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 m²/s |
| columns | 40 | Anisotropy K _{hor} /K _{ver} | 1 |
| Δχ | 0.025 m | n _e | 0.1 |
| Δу | 1 m | αL | 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.

In past IHE courses, this conceptual model has always been simulated with MOCDENS3D. This code (which is MOC3D (Konikow et al., 1996) adapted for density differences) is similar to SEAWAT, and pretty powerful in solving salt 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 simulated 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

| lumber of Layers: | 20 | | | |
|------------------------|-----|-----------|--------------|--|
| fodel Thickness: | 0.5 | Model Top | Elevation: 0 | |
| Row (I Dimension) — | | | | |
| lumber of Rows: | 1 | | | |
| fodel Extent: | 1 | | | |
| Column (J Dimension) | | | | |
| lumber of Columns: | 40 | | | |
| fodel Extent: | 1 | _ | | |
| Cross-Sectional Displa | y | | | |
| ertical Exaggeration: | 1 | | | |

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

| Lay | er Property | | | | | | | × |
|--------|-----------------------|--------------------------|------------------------|----------------|------------|------------------------|---------------|--------|
| low Pa | ckage: Block Centered | flow (BCF) | | | | | | |
| Layer | Туре | Horizontal Anisotropy | Vertical Anisotropy | Transmissivity | Leakance | Storage Coefficient | Inter Stor | rbei 🔨 |
| 1 | 0: Confined | 1 | VK | Calculated | Calculated | Calculated | Г | - |

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

| Lay | er Property | | | | | | |
|-----------------|-------------------------------|------------|------------------------|----------------|------------|------------------------|-----------|
| ow Pao Layer | ckage: Block Centered Type | Horizontal | Vertical Anisotropy | Transmissivity | Leakance | Storage Coefficient | Interbe A |
| 1 | 0: Confined | 1 | VK | Calculated | Calculated | Calculated | Г |
| 2 | 0: Confined | 1 | VK | User | Calculated | Calculated | |

4. Place a fixed head in the model



use this view (as we are 2D vertical):

Go to: Grid, Cell Status, IBOUND (MODFLOW)

Make layer=11, Row=1, Column=1: -1 (now this cell has a fixed head)

| | 1 + | 1.65 | - · | 5 1 5 | 9 H 9 9 | • • • • | 11 1 | | | | | | | | |
|------------------|-----|------|-----|-------|---------|---------|----------|------|--|--|--|--|--|--|--|
| | | | | | | | | | | | | | | | |
| | | | | | | | | | | | | | | | |
| | | | | | | | | | | | | | | | |
| $\left \right $ | | - | | | | | | - | | | | | | | |
| | | | | | | | | | | | | | | | |
| | | | | | | | | | | | | | | | |
| | | | | | | | | | | | | | | | |
| $\left \right $ | | - | | | | | | - | | | | | | | |
| F | | | | | | | | - | | | | | | | |
| | | | | | | | | | | | | | | | |

 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

| 🔮 Time | Paramet | ers | | | | | | | × |
|----------------------|----------|--------------|---------------|----------------------|----------------------|-----------------------|--------------------------------|---------------------------|-----|
| Period | Active | Transient | Period Length | No. of Time Steps | Multiplier (Flow) | Transport Stepsize | Max. No. of Transport Steps | Multiplier (Transport) | ^ |
| 1 | v | | 1E-05 | 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 | | Ξ., |
| | | | | | | | | | |
| Simulation Time Unit | | | | | | | | | |
| seconds | | | | | | | | | |
| 🔽 Auto | Update F | Period Lengt | n | | C Tr | ansient Flow Sin | nulation | | |

- 6. Go to: Parameter, Initial & Prescribed Hydraulic Heads [L] add "0" m to this cell where the head is fixed (IBOUND=-1) 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')

| 🏠 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 Apply to the current cross section | 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]: 00 | | | | | | | |
| 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 C Apply to the current cross section | | | | | | | |

Leave Editor, save

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

| S | Set to 0.1 | |
|---|---|---|
| | Ng Reset Matrix | × |
| _ | Effective Porosity [-]: 0.1 | |
| _ | Select "Apply to the entire model" to set the value to all cells of the model. Select "Apply to the current layer" to set the value to all cells of the current layer. | |
| | C Apply to the entire model Apply to the current cross section OK Cancel Help | |

Leave Editor, save

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

| 🌱 Preconditioned Conjugate Gra | dient Package 2 X |
|---|--|
| Preconditioning Method Modified Incomplete Cholesky Neuman Series Polynomial | |
| Calculate the upper bound on the Relaxation Parameter: 1 | e maximum eigenvalue |
| Allowed Iteration Numbers: Outer Iteration (MXITER): 50 | Convergence Criteria Head Change (L): |
| Inner Iteration (ITER1): | Residual (L^3/T): .001 |
| Printout From the Solver All available information The number of iterations only None | Damping Damping Parameter: |
| Printout Interval: 1 | |
| 0 | K Cancel Help |

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

| Sin | Simulation Settings (MT3DMS/SEAWAT) | | | | | | | | |
|--|-------------------------------------|--------|----------|-------------|------------|--------|---------|----------|--|
| Simulation Mode: Variable Density Flow and Transport with SEAWAT | | | | | | | | | |
| Type of Reaction: No kinectic reaction is simulated | | | | | | | | | |
| Species Stoichiometry (MT3D99) SEAWAT | | | | | | | | 1 | |
| | | Number | Active | Description | Density On | DRHODC | CRHOREF | <u>^</u> | |
| | | 1 | N | new Species | N | 25 | 0 | | |
| | | | | | | | | | |
| | | | | | | 10 | 10 | | |

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 (| MOC) 🔽 | | | | | |
| Weighting Scheme: Upstream weighting | v | | | | | |
| Particle Tracking Algorithm: Hybrid 1st order Euler and 4th 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 Canc | el Help | | | | | |

14. Go to Model, MT3DMS/SEAWAT, Dispersion, Edit, Ok Go to Value, Reset Matrix Longitudinal Dispersivity=0 (m), Ok

Leave Editor, save

15. Go to: Model, MT3DMS/SEAWAT, Output Control, Output Times Set Output frequency=11

| sei | Out | puι | rreq | uency | y=11 |
|-----|-----|-----|------|-------|------|
| | | | | | |

| Output Control (MT3D/MT3DMS) | | | × |
|---|--------|--------|----------|
| Output Terms Output Times Misc. | | | 1 |
| Output Frequency: | Number | r Outj | put 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 | | | |
| | ОК | Cancel | Help |

Set Output Time...

| 🚱 Output Time 🛛 🗙 |
|-------------------|
| Minimum= 0 |
| Maximum= 21600 |
| Interval= 2160 |
| OK Cancel |

CHANGE Number=1, Output Time 0 to 1!

| Output Frequency: 11 | Number | Output Time |
|--|--------|-------------|
| | 1 | 1 |
| _ | 2 | 2160 |
| | 3 | 4320 |
| Method 1: | 4 | 6480 |
| > Type in Uutput Frequency then Press TAB | C | 10000 |
| > Specify the Uutput Time(s) | 7 | 10000 |
| | | 12300 |
| Method 2: | 9 | 17280 |
| > Click on the column header Output Time | 10 | 19440 |
| > Speciry Min, Max output times and interval | 11 | 21600 |
| | | |

16. Run the model

Go to: Model, MT3DMS/SEAWAT, Run

| Generate | Description | Destination File |
|----------|---|--|
| • | Basic Package | c:\goe\lihe2019\practicals.2019\vertint001\make_ca |
| | Block-Centered Flow (BCF6) | c:\goe\lihe2019\practicals.2019\vertint001\make_ca |
| • | Output Control | c:\goe\!ihe2019\practicals.2019\vertint001\make_ca |
| v | Solver - PCG2 | c:\goe\lihe2019\practicals.2019\vertint001\make_ca |
| 2 | Basic Transport Package | c:\goe\lihe2019\practicals.2019\vertint001\make_ca |
| • | Advection Package | c:\goe\!ihe2019\practicals.2019\vertint001\make_ca |
| v | Dispersion Package | c:\goe\lihe2019\practicals.2019\vertint001\make_ca |
| • | Generalized Conjugate Gradient Solver F | c:\goe\!ihe2019\practicals.2019\vertint001\make_ca |
| • | Sink and Source Mixing Package | c:\goe\lihe2019\practicals.2019\vertint001\make_ca |
| | Variable Density Flow Package | c:\goe\lihe2019\practicals.2019\vertint001\make_ca |
| | <u>-</u> - | |
| Dptions | rate all input files | |

| ١ | C:\WINDOWS\system32\cmd.exe | - | × |
|---|---|---|---|
| | Outer Iter. 1 Inner Iter. 1: Max. DC = 0.000 [K,I,J] 1 1 1 | | |
| | STRESS PERIOD 15 TIME STEP 59 FROM TIME = 21540. TO 21570. | | |
| | Transport Step: 1 Step Size: 30.00 Total Elapsed Time: 21570. Outer Iter. 1 Inner Iter. 1: Max. DC = 0.000 [K,I,J] 1 1 1 | | |
| 1 | STRESS PERIOD 15 TIME STEP 60 FROM TIME = 21570. TO 21600. | | |
| | Transport Step: 1 Step Size: 30.00 Total Elapsed Time: 21600. Outer Iter. 1 Inner Iter. 1: Max. DC = 0.000 [K,I,J] 1 1 1 Transport Step: 2 Step Size: 1.0004E-00 Total Elapsed Time: 21600. | | |
| | Outeriter. i Inner Iter. 1: Max. DC = 0.000 [K,I,J] 1 1 1 Run end date and time (yyyyymm/dd hh:mm:ss): 2019/06/23 22:19:43 Elapsed run time: 5.055 Seconds | | |
| 2 | Normal termination of SEAWAT | | |
| | PMUTH Message SEAWAT run is complete. See the following file for full run details :.doclimeSupMacTicals.2019/ERTINGO1/WAKE_CASE\OUTPUT.SwT | | |
| | tn case of difficulties: 1. Check the version, path and file name of the SEAMAT program. 2. Regenerate all input files and run SEAWAT again. | | |
| | Make 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 on Modflow, consult your program documents. | | |
| | End of PMUIN Message | | |

Output:

17. Go to: 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 | |
| OK Cancel He | lp |

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



21. Printing the velocity field

Go to: Models, PMPATH (Advective Transport)

Go to: PMPATH: Options, Environment, Velocity vectors, click on Visible

| Appearance Cr | Velocity Vectors Contours |
|--|---------------------------|
| | |
| | OK Cancel |
| | |
| Dr a different Stress Period: o to: Options, Particle Track (Tim Particle Tracking (Time) Properties Simulation Mode/Time Pathline Colors RCH/EV/T Options | ne) Properties |
| Stress Period: Step Length: Step Length: | |
| Interval: 1 Cross Sections Visible Size: 10 Size: 3 | |
| Simulation Mode © Flowines, use that flow field from the current time step C Pathlines, use transient flow fields Stop Condition © Particles stop, when they enter cells with internal sinks Particles stop, when the simulation time limit is reached | |

HERE FOLLOWS THE ORIGINAL PRACTICAL EXERCISES (using vertint001.zip)

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 Mode: | Varial | ble Density Flow and Transport with SE | EAWAT | | | • |
|-------------------|-----------|--|---------------|--------|---------|---|
| Type of Reaction: | No kir | nectic reaction is simulated | | | | • |
| Species Stoich | iometry (| MT3D99) SEAWAT | | | | |
| Number | Active | Description | Density On | DRHODC | CRHOREF | • |
| ▶ 1 | V | new Species | <u></u> | 50 | 0 | |
| | | Reference fluid density | / (DENSEREF): | 1000 | | |
| | | Minimum fluid density | y (DENSEMIN): | 1000 | | |
| | | | | | | |

• 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!

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.