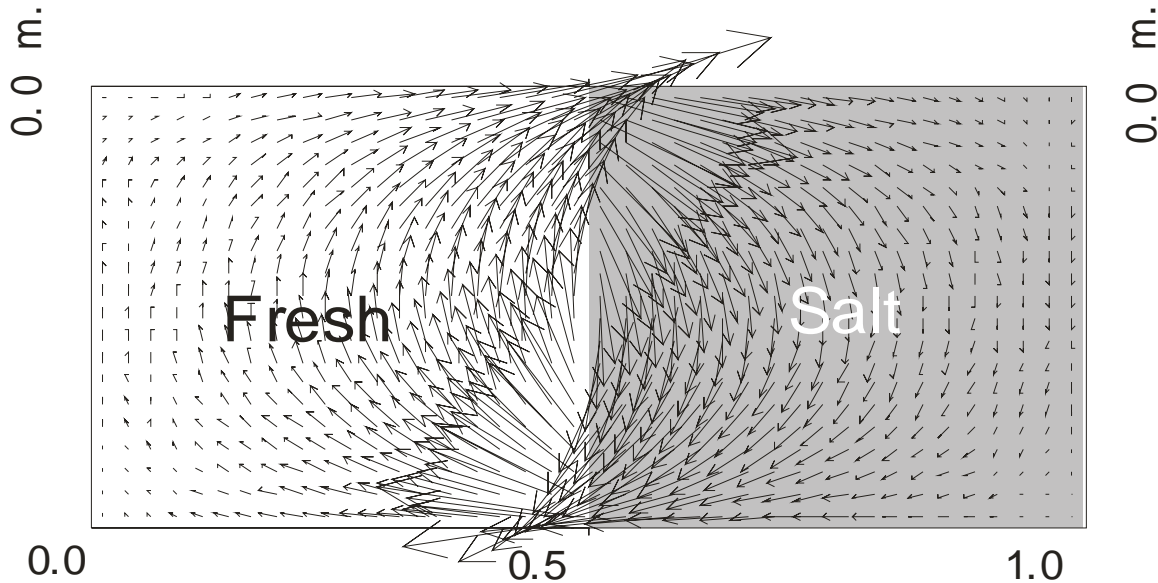


Vertical interface between fresh and saline groundwater

Variable-density groundwater flow modelling with SEAWAT



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Introduction

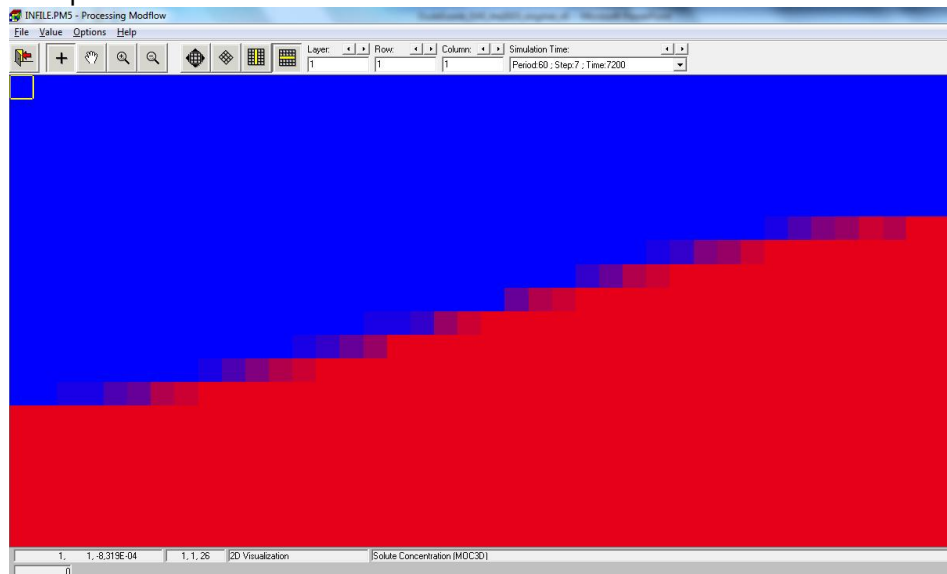
A hypothetical problem: a vertical fresh-saline interface in a homogeneous aquifer with the following geometry: horizontal $L=1.0$ m by vertical $D=0.5$ m. Interface approximation is simulated, which means: $D_{mol}=0$ m²/s, $\alpha_L=\alpha_{TH}=\alpha_{TV}=0$ m en $R_d=1$ (so no retardation). The other soil parameters are: hydraulic conductivity $k=10^{-3}$ m/s and porosity $n_e=0.1$.

Parameters

Layers	20	K_{hor}	$1 \cdot 10^{-3}$ m/s
Rows	1	$T (=K_{hor} \cdot \text{thickness cell})$	$2.5 \cdot 10^{-5}$ m/s
columns	40	Anisotropy K_{hor}/K_{ver}	1
Δx	0.025 m	n_e	0.1
Δy	1 m	α_L	0 m
Δz	0.025 m	α_T	0 m
Stress periods	15		
Initial concentration	0 and 35000 mg/l		
density buoyancy	0.025		

The total simulation consists of 720 time steps Δt of 30 s, divided over 15 'stress periods': the simulation time is 360 min=0.25 day.

This conceptual model has always been simulated with MOC3D. This code (MOC3D adapted for density differences) is similar to SEAWAT, and pretty powerful in solving solute transport issues. The result with this code is after 7200sec is:



The number of initial particles is 16, which appears to be enough for this case.

Some tips on modelling

When numerical modelling, learn to be as neatly as possible because this behaviour helps you avoiding vague modelling results with you cannot explain nor understand anymore. In modelling practices, you normally forget within days where a specific model with specific model input parameters and variables run was about. Try to keep up a smart and clear logbook system (e.g. in EXCEL) explaining about the changed model input data files, and describe what you see as significant or major modelling results that are different than in the previous model run(s). Create a new subdirectory for every new model run, e.g. by copying an old previous one and rename it. Important is to set up about a proper naming system: number every new model with enough digits, e.g. vertint001, vertint002, etc. Avoid spaces in names in files and subdirectories. Under normal circumstances running big 3D models, you also have to limit model output which easily can end up in hundreds of Gb's of memory when you testing around. Better zip input data of old model runs. Big modelling output files could be zipped and saved too, but those output files are not essential (a new model run could be executed again). By experience, it is strongly recommended to use Total Commander (freeware), which helps you in better manage model runs, use short cuts like file and directory content comparison. Note you also need good freeware text editors like the Med Editor, Textpad and Notepad ++.

Exercise 1: geometry of the problem

- This model vertint001 has already been run.
- Check in PMWIN the input files: heads, time-characteristics, IBOUND, MODFLOW; SEAWAT parameters. You still understand the input files?
- Check the concentration and the flow face results and explain what is going on.

- Why do cells exist with a concentration not equal to fresh or saline groundwater? Why does a large number of these cells disappear as a function of time?
- Is the steady-state time reached after 0.25 day (21600sec), based on the concentration distribution?

Exercise 2: on the best solute solver to reproduce the SEAWAT result

As can be seen checking the results with the default Advection solver ('ULTIMATE'), it is not easy to get a sharp interface (remember that no hydrodynamic dispersion is simulated!). Try to find a proper solver among the Advection solvers ('Models'->'MT3DMS / SEAWAT'->'Advection'): Finite Difference Method, MOC, HMOC, MMOC, ULTIMATE. You must change parameters within the solvers themselves, such as number as particles in the MOC versions; if you want to know more about the different parameters, check e.g. the PMWIN manual of the MT3DMS manual¹. Run SEAWAT.

NOTE: to be sure the old model runs remain and that you can compare the results; make new model runs in new subdirectories: e.g. vertint002, vertint003, etc.!

Exercise 3: effect of a larger density of saline groundwater

Use the best solute solver from Exercise 2. Change within 'MT3DMS / SEAWAT'-> 'Simulation settings' the value DRHODC in such a way that the saline/brine groundwater has a density of 1050 kg/m³. Run SEAWAT.

- Check the concentration results.

NOTE: to be sure the old model runs remain and that you can compare the results; make new model runs in new subdirectories!

Exercise 4: effect of dispersion

Use the best solute solver from Exercise 2. Add dispersion to the system: $\alpha_L=1.0$ m; $\alpha_{TH}=\alpha_{TV}=0.1$ m. 'MT3DMS / SEAWAT'-> 'Dispersion'. Run SEAWAT.

- Run the file with 'run.bat' in the same subdir.
- Analyse the effect due to the differences compared with the reference case.

NOTE: to be sure the old model runs remain and that you can compare the results; make new model runs in new subdirectories!

Exercise 5: effect of length of time step Δt : from 30 sec to 900 sec

'Parameters'-> 'Time'. Change the length of each time step to 900 sec by changing the 'No. of time step'. Run SEAWAT.

- Analyse the effect on the concentration distribution, especially during the first time steps.

NOTE: to be sure the old model runs remain and that you can compare the results, make new model runs in new subdirectories!

¹ Zheng, C., & Wang, P. (1999). *MT3DMS: A modular three-dimensional multispecies transport model for simulation of advection, dispersion, and chemical reactions of contaminants in groundwater systems. Technical report, Waterways Experiment Station, US Army Corps of Engineers.*