VERIFICATION OF A MODIFIED VERSION OF THE FEMWATER 3D SATURATED-UNSATURATED, VARIABLE-DENSITY FLOW AND TRANSPORT CODE.

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ABSTRACT
The groundwater flow and transport code FEMWATER was selected for modelling saturated-unsaturated, variable-density flow and brine transport at the ten tailings management areas (TMA) associated with potash mining in Saskatchewan. FEMWATER was originally developed for the U.S. Environmental Protection Agency and later updated and adopted as one of the codes supported by the U.S. Department of Defence groundwater modelling system (GMS). For application to TMA problems, the GMS-release of the FEMWATER code (version 2.1) was modified to allow pore-pressure response to total stress changes as a result of pile-loading at the surface to be modelled. The changes made it necessary to independently verify the revised code by running an extensive series of benchmark simulations. The benchmark solutions were compared with analytic solutions and numerical simulations using independent codes (such as FEFLOW, SEAWAT, SUTRA and TOUGH2). A large number of benchmark problems were assembled involving steady-state and transient flow, variable-density flow, variably saturated flow and pore-pressure dissipation and generation involving soil consolidation. Various aspects of the performance of FEMWATER are discussed as they relate to general problems and pitfalls encountered in code validation.

RÉSUMÉ
The groundwater flow and transport code FEMWATER was selected for modelling saturated-unsaturated, variable-density flow and brine transport at the ten tailings management areas (TMA) associated with potash mining in Saskatchewan. FEMWATER was originally developed for the U.S. Environmental Protection Agency and later updated and adopted as one of the codes supported by the U.S. Department of Defence groundwater modelling system (GMS). For application to TMA problems, the GMS-release of the FEMWATER code (version 2.1) was modified to allow pore-pressure response to total stress changes as a result of pile-loading at the surface to be modelled. The changes made it necessary to independently verify the revised code by running an extensive series of benchmark simulations. The benchmark solutions were compared with analytic solutions and numerical simulations using independent codes (such as FEFLOW, SEAWAT, SUTRA and TOUGH2). A large number of benchmark problems were assembled involving steady-state and transient flow, variable-density flow, variably saturated flow and pore-pressure dissipation and generation involving soil consolidation. Various aspects of the performance of FEMWATER are discussed as they relate to general problems and pitfalls encountered in code validation.

1. INTRODUCTION

Groundwater flow and transport models are finding increasing application as tools to assist in making complex decisions. They have been extensively applied in the areas of groundwater remediation, regulation, management, and litigation. It is vital for these applications that the computer codes are reliable and consistent and that they are subjected to stringent QA/QC requirements. There are three levels at which quality assurance and quality control procedures can be applied: verification, calibration and validation.

Calibration and validation of models take place at the site-specific application level to ensure that model simulations can match observed system responses. Calibration essentially involves tuning of model parameters within data constraints to obtain the best match to the measured response of a real system. Validation is a more stringent process requiring that models match data independent of the calibration. Such data should ideally be gathered after predictions have been made using a calibrated model to measure the predictive performance.

Code verification is a more fundamental level of QA/QC to establish that a computer code can correctly reproduce known solutions to problems generated using both analytical and numerical methods. This study describes the verification of the FEMWATER code (Lin *et al*, 2001).

2. FEMWATER VERIFICATION

The groundwater flow and transport code FEMWATER was selected for modelling saturated-unsaturated, variable-density flow and brine transport at the ten tailings management areas (TMA) associated with potash mining in Saskatchewan. FEMWATER was originally developed for the U.S. Environmental Protection Agency and later updated by the U.S Army Corps of Engineers, Waterways

Experiment Station and adopted as one of the codes supported by the U.S. Department of Defence groundwater modelling system (GMS).

For application to TMA problems, the GMS-release of the FEMWATER code (version 2.1) was modified to allow pore-pressure response to total stress changes as a result of pile-loading at the surface to be modelled. The changes made it necessary to independently verify the revised code by running an extensive series of benchmark simulations.

The ongoing verification exercise involves sixteen to twenty problems testing the saturated-unsaturated flow, variable density solute transport, and pore pressure response to total stress change; behaviours predicted by the code.

It is not possible to describe all the work in a short summary document. For this report, five problems relating to variable density solute transport are discussed. The cases considered are:

- Patch source problem (Cleary & Ungs, 1978)
- Density driven convection problem (Elder, 1967)
- Saline intrusion problem (Henry, 1964)
- Salt dome problem (Konikow *et al*, 1997)
- Layers cross-flow problem (Thiele & Diersch, 1986)

For each problem, parameter values and both boundary and initial conditions are briefly reviewed and the results of FEMWATER simulations are compared with analytical solutions and/or the results of other comparable codes including FEFLOW (Diersch, 2002), NAMMU (Atkinson *et al*, 1998), SUTRA (Voss & Sousa, 1987), SEAWAT (Guo & Langevin, 2002) and TOUGH2 (Oldenburg & Pruess, 1995).

2.1 Patch Source Problem

The idealized "patch-source" problem describes the transport of solute from a boundary source of finite extent into a rectangular domain subjected to a uniform, unidirectional velocity field.

Cleary and Ungs (1978) provide an analytical solution for the patch-source problem assuming homogeneous, semi-infinite domain with unidirectional flow with the solute source located along a finite length of y axis. Figure 1 shows the simplified 2D model domain for the patch source problem as defined by Daus and Frind (1985).

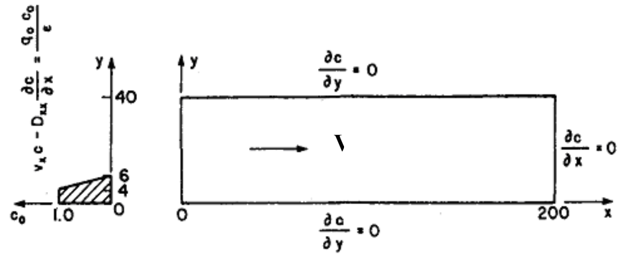

Figure 1: Idealized model domain for the patch source problem (Adapted from Daus and Frind, 1985)

Daus and Frind (1985) formulated the problem using an alternating direction Galerkin (ADG) finite element method with the source is located at the origin of the model domain considering both Dirichlet and Cauchy boundary conditions. Elnawawy *et al* (1990) solved the problem using cell analytical-numerical technique (CAN) for mass transport simulation. Leismann and Frind (1989) and Sudicky (1989) also simulated the patch source problem.

Figure 2 compares the numerical solutions obtained by Daus and Frind (1985) using the Dirichlet boundary condition after 160, 480 and 800 days, with the Cleary-Ungs analytical solution.

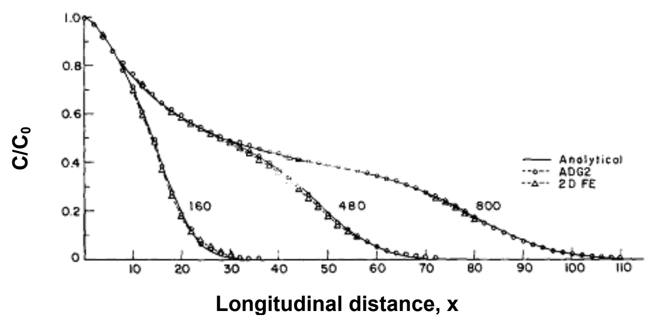

Figure 2: Longitudinal concentration profiles for Dirichlet boundary condition at y = 0 (Adapted from Daus and Frind, 1985)

Elanwawy *et al* (1990) also solved the patch problem using a Cell Analytical-Numerical (CAN) method. The results for various values of Peclet and Courant numbers are shown in Figure 3.

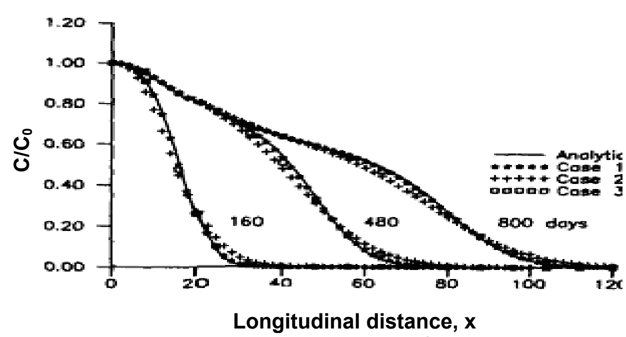

Figure 3: Longitudinal concentration profiles at y = 0 (Adapted from Elnawawy *et al*, 1990)

The FEMWATER model domain and boundary conditions were identical to those used by Daus and Frind (1985). It consisted of a 200 m x 40 m rectangle with a Dirichlet concentration source located on y-axis and extending a distance of 4 m from the origin (as shown in Figure 1) subjected to a 1D flow field parallel to the x-axis.

Figure 4 shows the concentration distribution predicted by FEMWATER for the model domain after 800 days. The ragged contours illustrate that the simulation is exhibiting some numerical oscillation.

Despite this problem (which can be eliminated by mesh refinement), the results shown in Figure 5 indicate a close fit with the analytical solution.

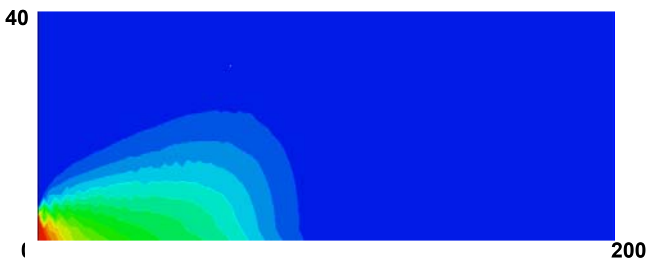

Figure 4: Model domain concentration distribution after 800 days using FEMWATER

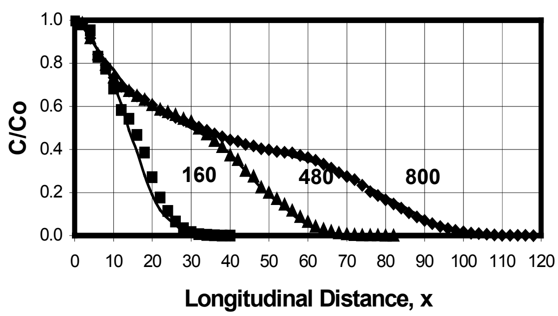

Figure 5: Longitudinal concentration profiles for Dirichlet boundary condition at y = 0 using FEMWATER

2.2 Density Convection Problem

The classic Elder's problem describes flow arising from a thermal instability in a porous medium which results in a plume driven by fluid density differences. This has been used by many authors, starting with Voss and Sousa (1987), as an analogue of density driven flow in groundwater systems created by solute concentration differences.

Figure 6 shows the model domain and boundary conditions used by Voss and Sousa (1987), Diersch (2002) and the current study to simulate density-driven plumes.

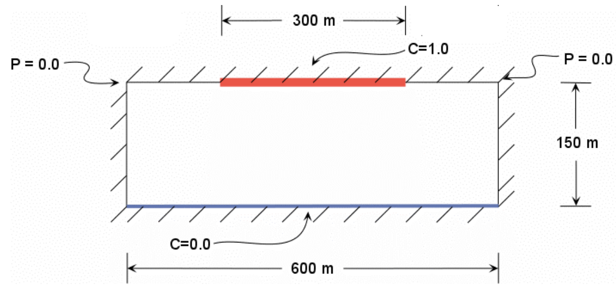

Figure 6: Definition of modified Elder's problem (Adapted from Reeves and Uweira, 2000)

Elder (1967) used a finite difference method to simulate the results of laboratory experiments. These FD numerical solutions to Elder's problem, shown in Figure 7, have been used by many researchers as a benchmark to verify numerical codes.

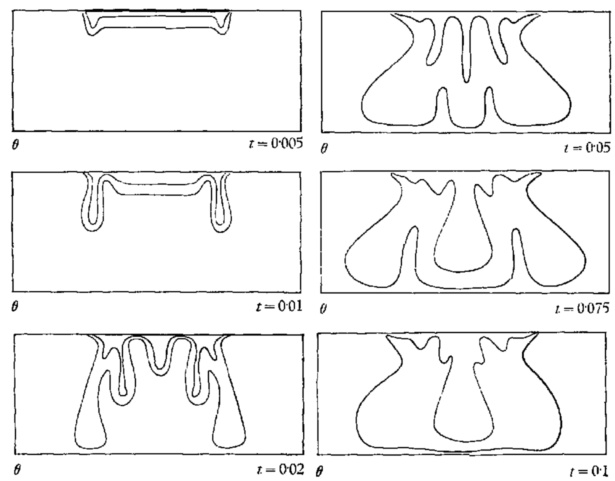

Figure 7: Results of Elder's FDM simulations (Adapted from Elder, 1967)

The original results presented in Figure 7 were computed in dimensionless time units and show contours for 20% and 60% of maximum fluid density. For comparison with more recent results, the times 0.005, 0.01, 0.02, 0.05, 0.075 and 0.1 correspond to 1, 2, 4, 10, 15 and 20 years.

Figure 8 shows the results from SEAWAT and SUTRA compared with the original Elder results.

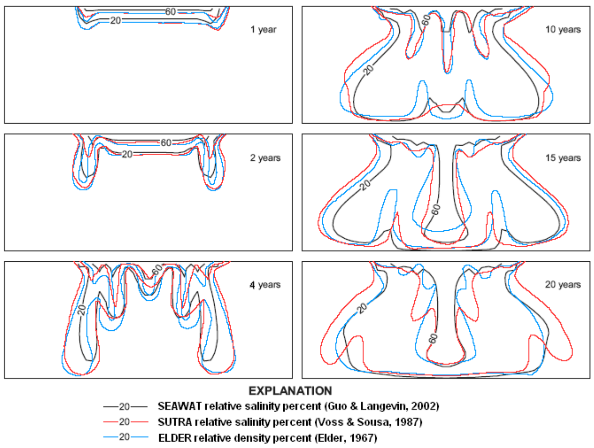

Figure 8: Comparison between SEAWAT, SUTRA and Elder's solution (Adapted from Guo & Langevin, 2002)

The mesh used for the FEMWATER simulation involved 1100 3D elements with mesh dimensions of 44 x 25. The simulation ran for a period of 20 years (7300 days). This is similar to the original 2D finite-difference grid of Elder (1967) with 1100 cells. Voss and Souza (1987) used a mesh 1600 elements. Diersch (1996) also used a mesh with 1100 elements. Guo and Langevin (2002) used a finite difference grid with 1188 cells.

The FEMWATER results (Figure 9) are similar (but not identical) to those generated by the original Elder model, by Voss and Souza using SUTRA, by Guo and Langevin using SEAWAT and by Diersch using FEFLOW.

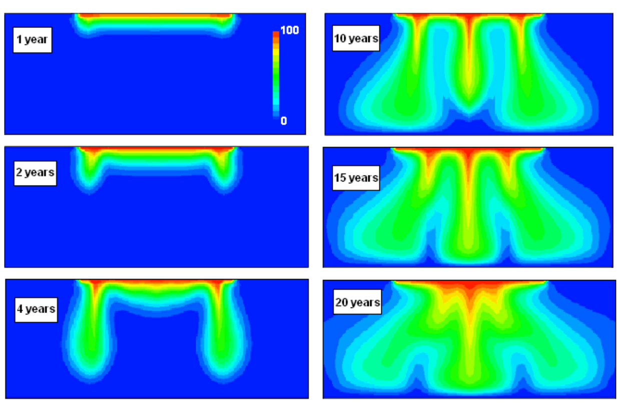

Figure 9: Results of FEMWATER simulation of Elder's problem.

Solutions to Elder's problem have been found by other authors (most recently Diesrsch, 2002) to be sensitive to small changes in initial conditions and boundary conditions. The solutions can also be sensitive to mesh spacing, time stepping and the solution method, particularly the "sweep-direction" of some solvers. Given these known sensitivities, the differences in detail in the various simulation results are understandable.

2.3 Saline Intrusion Problem

The extent of encroachment of seawater and the location of the zone of brackish water are significant factors in determining the use of groundwater from coastal areas (Henry, 1964). The saline intrusion phenomenon has been investigated by several researchers making a variety of assumptions. Using the description of conditions at the interface in terms of the velocity potential of the freshwater and saltwater, Hubbert (1940) suggested the boundary condition for an interface. Glover (1959) found an analytical solution technique for salt encroachment problem for an artesian aquifer of infinite thickness.

In the process of advance of saltwater into freshwater, saltwater merges with the freshwater in a zone of diffusion. there is a motion of saltwater from the ocean into the zone of diffusion (Henry, 1964). If the zone of diffusion is extensive, he process takes the form of dispersion and the entrainment of saltwater by moving freshwater. Cooper (1959) found that the dispersion is sufficient to cause a large amount of saltwater to become entrained in the otherwise freshwater flowing seaward.

Henry (1964) investigated the advance of a saltwater front in a confined aquifer that is initially charged with uncontaminated freshwater, assuming that the interface between freshwater and saltwater is sharp and well defined. The effect of dispersion at the saltwater front was also taken into consideration. Henry derived analytical expressions for the stream function and the concentration in the form of a Fourier series that enable to calculate the steady state solute distribution for the system.

Henry's (1964) approximate analytical solution for steady state seawater intrusion is widely used for verification of variable density transport models.

No model to date has successfully matched the Henry's solution. This may be due to inaccuracy of Henry's results, possibly due to missing of higher order terms that were originally dropped for the sake of reducing computational time (Voss and Souza, 1987). And another possible reason is that the neglect of velocity dependent dispersion in order to make the semi analytical solution tractable (Voss and Souza, 1987).

Figure 10 shows the idealized aquifer system commonly used for numerical verifications for the Henry's problem.

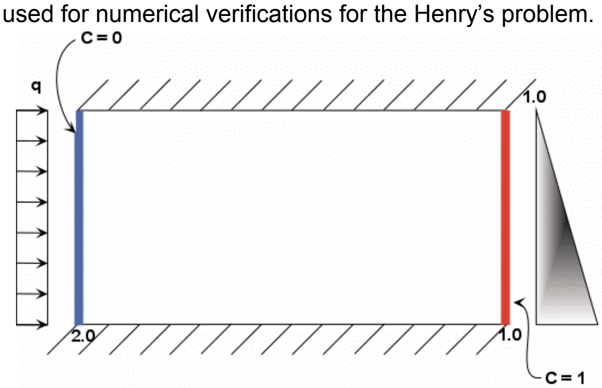

Figure 10: Definition of the Henry's problem (Adapted from Reeves and Uwiera, 2000)

Zero flux boundaries are defined along the top and the bottom of the aquifer. Hydrostatic pressure distribution is assumed along the RHS saltwater boundary. The aquifer is charged with at a constant flux along the LHS freshwater boundary. A constant nonzero concentration is applied on the RHS saltwater boundary together with a zero concentration on the LHS freshwater boundary.

Figure 11 shows the streamlines predicted by Henry's semi-analytical solution.

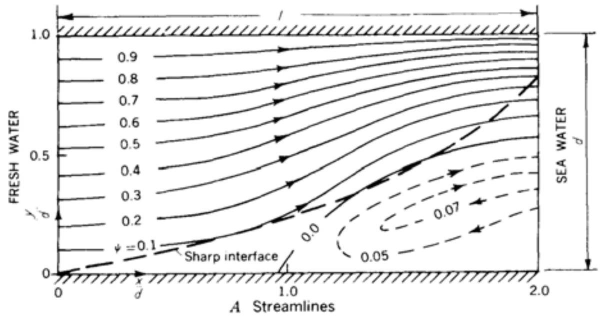

Figure 11: Stream Functions obtained by Henry (Adapted from Henry, 1964)

The sharp interface (dashed line) is the analytical prediction if mixing is ignored. Notice the converging streamlines on the freshwater side and the vortex beneath the interface on the seawater side.

Figure 12 shows the concentration profiles obtained by Henry using his semi analytical solution.

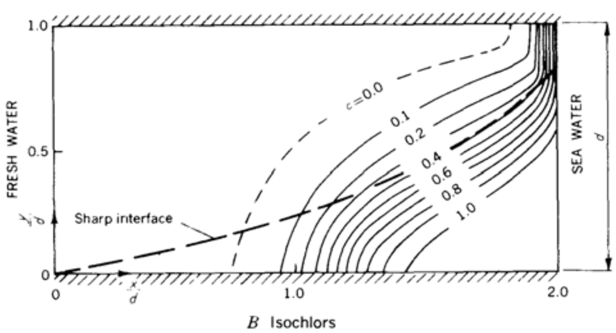

Figure 12: Concentration profiles obtained by Henry (Adapted from Henry, 1964)

Henry's solution predicts a relatively steep broad zone of mixing rather than a sharp interface. The width and rate of development of the zone depend on the diffusion and dispersion characteristics of the porous medium.

A number of numerical models based on significantly different methods give nearly identical results for the Henry's problem (Figure 13). These include a particle tracking model by Pinder and Cooper (1970), FEM codes by Segol et al. (1975), Huyakorn and Taylor (1976), Desai and Contractor (1977) and Frind (1982), an FDM code by INTERA (1979), and the USGS FEM model SUTRA (Voss, 1984; Voss and Souza, 1987). The results were assembled by Diersch, 2002 for comparison with results from the FEFLOW code shown on the LHS in Figure 13.

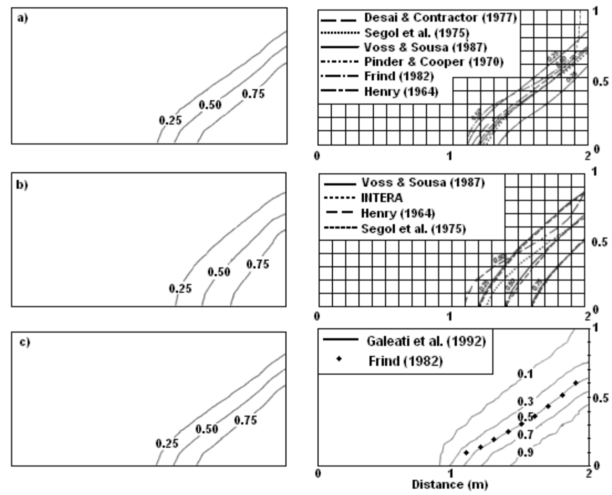

Figure 13: Comparison of FEFLOW simulation results with earlier authors (Adapted from Diesrch, 2002)

Simulation parameters used for the FEMWATER analysis were similar to those of FEFLOW except for details of time stepping and the solver. The point-wise iterative solver was used. Simulations were run for two values of dispersion coefficient: 6.60 x 10^{-6} m^2/s (Low D_d) and 18.9 x 10^{-6} m^2/s (high D_d).

The relative concentration (C/C_0) results are shown in Figure 14. The figure shows the results for a coarse (20 x 10) FEMWATER mesh. The contours represent fractional salinities of 0.05, 0.1, 0.2, 0.3, 0.5, 0.7, 0.8, 0.9 and 0.95.

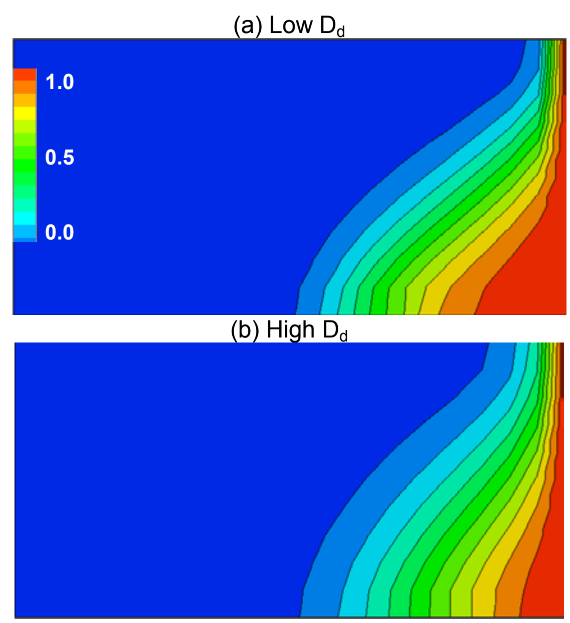

Figure 14: Relative concentration (C/C_0) contours for the 20 x 10 mesh with low (a) and high (b) diffusion coefficients.

The FEMWATER results closely match the results from other codes for the “standard” 20 x 10 mesh for similar assumptions for diffusion coefficient. All model codes predict a clear difference for the advance of the interface for low and high D_d cases.

2.4 Salt Dome Problem

HYDROCOIN Case 5, level 1 of the international groundwater flow modeling test suite is an attempt to investigate an idealized flow over a salt dome in which groundwater flow and solute transport taking place in a two dimensional vertical plane where fluid density depends on the dissolved solids concentration. The problem was developed to represent a rough approximation of conditions existing at the Gorleben salt dome in Germany (Konikow *et al*, 1997).

Figure 15 shows the idealized model domain with the basic geometry and boundary conditions. The domain is simplified to a 900m long and 300m thick 2D cross section. A homogeneous and isotropic aquifer with freshwater recharge at the surface is considered. No flow boundary conditions are applied at the sides and bottom while the top boundary is represented by a linearly varying specified pressure condition. The pressure gradient along the top boundary induces a flow from left to right but does not predetermine either the rates of recharge and discharge or the separation point between recharge and discharge zone (Konikow *et al*, 1997).

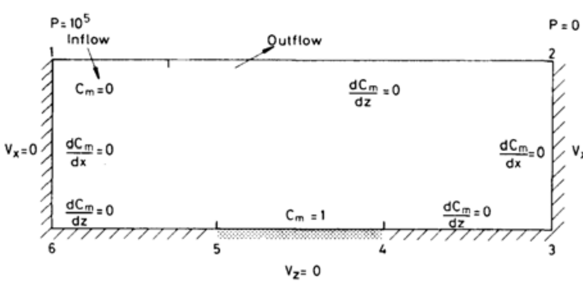

Figure 15: Geometry and boundary conditions of the HYDROCOIN salt dome problem (Adapted from Younes *et al.,* 1999)

It is assumed that the top of the salt dome is exposed to circulating groundwater in the overlying aquifer and that saturated brine is released from this surface by a diffusive or dispersive process. Salt is enters the flow system by transverse dispersion only along the central third of the bottom boundary and that flow velocity is zero within the salt dome. Only numerical solutions are available for this verification problem.

Numerical codes that have been tested using the HYDROCOIN problem include NAMMU (Atkinson et al., 1985), SUTRA (Voss, 1985), FEFLOW (Diersch and Kolditz, 1998) and TOUGH2 (Oldenberg and Pruess, 1995). Pure diffusive, diffusive-dispersive and pure dispersive regimes have been considered.

Figure 16 shows the steady state solute distribution for diffusive-dispersive model with dispersivities β_L = 20m, β_T = 2m and diffusion coefficient $D_d = 5x10^{-8}$ m^2/s.

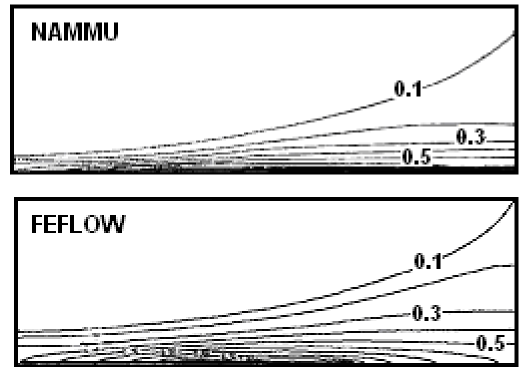

Figure 16: Comparison of steady state salt distribution using NAMMU and FEFLOW codes for diffusive-dispersive model (Adapted from Diersch, 2002).

The figure compares the results of NAMMU (Herbert *et. al.*, 1988) with FEFLOW results (Diersch and Kolditz, 1998). The flow patterns are similar in shape for both NAMMU and FEFLOW.

Figure 17 compares the TOUGH2 results with FEFLOW for the dispersive model with β_L = 20m and β_T = 2m and zero diffusion coefficient. Oldenburg and Pruess (1995) showed that clockwise recirculation of salt against the anticlockwise flow is possible in case of a large diffusivity. But for small diffusivity, the convection forces are insufficient to develop such a circulation and hence salt is swept forward from left to right with the flow as shown in Figure 17.

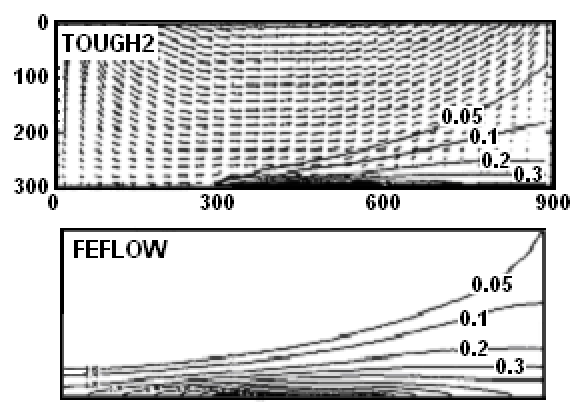

Figure 17: Comparison of FEFLOW and TOUGH2 results for pure dispersive model (Adapted from Diersch, 2002).

Figures 18a shows the FEMWATER relative concentration results for the NAMMU-FEFLOW diffusive-dispersive case. Figure 18b illustrates the steady state salt distribution after 100 years for the FEMWATER simulation for the TOUGH2-FEFLOW zero-diffusion case.

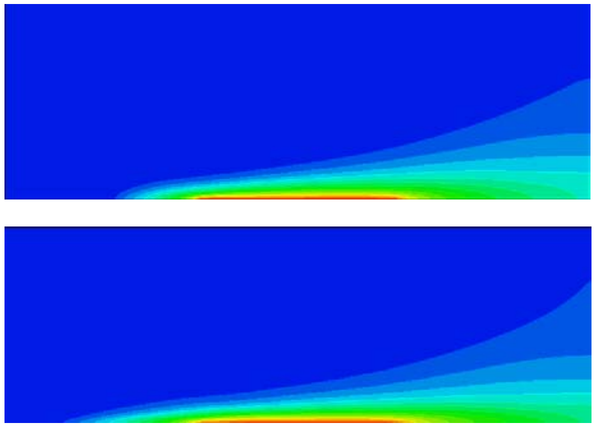

Figure 18: FEMWATER results for (a) diffusive-dispersive and (b) pure dispersive cases.

FEMWATER results (contour interval 0.1) are similar to those obtained using FEFLOW, NAMMU and TOUGH2.

2.5 Layers Problem

Saltwater encroachment problems from deep aquifers are important in the field of water supply. Transient effects can result in an elevation of salinity in shallow aquifers arising from induced interflow as a result of shallow pumping. Typically contaminant concentrations rise to a maximum, then fall back to a lower equilibrium value. This phenomenon is known as “overshooting”.

Figure 19 shows a sketch (a) of a typical saltwater layer problem. The model representation of the system is shown as (b). The upper layer of the aquifer contains groundwater with low salinity freshwater and the underlying layer contains higher salinity saltwater.

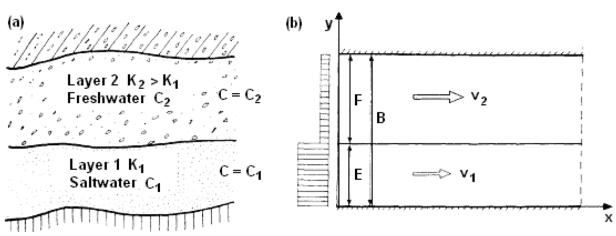

Figure 19: Schematic sketch of a layered aquifer system (Adapted from Thiele and Diersch, 1986)

Under a uniform horizontal flow gradient, permeability differences between the lower and upper layers will result in the development of differential velocities v_1 and v_2. Assume that the initial saltwater concentrations of lower and upper layers are C_1 and C_2 respectively. The boundary conditions, illustrated in Figure 19b, assume no vertical concentration gradient (zero mass flux) at the upper boundary and no change in concentration within the horizontal layers. Two boundary conditions are considered for bottom boundary; Case1: zero flux and Case2: constant concentration C_1. The saltwater concentrations are maintained at C_1 and C_2 on the LHS boundary for all times.

Bruch and Street (1967) studied the layered aquifer system and derived an analytical expression for saltwater concentration. Their investigation was based on transient pollution of an initially uncontaminated semi-infinite layered aquifer, that is, initially the system had uniform concentration C_2. Their solution failed to explain “overshooting”.

Thiele and Diersch (1986) derived a more general analytical expression for 2D, unsteady, convective and hydro-dispersive saltwater spreading in finite layers. In this study, an initially pre-contaminated finite layered aquifer was considered, that is, the initial concentrations in the two layers were not equal. Figure 20 compares the two transient analytical solutions.

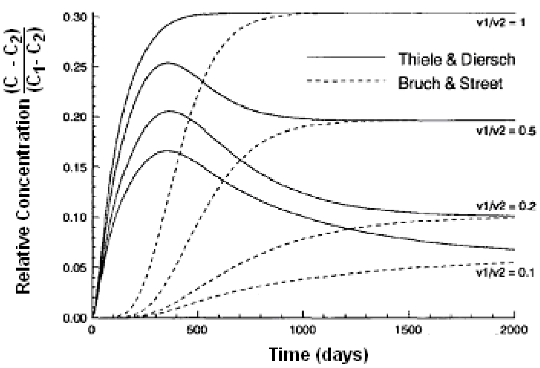

Figure 20: Analytical solutions for field point x=200, y=20 (Adapted from Thiele and Diersch, 1986)

For the inhomogeneous initial condition, the predicted concentration change is no longer monotonic. A peak transient value is predicted above the eventual equilibrium concentration. The Thiele and Diersch solution captures the “overshooting” phenomenon.

Figure 21 shows the transient numerical solution obtained using the FEFLOW code for the field point (200m, 20m). Comparing Figures 20 and 21 it can be seen that the numerical results generally agree with the analytical solution obtained by Thiele and Diersch (1986).

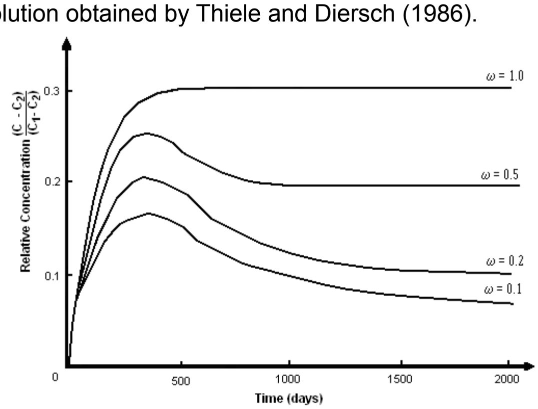

Figure 21: Predicted saltwater relative concentration curves at different velocity ratios using the FEFLOW code (Adapted from Diersch (2002).

For the verification study, a FEMWATER mesh of 1938 elements (102x19) was used. The simulation period was 2000 days. The simulation was performed using variable time steps with coupled flow and transport options of the FEMWATER package. The precondition conjugate gradient (PCG) solver was utilized.

Figure 22 shows that the system reaches a constant equilibrium value of 0.20 after an extended period of time (2000 days). The relative concentration $(C-C_2)/(C_1-C_2)$ distributions are shown in the figure.

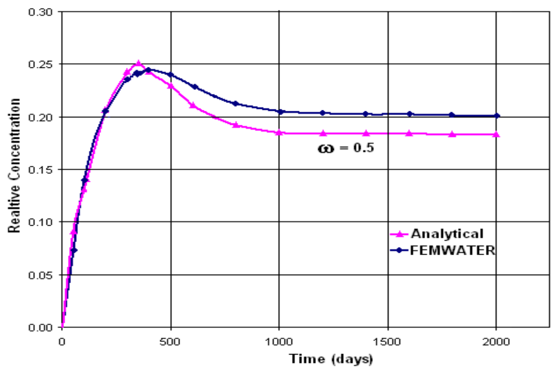

Figure 22: Predicted saltwater relative concentration curves using FEMWATER for velocity ratio 0.5.

The FEMWATER numerical results compare well with the Thiele and Diersch (1986) analytical solution although they are not coincident. The maximum saltwater concentration occurs after about 400 days. After 1000 days, the saltwater concentration reaches a constant value. The shape of the breakthrough curves obtained using FEMWATER are comparable with the results using FEFLOW.

3. CONCLUSIONS

The modified FEMWATER code has been successfully verified for variable density flow and transport problems by comparing simulation results with analytical and numerical solutions for a wide range of problems.

4. ACKNOWLEDGEMENTS

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