Suite of Simulations for Evaluating Groundwater Well Concentrations

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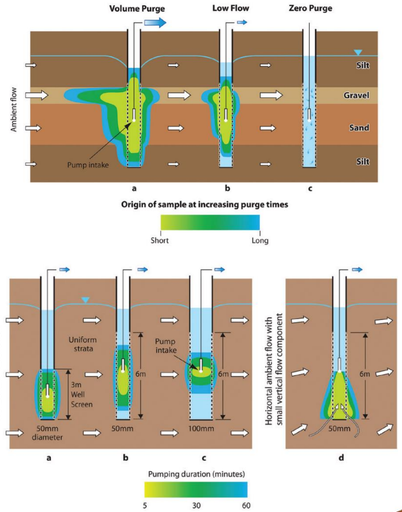
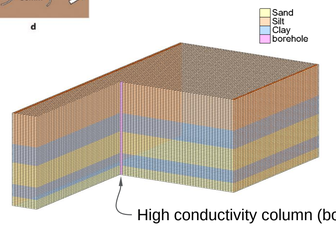
Challenge

Groundwater sample results may not reflect the actual concentrations and contaminant distribution in the subsurface when a well screen intersects multiple hydrogeologic units.

- Different transmissivity or flow regimes can result in different mass fluxes
- Vertical flow within a well bore can bias the water being sampled.



Influence of formation properties and sampling approach on water being sampled (top). Screen length, diameter, and ambient vertical flows affect the water being sampled (bottom). Figures from McMillan et al. (2015).



Approach

Approaches exist for assessing sample concentrations.

- Flow-weighted average and inverse modeling (e.g., Day-Lewis et al., 2023)
- Mass flux measurements (e.g., ITRC, 2010)

Evaluation and application of calculational / interpretation approaches requires suitable data.

- Can collect field measurements (concentrations, borehole flow)
- Can use numerical simulations (known inputs + simulation outputs)

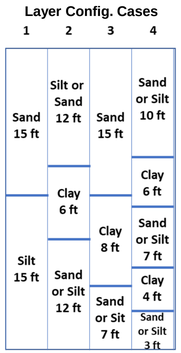
This work compiled a suite of 28 numerical simulations using the MODFLOW and MT3DMS codes, with simulations configured and visualized using FloPy, to provide data for looking at a range of groundwater flow and concentrations scenarios.

Model Config. & Simulation Plan

The model uses a uniform grid of 0.3 m square cells across 51 columns and 101 rows, with a layer thickness of 0.15 m in each of 60 layers.

Simulations used selected combinations of hydrogeologic layer configurations (at right), source definitions, and flow conditions from the following options:

- Kh (m/d): sand (50), silt (2), clay (0.001)
- Source: 1000, 500, or 0 mg/ L
- Gradient: 0.01, 0.001, or 0.0001 m/m



Outcome

FloPy was used to configure and execute MODFLOW and MT3DMS simulations, and then to visualize results for hydraulic head, flow vectors, and concentration contours. See example code at right for the MODFLOW DIS package.

Example results are shown below for simulations 9 and 25, which use layer configuration 4 with a silt-clay-sand-clay-sand sequence. Simulation 9 has a uniform head gradient, whereas the gradients differ by hydrogeologic layer in simulation 25.

Future work will examine radial flow with a pumping well, make use of the AnalyzeHole software, and consider a transect of wells.

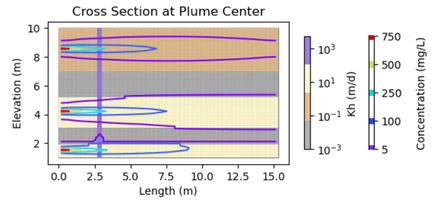
Example FloPy Code:

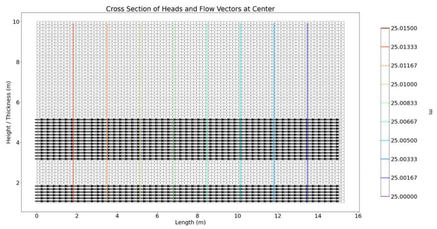
```
# DIS file
Lx = 15.3 # in meters
Ly = 30.3 # in meters
ncol = 51
nrow = 101
nlay = 60
delr = Lx / ncol
delc = Ly / nrow
top = 10
botm1 = (list(np.arange(1, 10,.15)))
botm1.reverse()
nper = 1
perlen = 1500
nstp = 1

dis = mf.ModflowDis(mf_model,
                    nlay = nlay,
                    nrow = nrow,
                    ncol = ncol,
                    delr = delr,
                    delc = delc,
                    top = top,
                    botm = botm1,
                    itmuni = 4,
                    nstp = nstp,
                    nper = nper,
                    perlen = perlen)
```

Simulation 9 configuration, concentrations & hydraulic heads:

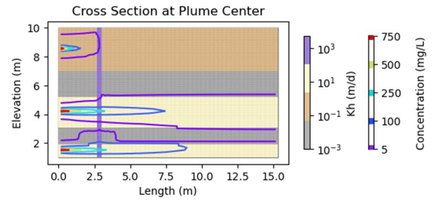
Sim. #	Layer Config.	Layers	K (m/d)	Left BC (m)	Right BC (m)	Gradient (m)	Source (mg/L)
9	4	Silt	2	25.015	25	0.001	1000
		Clay	0.001				0
		Sand	50				1000
		Clay	0.001				0
		Sand	50				1000

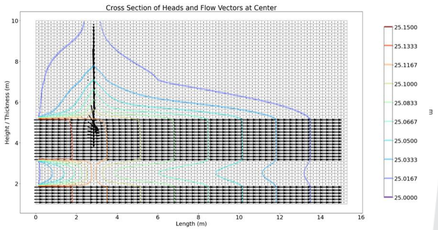




Simulation 25 configuration, concentrations & hydraulic heads:

Sim. #	Layer Config.	Layers	K (m/d)	Left BC (m)	Right BC (m)	Gradient (m)	Source (mg/L)
25	4	Silt	2	25.015	25	0.001	1000
		Clay	0.001	25.015	25	0.001	0
		Sand	50	25.15	25	0.01	1000
		Clay	0.001	25.015	25	0.001	0
		Sand	50	25.15	25	0.01	1000





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References:

Day-Lewis, F.D., R.D. Mackley, and J. Thompson. 2023. "Interpreting Concentrations Sampled in Long-Screened Wells with Borehole Flow: An Inverse Modeling Approach." *Groundwater*, 61(6):834-845. https://doi.org/10.1111/gwat.13300

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McMillan, L.A., M.O. Rivett, J.H. Tellam, and P. Dumble. 2015. "Groundwater Quality Sampling at Contaminated Sites: The Long And The Short Of It." Int. Environ. Technol., 25(2):50-51.

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