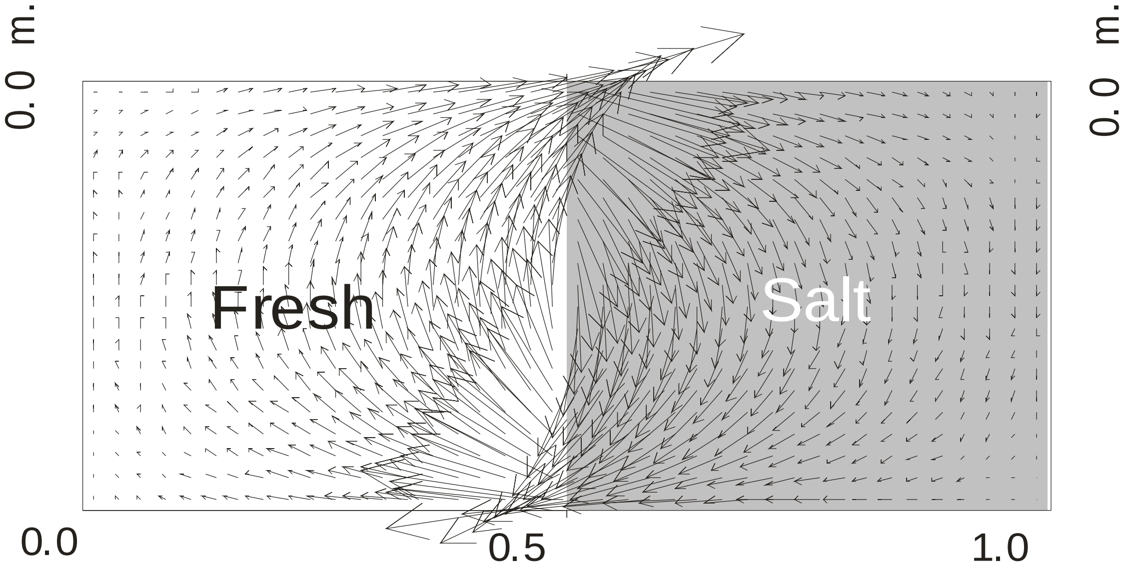
Vertical interface between fresh and saline groundwater

Variable-density groundwater flow modelling with SEAWAT



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Enabling Delta Life

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Introduction

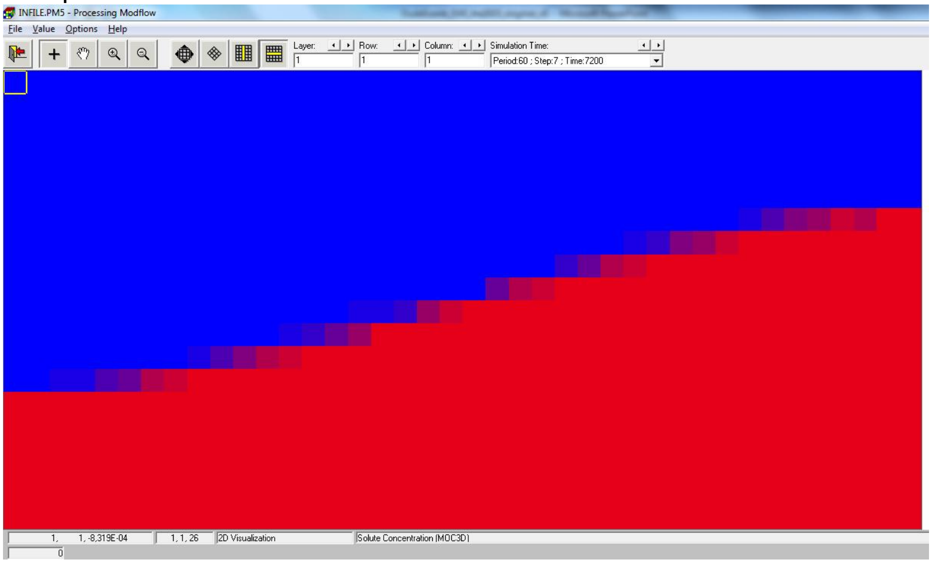
A hypothetical problem: a vertical fresh-saline interface in a homogeneous aquifer with the following geometry: horizontal L=1.0 m by vertical D=0.5 m. Interface approximation is simulated, which means: D_{mol}=0 m^2/s, $\alpha_L=\alpha_{TH}=\alpha_{TV}$= 0 m en R_d=1 (so no retardation). The other soil parameters are: hydraulic conductivity $k=10^{-3}$ m/s and porosity n_e=0.1.

Parameters

Layers	20	K_{hor}	$1*10^{-3}$ m/s
Rows	1	T (=K_{hor}*thickness cell)	$2.5*10^{-5}$ m^2/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 MOCDENS3D. 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:



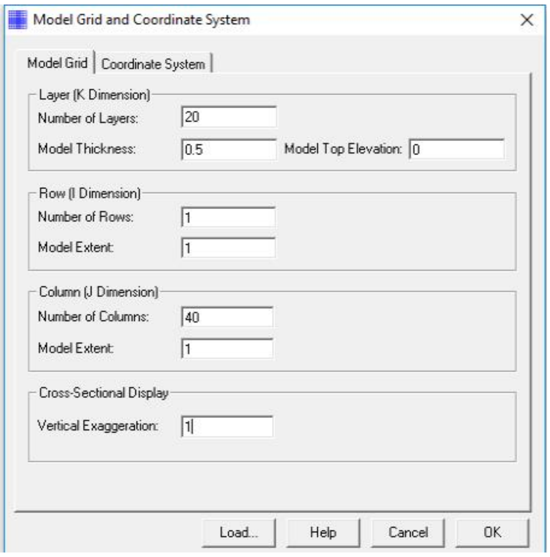
The number of initial particles is 16, which appears to be enough for this case.

Some tips on modelling

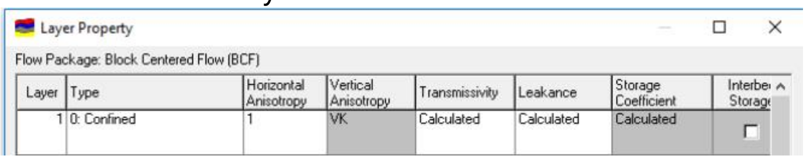
When numerical modelling, learn to be as neatly as possible because this behaviour helps you avoiding vague modelling results with you cannot explain nor understand anymore. In modelling practices, you normally forget within days where a specific model with specific model input parameters and variables 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. verint001, 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: link), which helps you in better manage model runs (some hotkeys: link), 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 000: making of the model

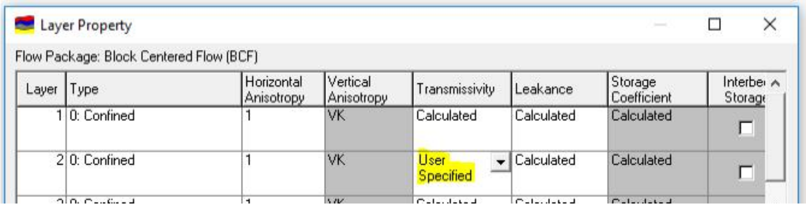
1. Go to: File, New Model
   Name the new model: e.g. 'vertint000'
2. Go to: Grid, Mesh Size



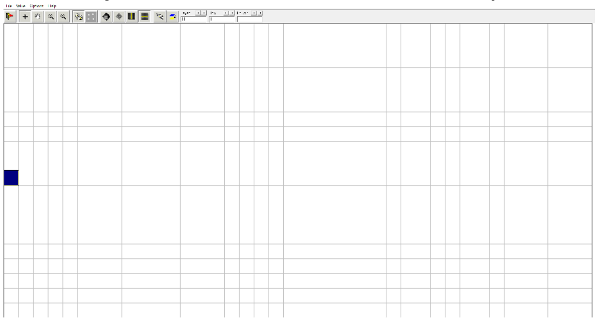
3. Go to: Grid, Layer Property
   Make all 20 model layers '0: Confined'



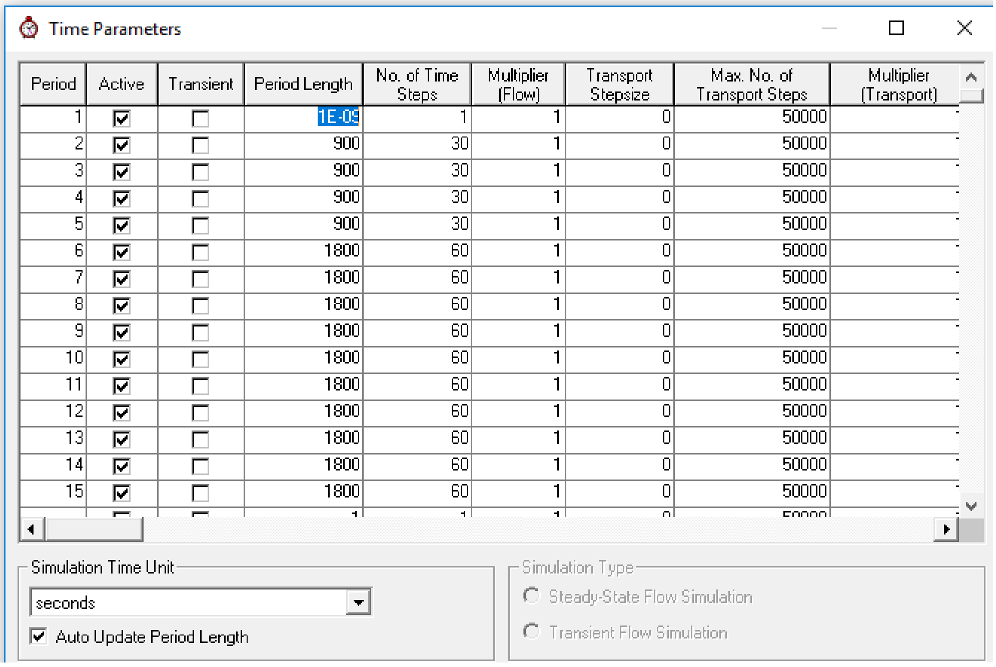
   Make sure that Transmissivity and Leakance are 'Calculated' for all model layers



4. Place a fixed head in the model
   Go to: Grid, Cell Status, IBOUND (MODFLOW)
   Make layer=11, Row=1, Column=1: -1 (now this cell has a fixed head)

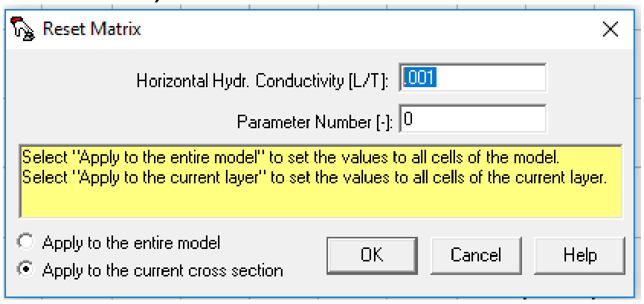


5. Go to: Parameter, Time
   Make 15 stress periods
   SP1: period length 1E-09 sec, No. of Time Steps 1
   SP2-5 period length 900 sec, No. of Time Steps 30
   SP6-15 period length 1800 sec, No. of Time Steps 60

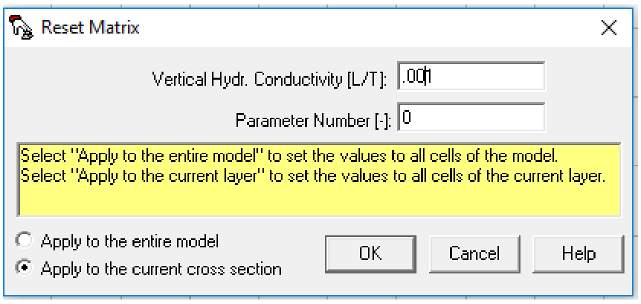


Period	Active	Transient	Period Length	No. of Time Steps	Multiplier (Flow)	Transport Stepsize	Max. No. of Transport Steps	Multiplier (Transport)
1	☑	☐	1E-09	1	1	0	50000	
2	☑	☐	900	30	1	0	50000	
3	☑	☐	900	30	1	0	50000	
4	☑	☐	900	30	1	0	50000	
5	☑	☐	900	30	1	0	50000	
6	☑	☐	1800	60	1	0	50000	
7	☑	☐	1800	60	1	0	50000	
8	☑	☐	1800	60	1	0	50000	
9	☑	☐	1800	60	1	0	50000	
10	☑	☐	1800	60	1	0	50000	
11	☑	☐	1800	60	1	0	50000	
12	☑	☐	1800	60	1	0	50000	
13	☑	☐	1800	60	1	0	50000	
14	☑	☐	1800	60	1	0	50000	
15	☑	☐	1800	60	1	0	50000	

6. Go to: Parameter, Initial & Prescribed Hydraulic Heads [L]
   Leave Editor, save (so now the value is saved).
7. Go to: Parameter, Horizontal Hydraulic Conductivity
   Go to: Value, Reset Matrix
   Set to 0.001 (in 2D, 'Apply to the entire model' or 'Apply to the current cross section is the same')

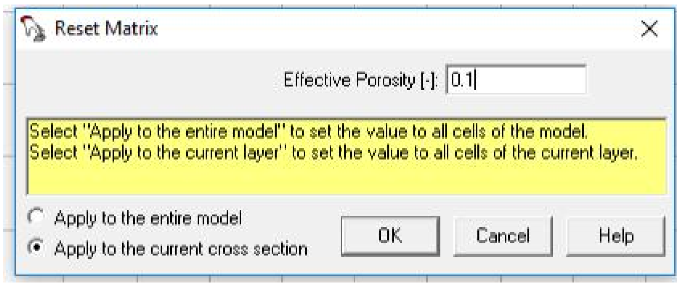


   Leave Editor, save
8. Go to: Parameter, Vertical Hydraulic Conductivity
   Go to: Value, Reset Matrix
   Set to 0.001

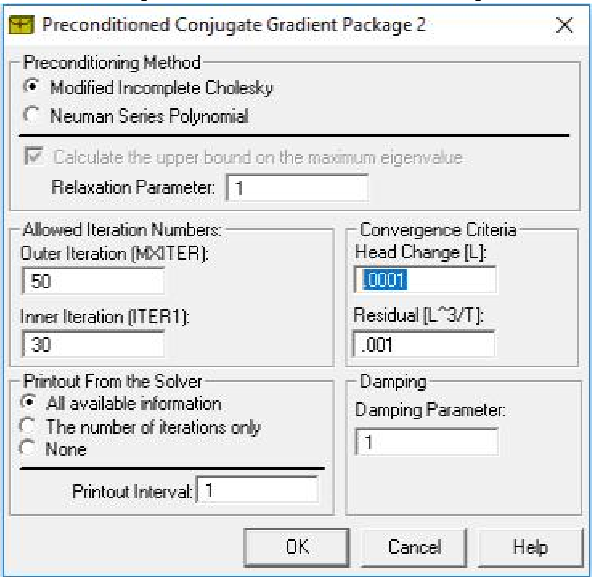


   Leave Editor, save

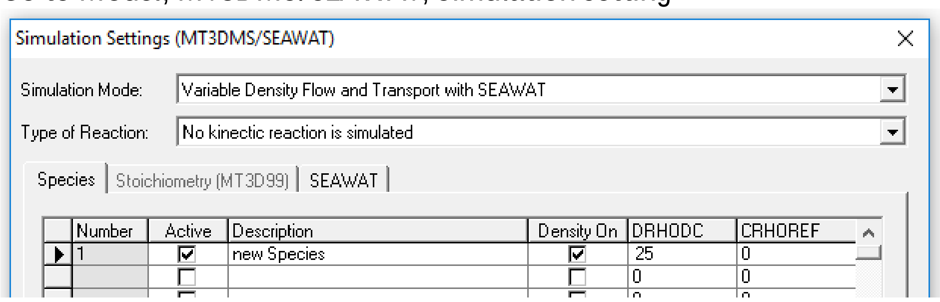
9. Go to: Parameter, Effective Porosity
   Go to: Value, Reset Matrix
   Set to 0.1



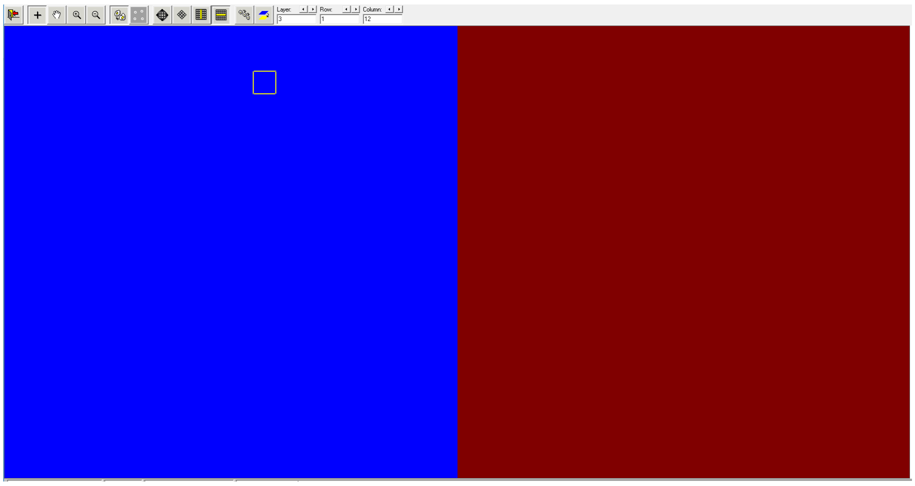
   Leave Editor, save
10. Go to Model, MODFLOW (Flow Simulation), Solvers, PCG2
   Set Convergence Criteria, Head Change to 0.001



11. Go to Model, MT3DMS/SEAWAT, Simulation setting

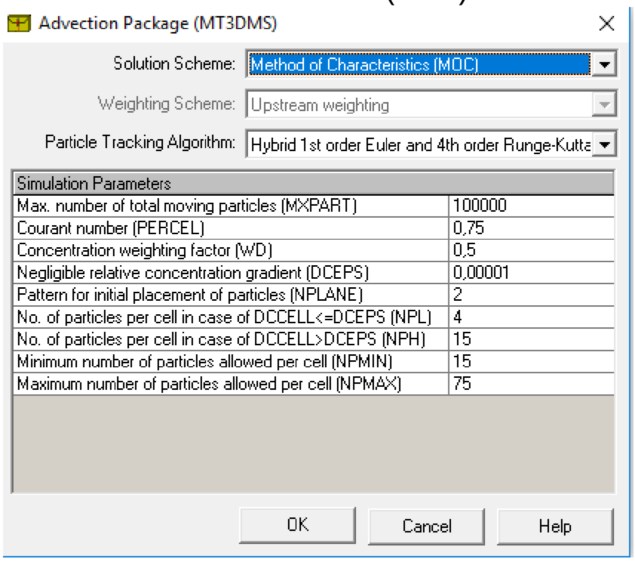


   Set Simulation Mode: Variable Density Flow and Transport with SEAWAT
   Set Species, Number 1, Active, ‘new Species’, Density ‘On’
   Set DRHODC=25 (this is the DRHODC term, Equation of State: $\partial \rho / \partial C$)
12. Go to Model, MT3DMS/SEAWAT, Initial Concentration
   Set cells 1-20: Initial concentration=0, cells 21-40: Initial concentration=1

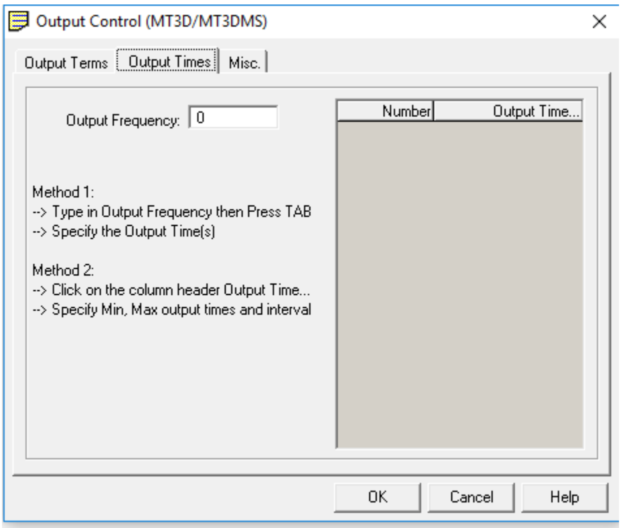


Leave Editor, save

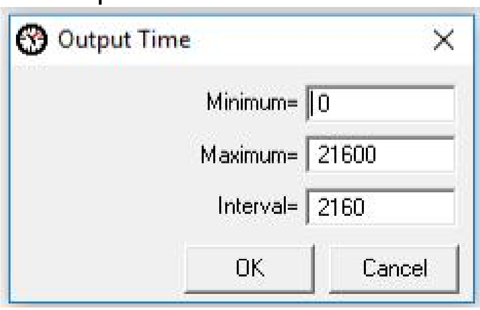
13. Go to Model, MT3DMS/SEAWAT, Advection
    Set Method of Characteristics (MOC)



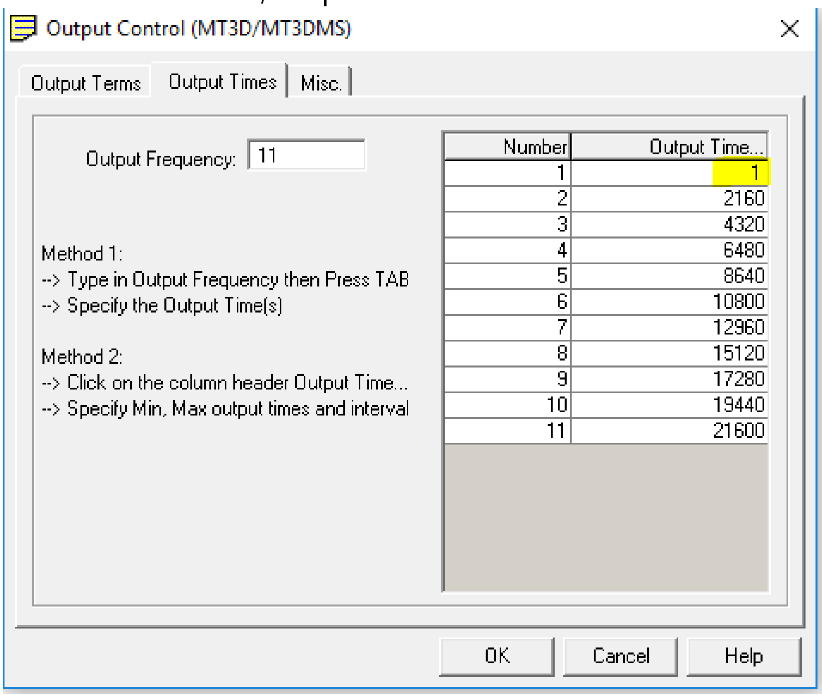
14. Go to Model, MT3DMS/SEAWAT, Dispersion
    Set TRPT=0.1, TRPV=0.1
    Set Longitudinal Dispersivity [L]=0
    Leave Editor, save
15. Model, MT3DMS/SEAWAT, Output Control, Output Times
    Set Output frequency=11



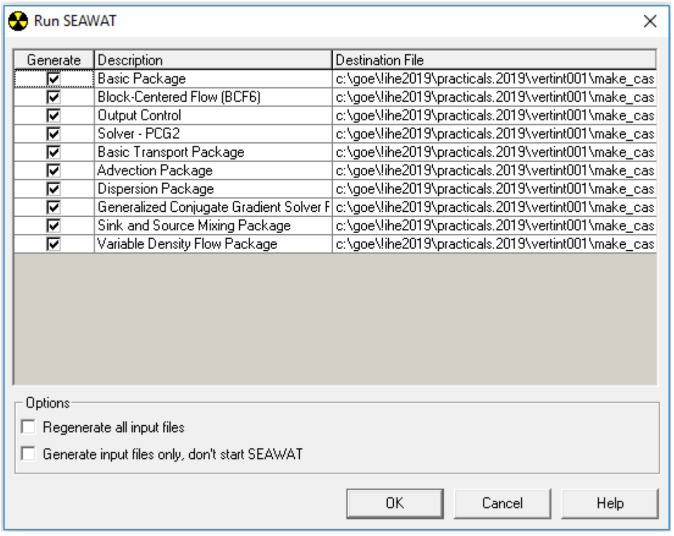
Set Output Time...

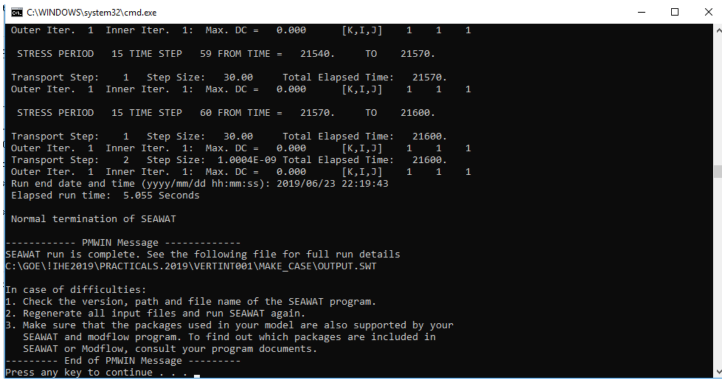


CHANGE Number=1, Output Time 0 to 1!



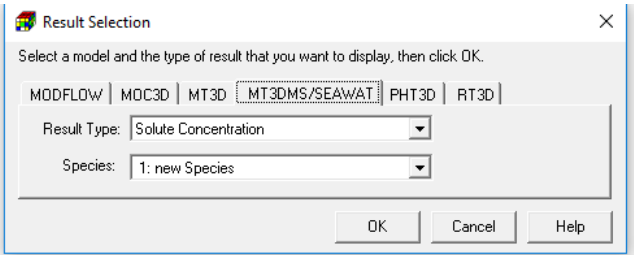
16. Run the model:
    Model, MT3DMS/SEAWAT, Run



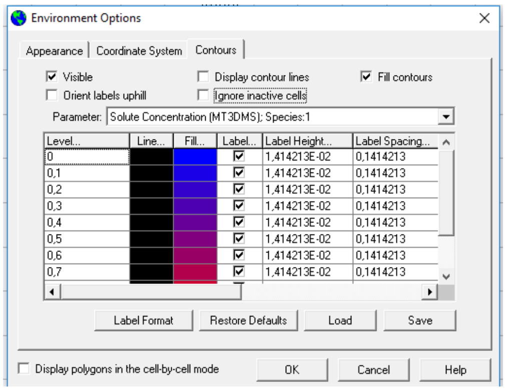


Output:

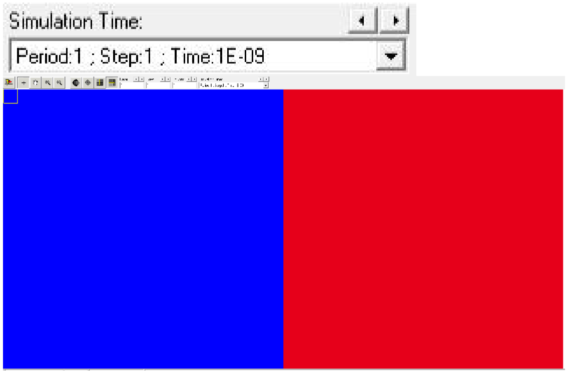
17. Tools, 2D-Visualization, MT3dMS/SEAWAT, Solute Concentration



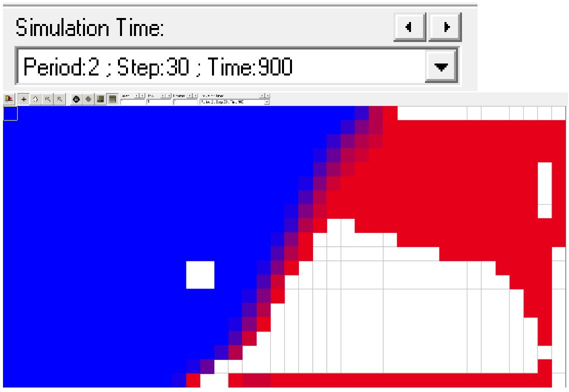
18. Options, Environment
    Set Visible, Fill Contours
    Make for instance red and blue



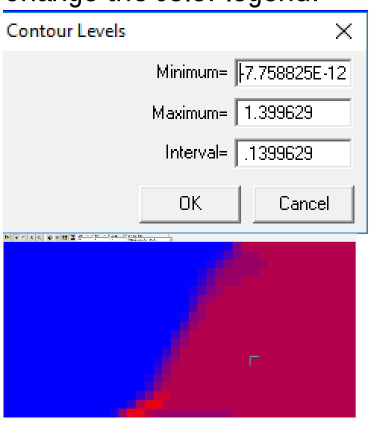
19. Time=1E-09 sec



Time=900sec



20. Over and underschooting:
Change the color legend:



HERE FOLLOWS THE ORIGINAL PARCTICAL EXERCISES

Exercise 001: geometry of the problem

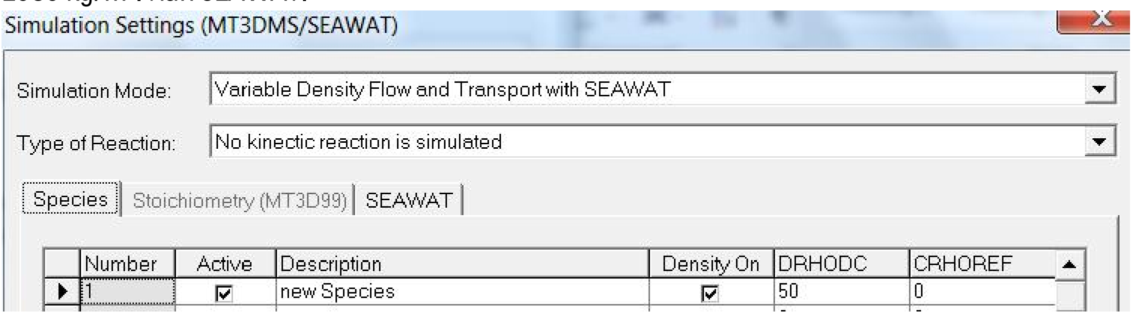
- This model vertint001 has already been run.
- Check in PMWIN the input files: heads, time-characteristics, IBOUND, MODFLOW; SEAWAT parameters. You still understand the input files?
- Check the concentration and the flow face results and explain what is going on.
- Why do cells exist with a concentration 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 002: on the best solute solver to reproduce the SEAWAT result

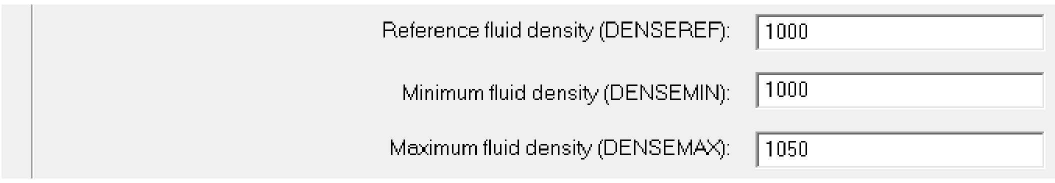
As can be seen checking the results with the default Advection solver ('ULTIMATE'), it is not easy to get a sharp interface (remember that no hydrodynamic dispersion is simulated!). Try to find a proper solver among the Advection solvers ('Models'->'MT3DMS / SEAWAT'->'Advection'): Finite Difference Method, 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 manual[1]. 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 003: 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/m^3. Run SEAWAT.



[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.*



- 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 004: effect of dispersion

Use the best solute solver from Exercise 2. Add dispersion to the system: α_L=1.0 m; α_{TH}=α_{TV} =0.1 m. ‘MT3DMS / SEAWAT’-> ‘Dispersion’. Run SEAWAT.

- 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!