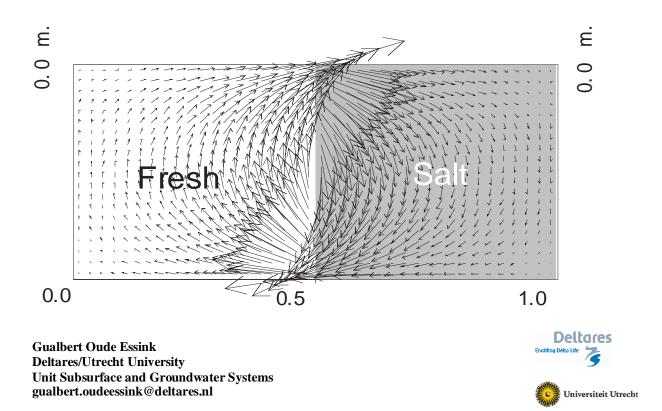
Vertical interface between fresh and saline groundwater



Variable-density groundwater flow modelling with SEAWAT

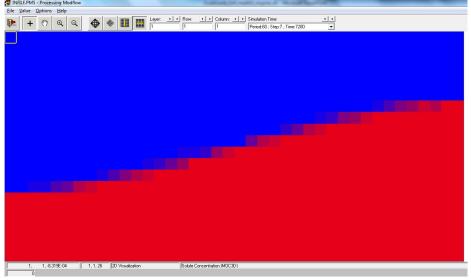
Introduction

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: $D_{mof}=0$ 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*10⁻³ m/s
Rows	1	T (=K _{hor} *thickness cell)	2.5*10 ⁻⁵ m ² /s
columns	40	Anisotropy Khor/Kver	1
Δχ	0.025 m	n _e	0.1
Δy	1 m	α_{L}	0 m
ΔΖ	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

Layer (K Dimension) Number of Layers:	20	
Model Thickness:	0.5 Model Top Elevation: 0	
Row (I Dimension)		
Number of Rows:	1	
Model Extent:	1	
Column (J Dimension)-		
Number of Columns:	40	
Model Extent:	1	
Cross-Sectional Display		
Model Extent:	1	

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

	J							
🥌 Lay	er Property					_		×
Flow Pac	ckage: Block Centered Flow (Bl	CF)						
Layer	Туре	Horizontal Anisotropy	Vertical Anisotropy	Transmissivity		Storage Coefficient	Interb Stora	
1	0: Confined	1	VK	Calculated	Calculated	Calculated		

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)

3	• 0	8	a 1	20	* 8	1 🖽	3	-	ter 11	a 11	Count 1	1												
						-																		
						-												-						
					-	-												-						
					-	-																		
					 _								-	_	_		_		_		_	_	_	

 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	V		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	V		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	V		1800	60	1	0	50000		-
•			4	4	4	n	E0000	[۶İ
Simulati	on Time U	nit			Simula	tion Type			
second	s		-]	C Ste	eady-State Flow	Simulation		
🗹 Auto	l Indata P	Period Lengt			O Tr	ansient Flow Sin	nulation		

- 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')

Ng Reset Matrix	×
Horizontal Hydr. Conductivity [L/T]:	
Parameter Number [-]: 0	
Select "Apply to the entire model" to set the values to all cells of the model. Select "Apply to the current layer" to set the values to all cells of the current layer	
C Apply to the entire model OK Cancel Help	

Leave Editor, save

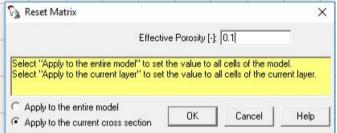
8. Go to: Parameter, Vertical Hydraulic Conductivity Go to: Value, Reset Matrix Set to 0.001

🙀 Reset Matrix	×
Vertical Hydr. Conductivity [L/T]:	DOţI
Parameter Number [-]:	
Select "Apply to the entire model" to set the values to Select "Apply to the current layer" to set the values to	
C Apply to the entire model C Apply to the current cross section OK	Cancel Help

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

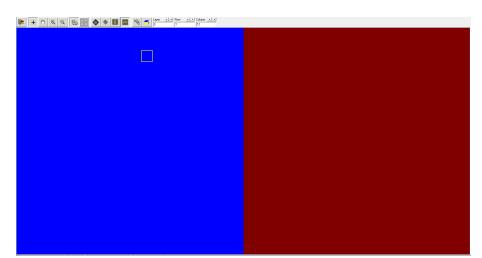
🕶 Preconditioned Conjugate	Gradien	t Package 2	×
Preconditioning Method Modified Incomplete Cholesi Neuman Series Polynomial	(y		
Calculate the upper bound on Relaxation Parameter:	on the ma	ximum eigenvalue	
Allowed Iteration Numbers: Outer Iteration (MXITER): 50		Convergence Cri Head Change [L]:	
Inner Iteration (ITER1):		Residual [L^3/T]:	-
Printout From the Solver All available information C The number of iterations only C None		Damping Damping Parame	ter:
Printout Interval: 1			
	OK	Cancel	Help

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

Simu	ulat	tion Settin	igs (MT3D	MS/SEAWAT)				×
Simu	ulat	ion Mode:	Variat	le Density Flow and Transport with SEAW.	AT			•
Тур	e ol	f Reaction:	No kir	nectic reaction is simulated				-
S	pec	cies Stoid	hiometry (N	1T3D99) SEAWAT				1
		Number	Active	Description	Density On	DRHODC	CRHOREF	<u>^</u>
	▼	1	ব	new Species	I	25	0	
						0	0	
						0	0	

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)

🌱 Advection Package (MT3DMS)	×
Solution Scheme: Method of Characteristics (N	40C) 🗾
Weighting Scheme: Upstream weighting	~
Particle Tracking Algorithm: Hybrid 1st order Euler and 4	lth order Runge-Kutta 💌
Simulation Parameters	
Max. number of total moving particles (MXPART)	100000
Courant number (PERCEL)	0,75
Concentration weighting factor (WD)	0,5
Negligible relative concentration gradient (DCEPS)	0,00001
Pattern for initial placement of particles (NPLANE)	2
No. of particles per cell in case of DCCELL<=DCEPS (NPL)	4
No. of particles per cell in case of DCCELL>DCEPS (NPH)	15
Minimum number of particles allowed per cell (NPMIN)	15
Maximum number of particles allowed per cell (NPMAX)	75
OK Cance	el Help

- 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

Output Control (MT3D/MT3DMS)	×
Output Terms Output Times Misc.	
Output Frequency: 0	Number Output Time
Method 1: > Type in Output Frequency then Press TAB > Specify the Output Time(s) Method 2: > Click on the column header Output Time > Specify Min, Max output times and interval	
	OK Cancel Help

Set Output Time...

Output Time	×
Minimum	= 0
Maximum	= 21600
Interval	= 2160
OK	Cancel

CHANGE Number=1, Output Time 0 to 1!

Uutput Control (MT3D/MT3DMS)

Output Frequency: 11	Number	Output Time
Output Frequency. 1 **	1	1
	2	2160
	3	4320
Method 1:	4	6480
-> Type in Output Frequency then Press TAB	5	8640
-> Specify the Output Time(s)	6	10800
	7	12960
Method 2:	8	15120
-> Click on the column header Output Time	9	17280
-> Specify Min, Max output times and interval	10	19440
	11	21600

16. Run the model:

Model, MT3DMS/SEAWAT, Run

×

Generate	Description	Destination File
T	Basic Package	c:\goe\lihe2019\practicals.2019\vertint001\make_ca
	Block-Centered Flow (BCF6)	c:\goe\lihe2019\practicals.2019\vertint001\make_ca
2	Output Control	c:\goe\lihe2019\practicals.2019\vertint001\make_ca
2	Solver - PCG2	c:\goe\!ihe2019\practicals.2019\vertint001\make_ca
V	Basic Transport Package	c:\goe\lihe2019\practicals.2019\vertint001\make_ca
2	Advection Package	c:\goe\lihe2019\practicals.2019\vertint001\make_ca
V	Dispersion Package	c:\goe\lihe2019\practicals.2019\vertint001\make_ca
2	Generalized Conjugate Gradient Solver F	c:\goe\!ihe2019\practicals.2019\vertint001\make_ca
V	Sink and Source Mixing Package	
	pirik anu pource Mixing Hackage	c:\goe\!ine2019\practicals.2019\vertint001\make_ca
<u>v</u>	Variable Density Flow Package	
Options		c:\goe\lihe2019\practicals.2019\vertint001\make_ca c:\goe\lihe2019\practicals.2019\vertint001\make_ca
Options Regene	Variable Density Flow Package	
Options Regene	Variable Density Flow Package	

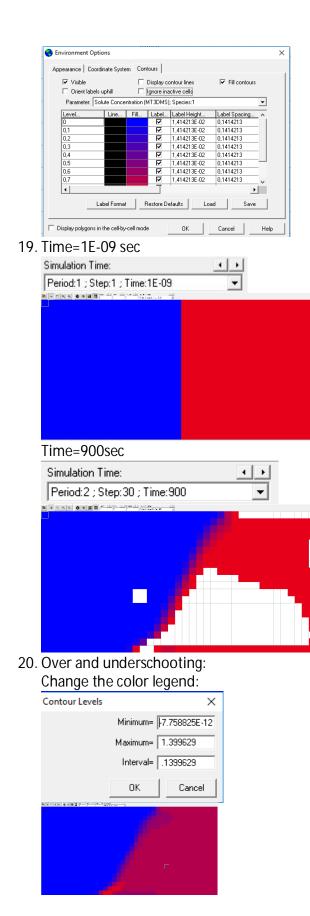
1	C:\WINDOWS\system32\cmd.exe	-	×
C	uter Iter. 1 Inner Iter. 1: Max. DC = 0.000 [K,I,J] 1 1 1		1
	STRESS PERIOD 15 TIME STEP 59 FROM TIME = 21540. TO 21570.		
	ransport Step: 1 Step Size: 30.00 Total Elapsed Time: 21570. Juter Iter. 1 Inner Iter. 1: Max. DC = 0.000 [K,I,J] 1 1 1		
	STRESS PERIOD 15 TIME STEP 60 FROM TIME = 21570. TO 21600.		
C	ransport Step: 1 Step Size: 30.00 Total Elapsed Time: 21600. uter Iter. 1 Inner Iter. 1: Max. DC = 0.000 [K,I,J] 1 1 1 ransport Step: 2 Step Size: 1.00046-09 Total Lapsed Time: 21600.		
E F	uter Iter, 1 Inner Iter, 1: Nax, DC = 0.000 [K,I,J] 1 1 1 un end data end time (yyyymm/dd hh:mm:ss): 2019/06/23 22:19:43 lapsed run time: 5.055 Seconds		ľ
N	Normal termination of SEAWAT		
SE	- WMITH Message		
1. 2. 3.	i case of difficulties: Check the version, path and file name of the SEAWAT program. Regenerate all input files and run SEAWAT again. Nake sure that the packages used in your model are also supported by your SEAWAT and modflow program. To find out which packages are included in SEAWAT or Modflow, consult your program documents. End of PMWIN Message		
	And the state of t		

Output:

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

🗊 Result Selection	×				
Select a model and the type of result that you want to display, then click OK.					
MODFLOW MOC3D MT3D MT3DMS/SEAWAT PHT3D RT3D					
Result Type: Solute Concentration	•				
Species: 1: new Species					
ОК	Cancel Help				

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



HERE FOLLOW 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 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 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/m³. Run SEAWAT.

Simulation Settings (MT3DMS/SEAWAT)

Simulation Mod	mulation Mode: Variable Density Flow and Transport with SEAWAT					1
Type of Reaction	in: No ki	nectic reaction is simulated				
Species Sto	ichiometry ((MT3D99) SEAWAT				
Species Sto		MT3D99) SEAWAT	Density On	DRHODC	ICBHOREF	

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.

Reference fluid density (DENSEREF):	1000
Minimum fluid density (DENSEMIN):	1000
Maximum fluid density (DENSEMAX):	1050

• 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!