SVFLUX are presented in Figure 19 and Figure 20. Again, there is good agreement between the simulated results and semi-analytical as shown in Figure 21.
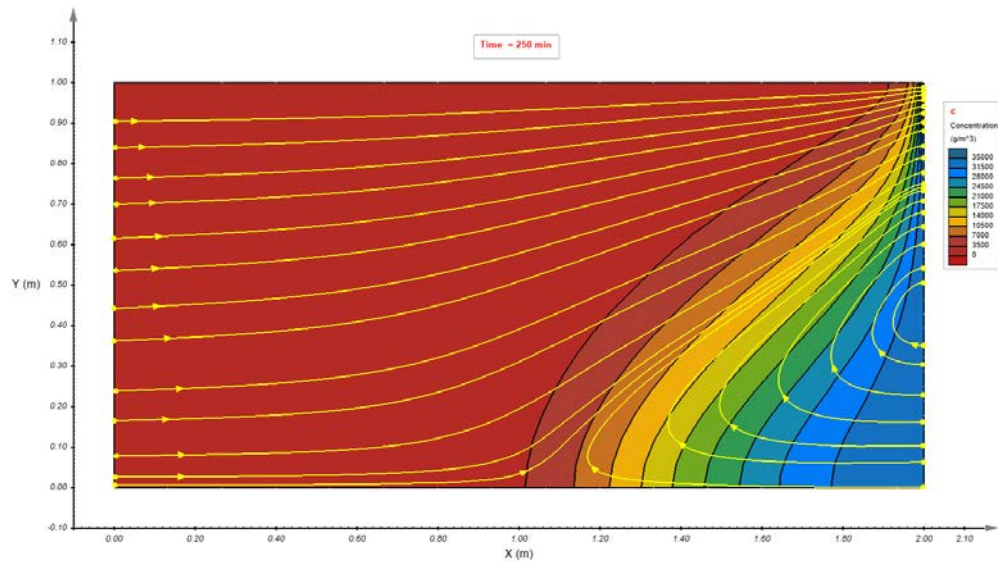
Figure 16 Salt concentration evolution and strealines for the Henry problem at steady state
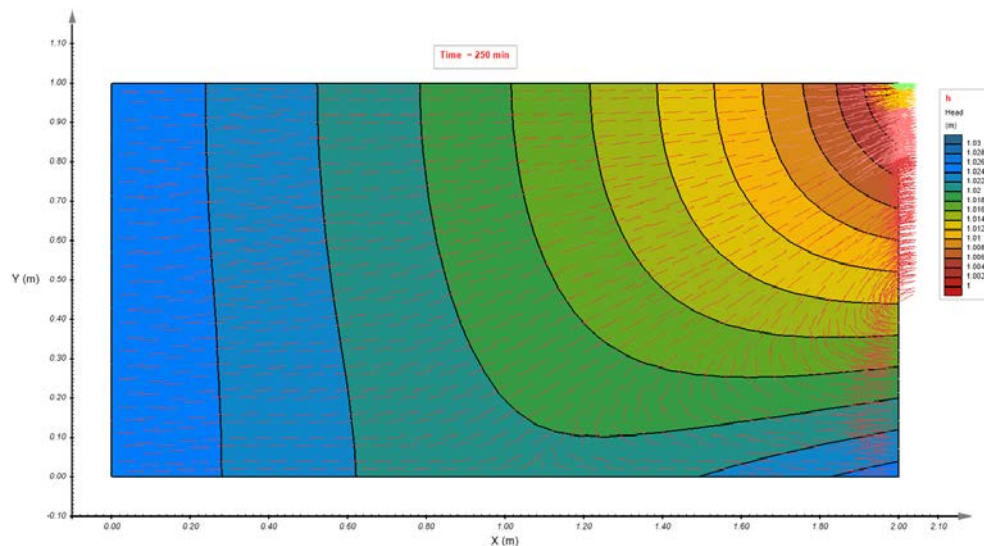

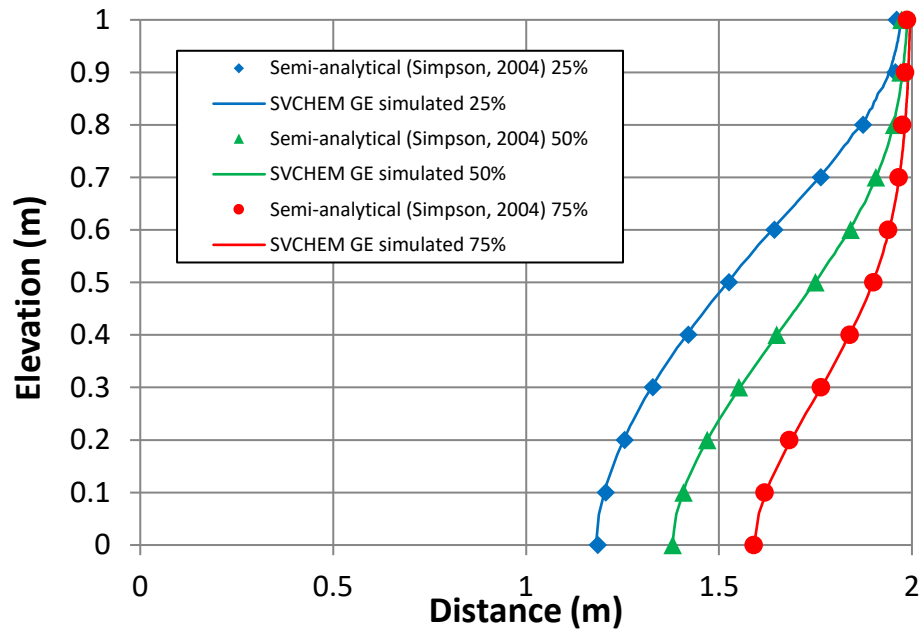**Figure 17 head contours and velocity vectors for the Henry problem at steady state**

Figure 18 Comparison of simulation of SVCHEM (formerly ChemFlux) with the semi-analytical results (Simpson 2004).
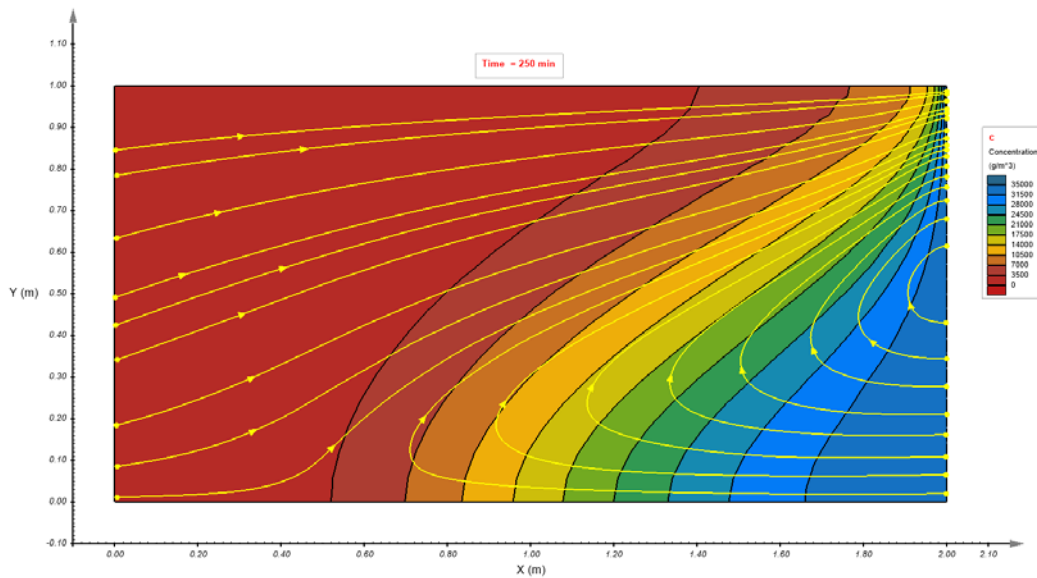

Figure 19 The profiles of salt concentration and streamlines for the modified Henry's problem in the case of fresh water flow rate = 3.3×10⁻⁵ *m/s*
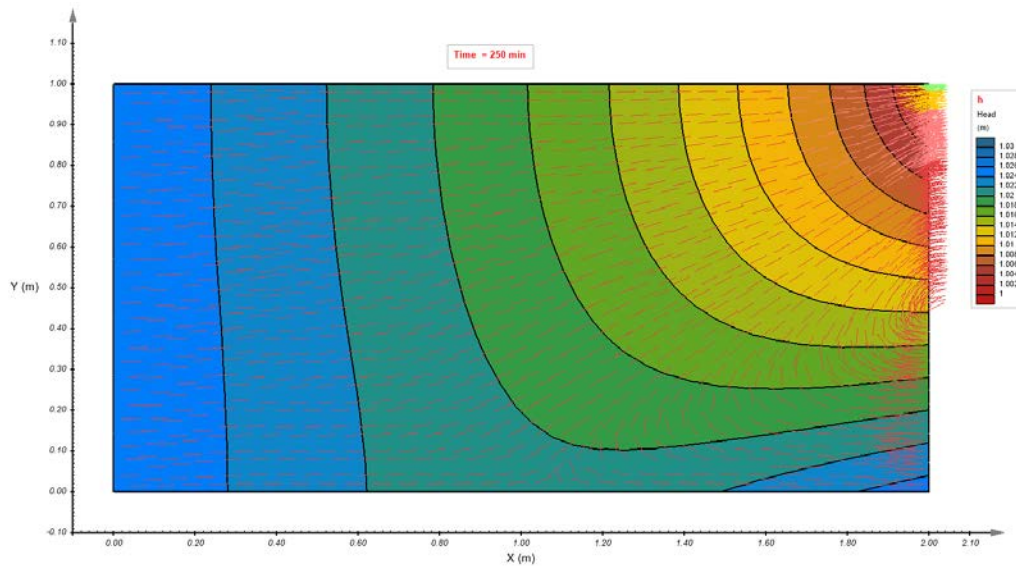
Figure 20 head contours and velocity vectors for the modified Henry's problem in the case of fresh water flow rate = 3.3×10^{-5} *m/s*
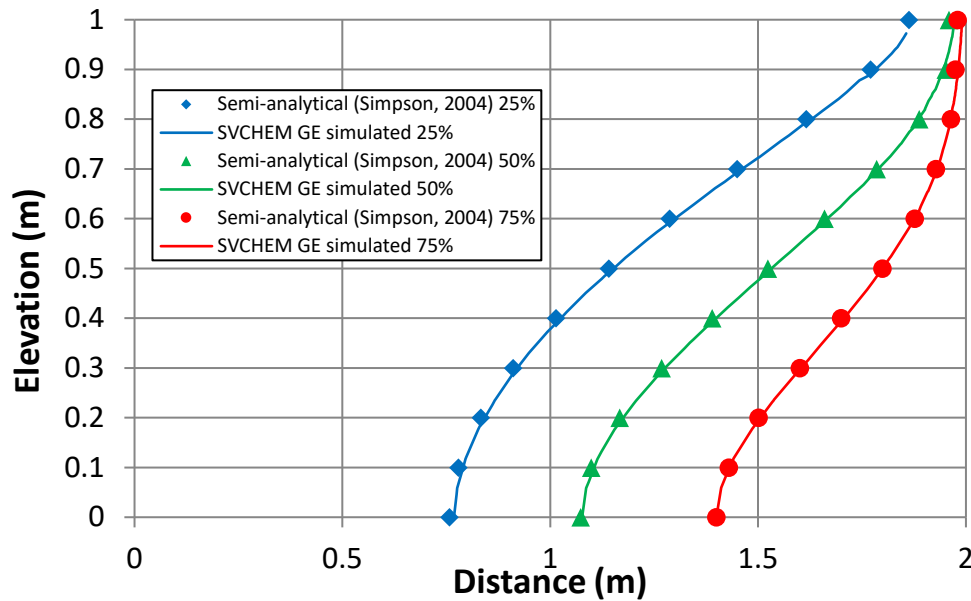

Figure 21 Comparison of the SVCHEM (formerly ChemFlux) simulation with the semi-analytical results for the modified Henry's problem in the case of fresh water flow rate = 3.3×10^{-5} *m/s*

4.4 ELDER PROBLEM (COUPLED WITH SVFLUX)

The Elder convection problem (Elder 1967) is a rigorous benchmark that has been widely used in the numerical analysis of the density-dependent solute transport (Boufadel, 1999, Guo, 2002, Simpson 2003, and Hassanzadeh 2005). This benchmark presents the solute flow patterns of Elder problem using SVCHEM coupled with SVFLUX.

Project: SoluteTransport
Model: ElderModel_10y

4.4.1   Model Geometry and Boundary Conditions

The model utilizes a rectangular geometry with a length of 160 *m* and a height of 150 *m*. A constant solute concentration with a value of 285.7 *g/m³* is applied on the upper boundary F-G of the model domain. On the bottom boundary A-D, the concentration is set to 0 *g/m³*. At the corner of upper-left B-E and upper-right H-C line segments, a zero water head is maintained. Zero water flux and concentration flux are applied on other boundary conditions as shown in Figure 22. The symbols used in the Figure 22 are defined as follows:

h = water pressure head, m,

C = the salt concentration, g/m^3,

$Cmax$ = the maximum salt concentration, g/m^3.

NOTE:

1. The density-dependent option must be selected in the SVFLUX model settings dialog for this model.
2. To include the buoyant force in seepage equation, the density-dependent flow option must be checked in the SVFLUX model settings dialog.

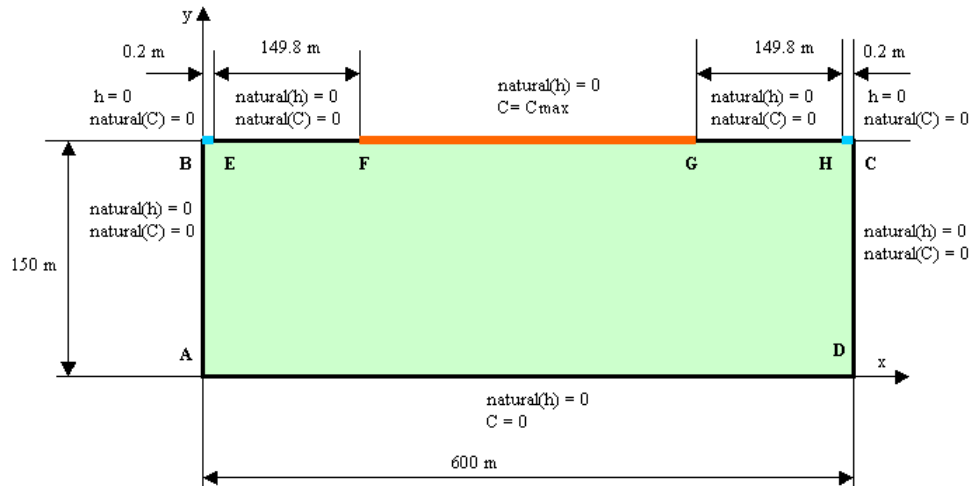3. *h, C, and Cmax are the valid PDE variables in a SVCHEM model.*

Figure 22 Model Geometry of Elder Problem

Initial Conditions:
Initial head: 150 *m,*
Initial concentration: 0 *g/m^3,*

Material Properties:
The material properties used in this benchmark is listed in Table 1:

Table 2 Material properties used in Elder's problem

| Symbol	Properties	Value	unit
Ksat	Saturated hydraulic conductivity	4.75×10^{-6}	*m/s*
SatVWC	Saturated water content	0.1	*m^3/m^3*
ρ_w	Fresh water density	1000	*kg/m^3*
ρ_{max}	The maximum seawater density	1200	*kg/m^3*
Cmax	The maximum solute concentration	285.7	*g/m^3*
D	Dispersion coefficient	3.56×10^{-5}	*m^2/s*

4.4.2   Results and Discussions

The concentration patterns simulated with SVCHEM/SVFLUX are illustrated in Figure 24. The concentration distribution is dependent on the mesh spacing of the model domain. An asymmetric concentration distribution is found in the simulation with the larger mesh spacing. Figure 25 is the numerical result simulated with the implicit settings of mesh spacing that is determined by the FlexPDE resolver. It can be seen from Figure 25 that the matching to the result presented by Simpson (2003) can be considered reasonable.

Boufadel (1999) suggested that the asymmetric concentration contour can be improved through reducing mesh spacing. Figure 26 shows the simulated result with the explicit setting of mesh spacing =3 *m* and nodes = 39,235. The pattern of concentration distribution is different from the original Elder problem, but the simulated result is similar to the numerical result obtained by Boufadel (1999).
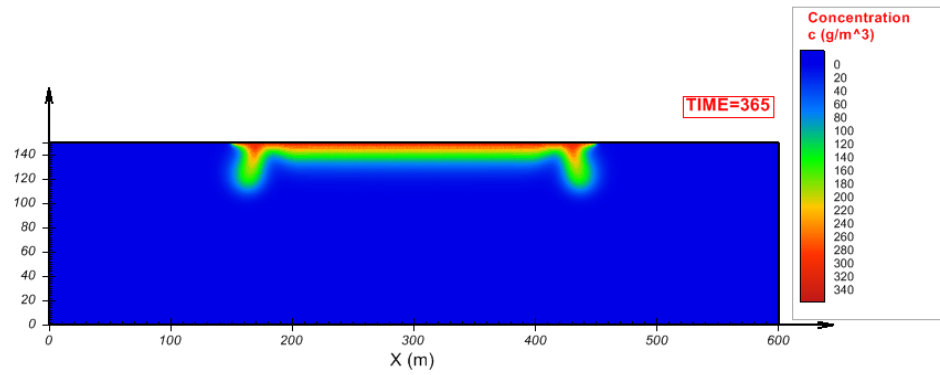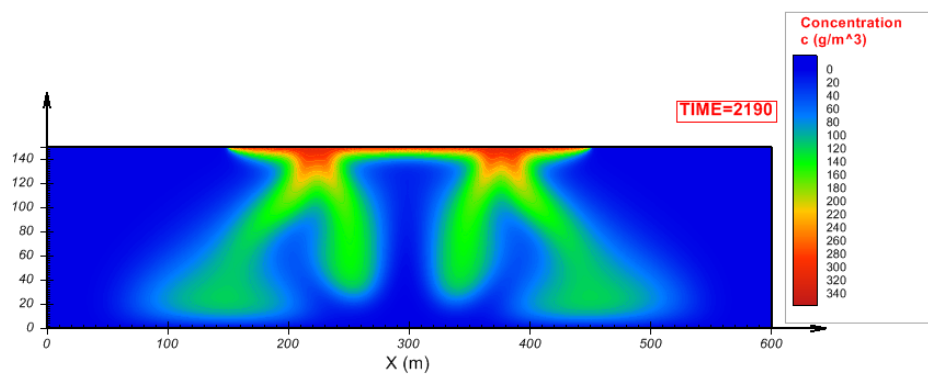
a. at the time of 1 year
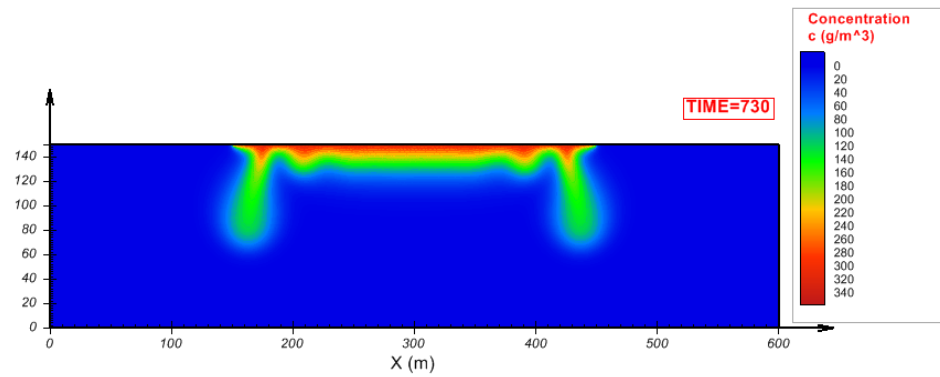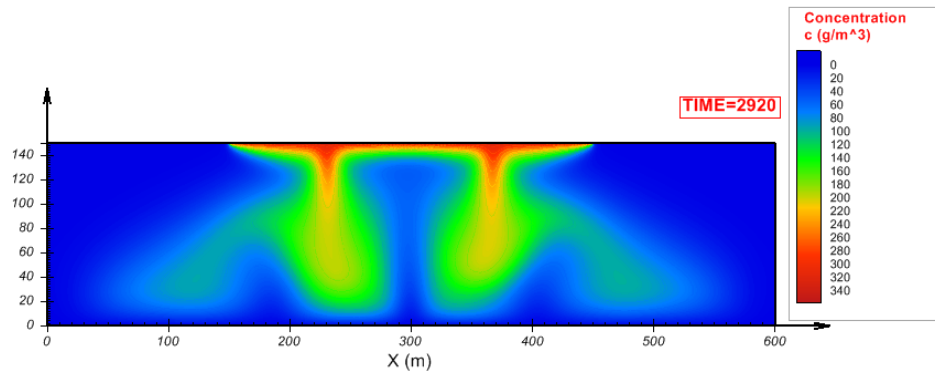

b. at the time of 2 year
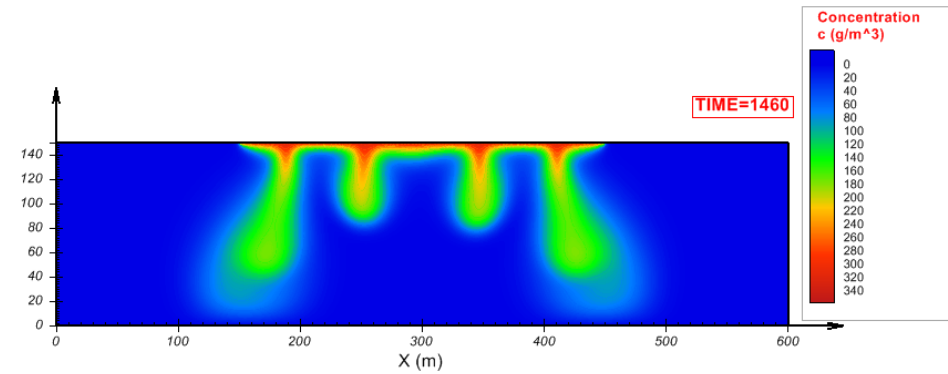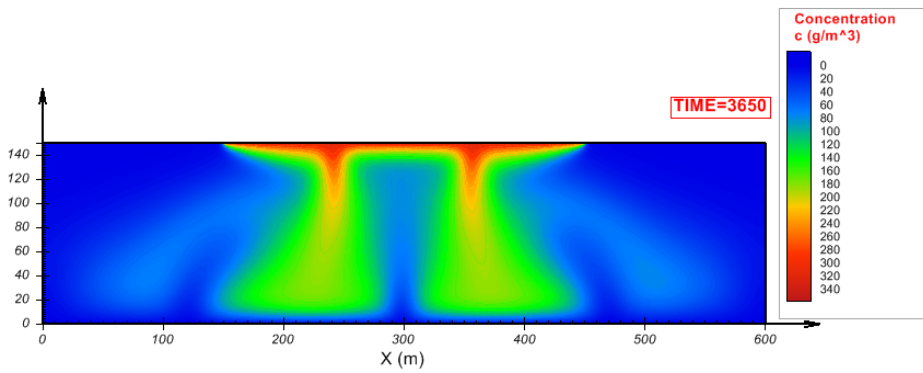

c. at the time of 4 year

Figure 23 Concentration patterns for the Elder problem at the time of 1 year, 2 years, and 4 years
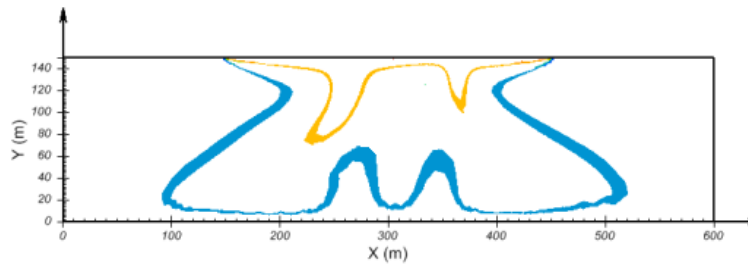

d. at the time of 6 years
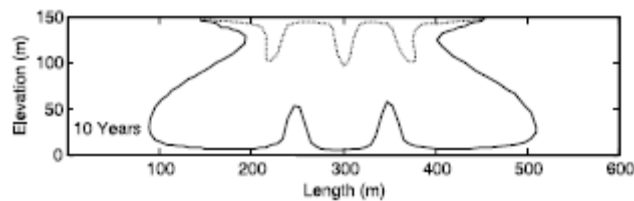
e. at the time of 8 years

f. at the time of 10 years

Figure 24 Concentration patterns for the Elder problem at the time of 6 years, 8 years, and 10 years
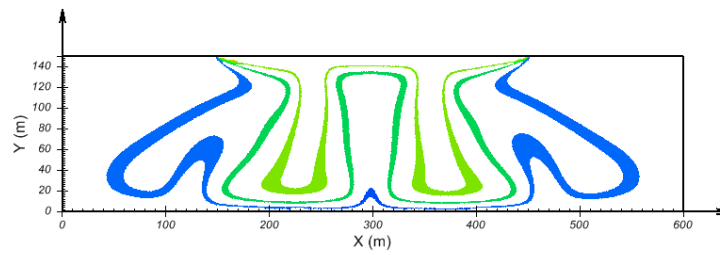

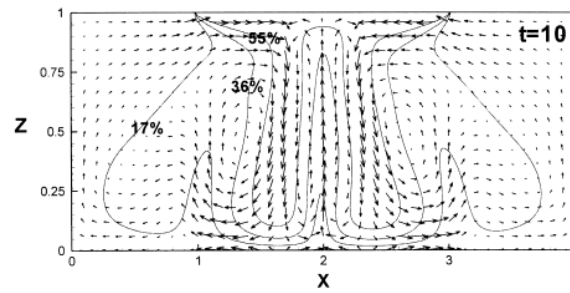**a. SVCHEM numerical result with the implicit settings of mesh spacing**

b. Simpson result of Elder problem (2003)

Figure 25 Comparison of simulation with Simpson's result (2003) of 20% and 60% of maximum concentration for Elder problem at the time of 10 years

a. SVCHEM simulation with the explicit settings of mesh spacing = 3 m and nodes = 39,235

b.   Boufadel result (1999) of 17%, 36%, and 55% maximum concentration for Elder problem

Figure 26 Comparison of Simulation with Boufadel result (1999) at the time of 10 years

5 REFERENCES

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