Investigating Managed Aquifer Recharge Impacts on Redox Potential: A HYDRUS 2D Modeling Approach

Alessandra Bonazzi[1], Kyounglim Kang[1], Zhe Zhao[1], Sharod Nandi[1], Scott Bradford[2], Salini Sasidharan[3], Helen Dahlke[4], Thomas Young[1], Jasquelin Peña[1], Veronica Morales[1]

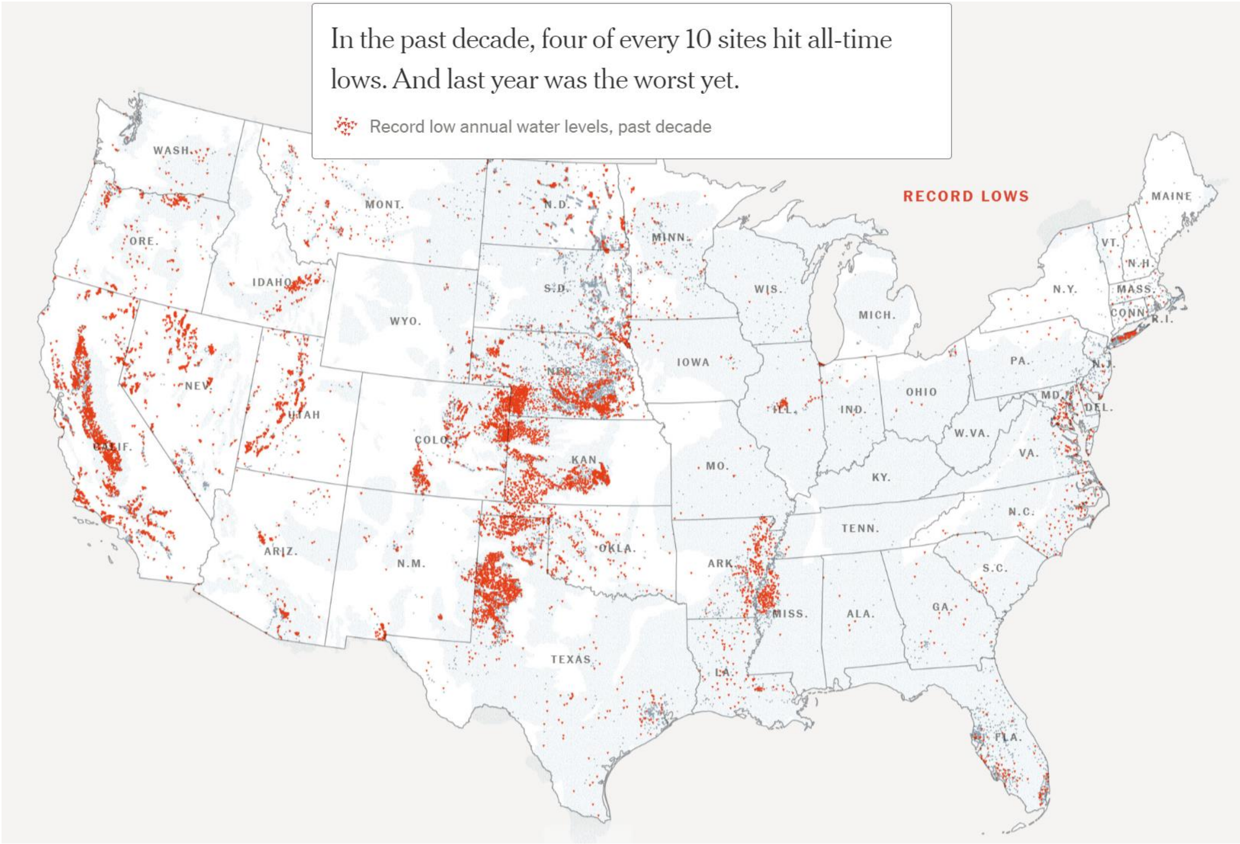
[1]Civil and Environmental Engineering, University of California, Davis

[2]USDA-ARS Sustainable Agricultural Water Systems Unit

[3]Dept. of Biological and Ecological Engineering, Oregon State University

[4]Dept. Land, Air, and Water Resources, UC Davis

Why Managed Aquifer Recharge (MAR)?



Source: The New York Times

Geogenic contaminants mobilization (As, U...)

- MAR practices can improve groundwater availability, but they can pose a risks to aquifer water quality. In California, spikes in concentration of arsenic and uranium have been observed at MAR sites.

- The injection of water rich in dissolved oxygen into the subsurface creates geochemical gradients (e.g., redox) that can mobilize pollutants (i.e., As and U) from the rock, yet the processes involved are poorly understood.

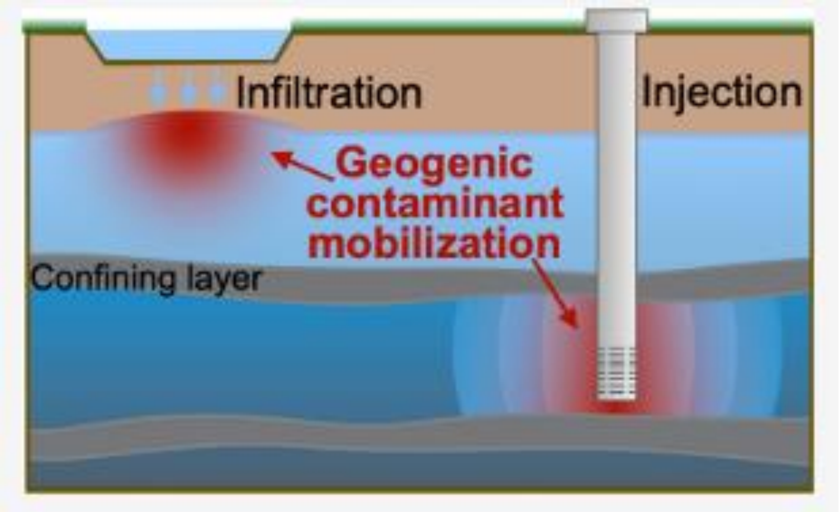
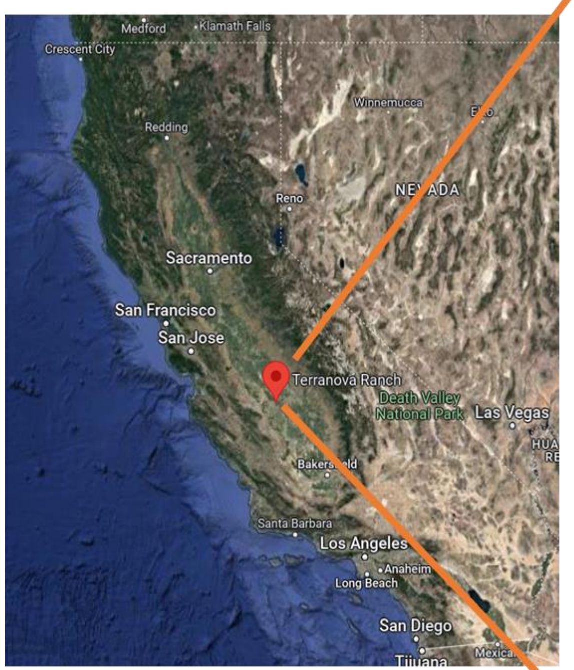
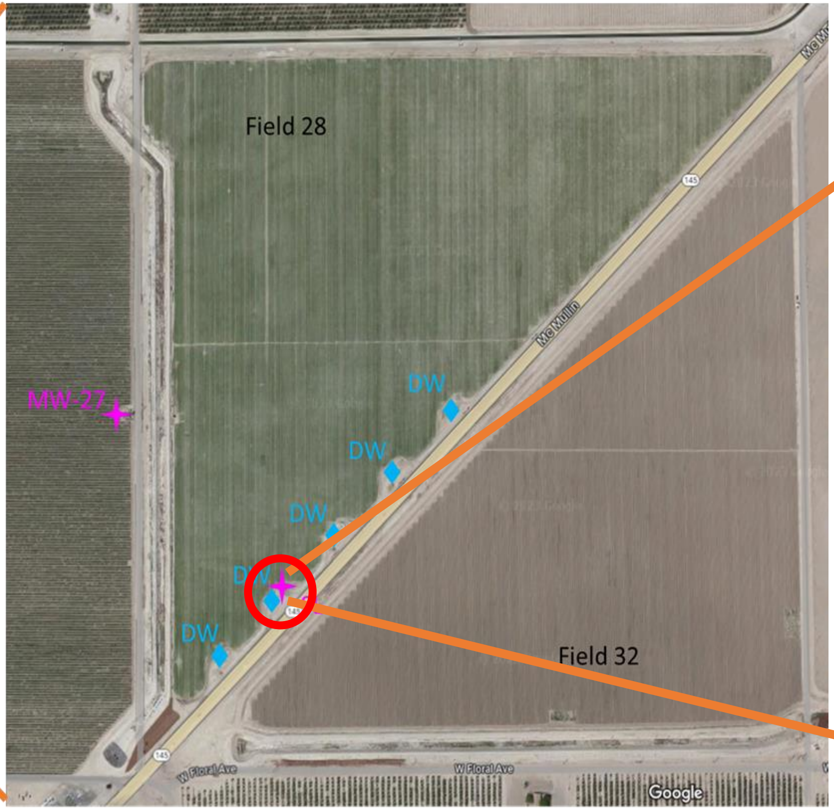
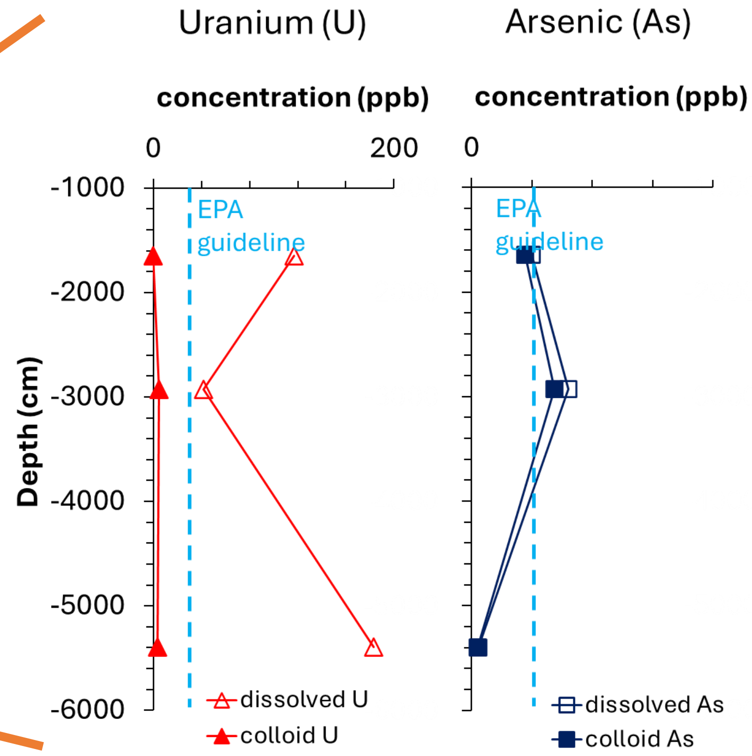


Image from Fakhreddine, Sarah, et al. "Mobilization of arsenic and other naturally occurring contaminants during managed aquifer recharge: a critical review." Environmental Science & Technology 55.4 (2021): 2208-2223.

Field site: Terranova Ranch







Left and central images from Google Maps.
Right: measured concentrations at the monitoring well at Terranova Ranch of Uranium and Arsenic at 17, 29 and 54 meters of depth.

Geogenic contaminants mobilization (As, U...)

Assess how :

1) *pore water residence time*
2) *soil water saturation*
3) *microbial oxygen consumption*

influence variations in redox conditions that cause contaminant mobilization (U and As) during MAR operations.

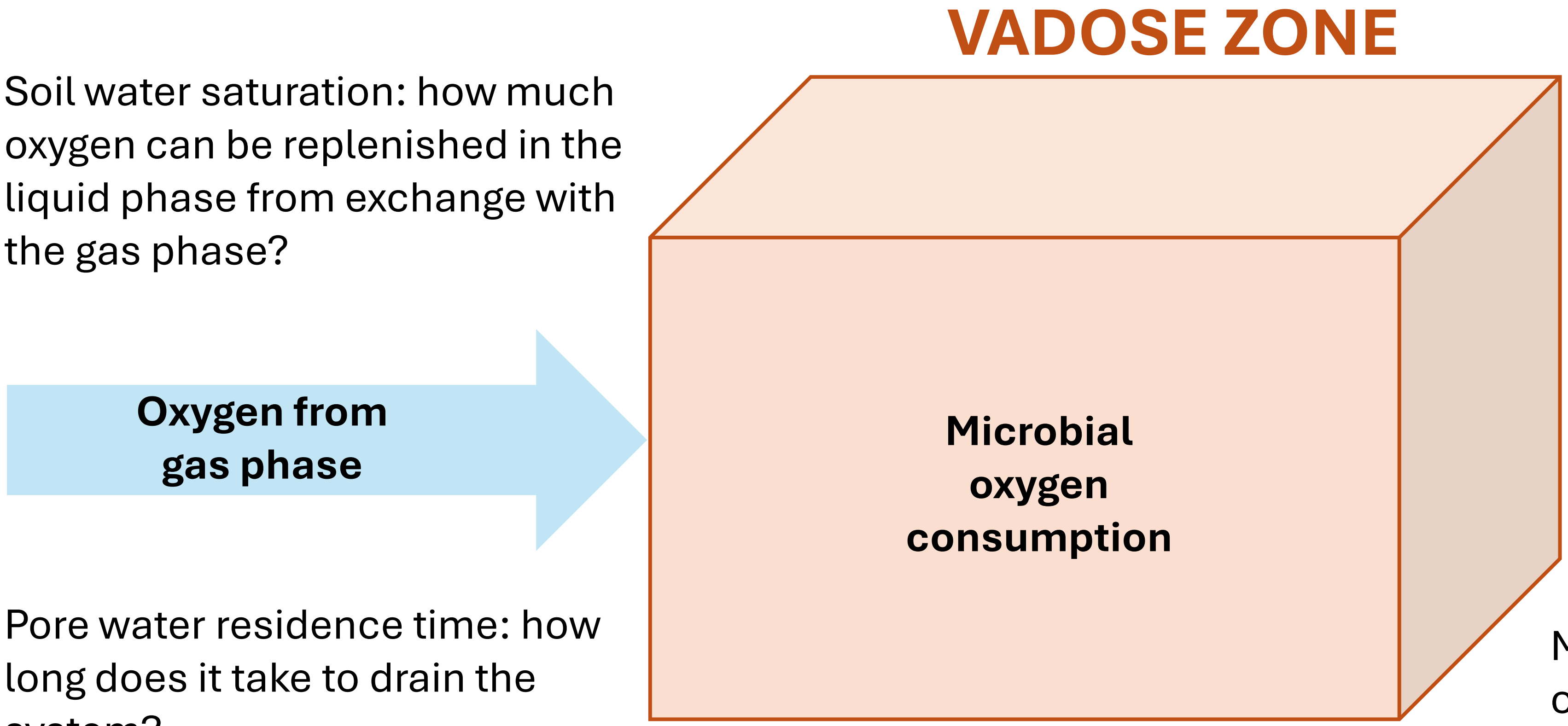
How can mitigate adverse redox conditions?

(e.g. faster injection, longer draining periods, etc...)

Numerical models can help assess that!

Oxygen content as a “proxy” for redox state

Soil water saturation: how much oxygen can be replenished in the liquid phase from exchange with the gas phase?

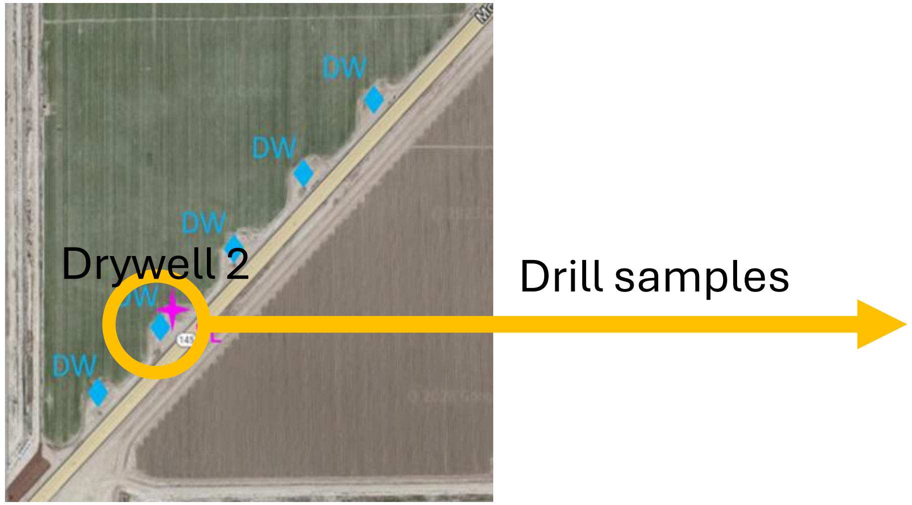


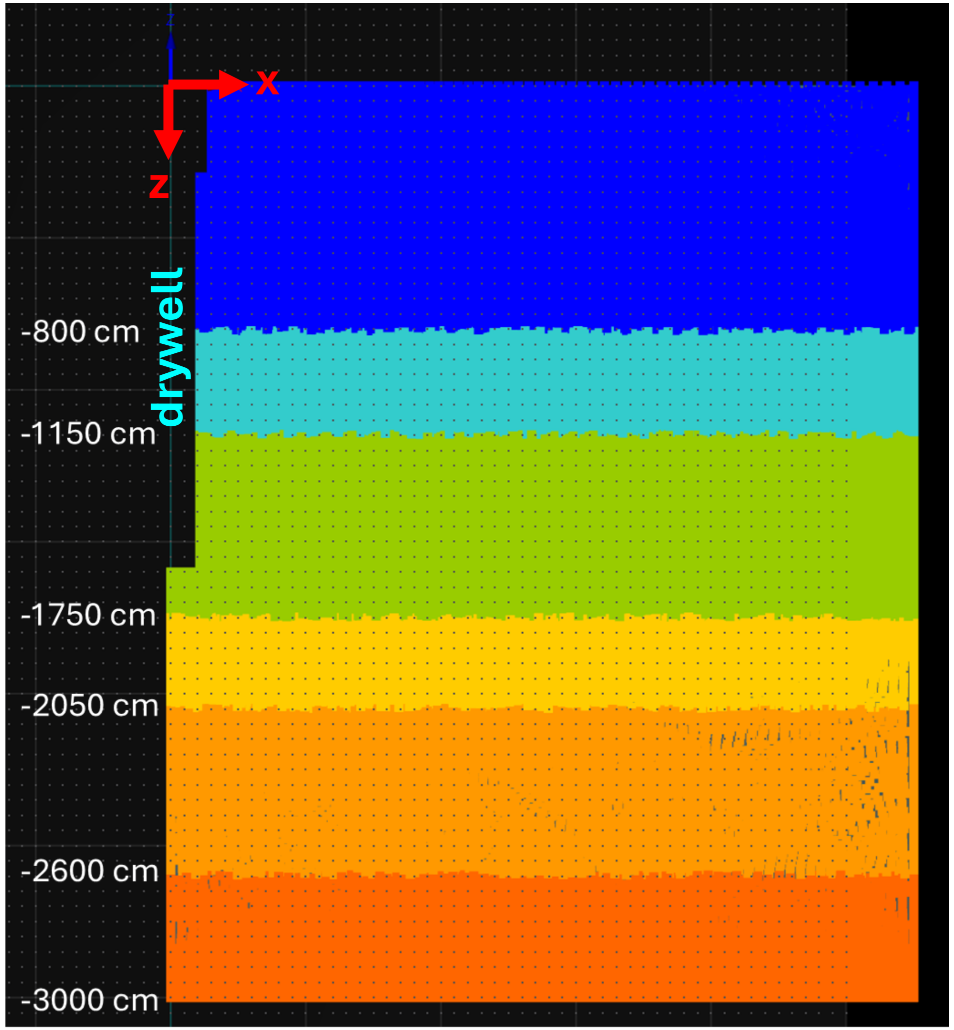
Pore water residence time: how long does it take to drain the system?

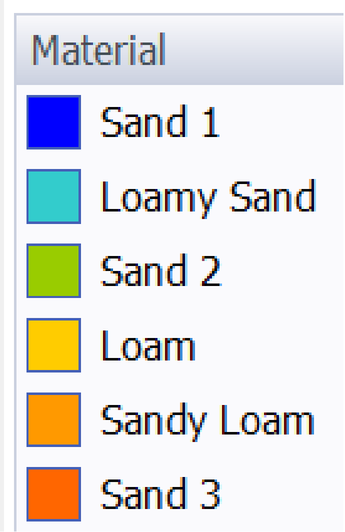
Pore water residence time: how much time do microbes have to consume oxygen?

Microbial activity: how much oxygen do microbes consume at those depths?

Building the model: Hydrus 2D

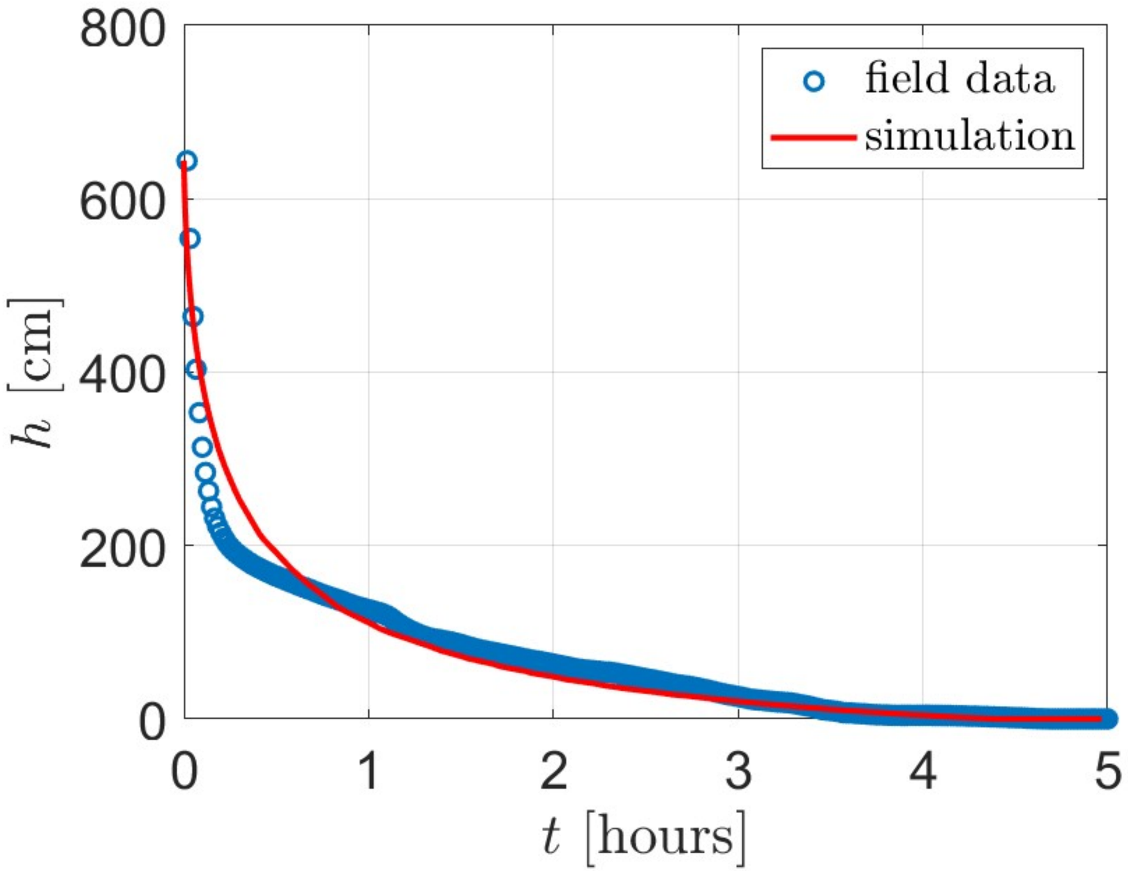






Axisymmetric soil profile at Drywell 2. Six profiles were identified by textural characterization of extracted soil cores.

Hydrologic parameters estimation



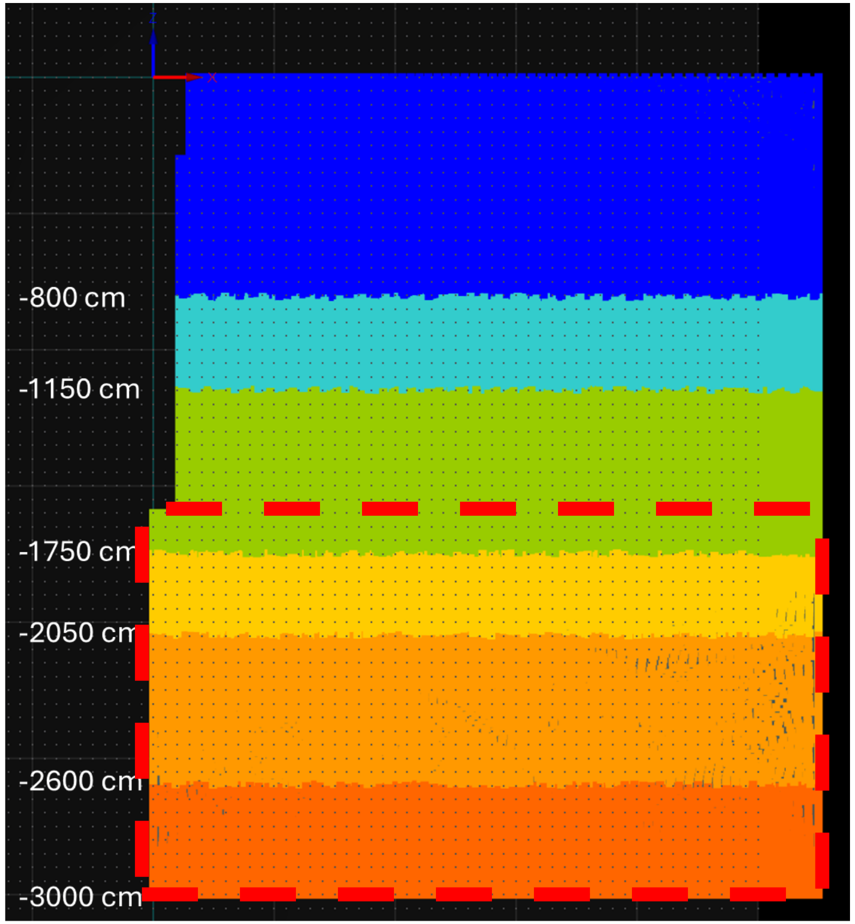
Water level in time in Drywell 2 measured in the field (blue circles), and as obtained through inverse modeling with Hydrus, using the "best" set of hydrological parameters (red line).

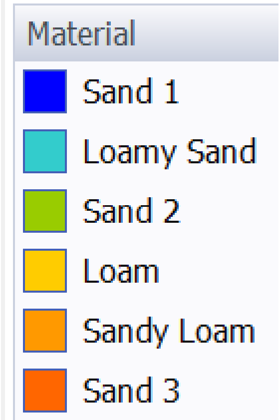
- First guess of van Genuchten's water retention parameters and saturated hydraulic conductivity provided by Rosetta [1]
- Inverse modeling of falling head pumping test performed in Drywell 2 (water level measurements, see figure)

[1] Schaap, M. G., Leij, F. J., and van Genuchten, M. Th., Rosetta: a computer program for estimating soil hydraulic parameters with hierarchical pedotransfer functions, J. of Hydrol., 251, 163-176, 2001.

Can we engineer the system?

Injection/drainage periods designed to control redox conditions.





Axisymmetric soil profile at Drywell 2. Six profiles were identified by textural characterization of extracted soil cores. In red is highlighted the area modeled using Hydrus 1D with different injection/drainage periods.

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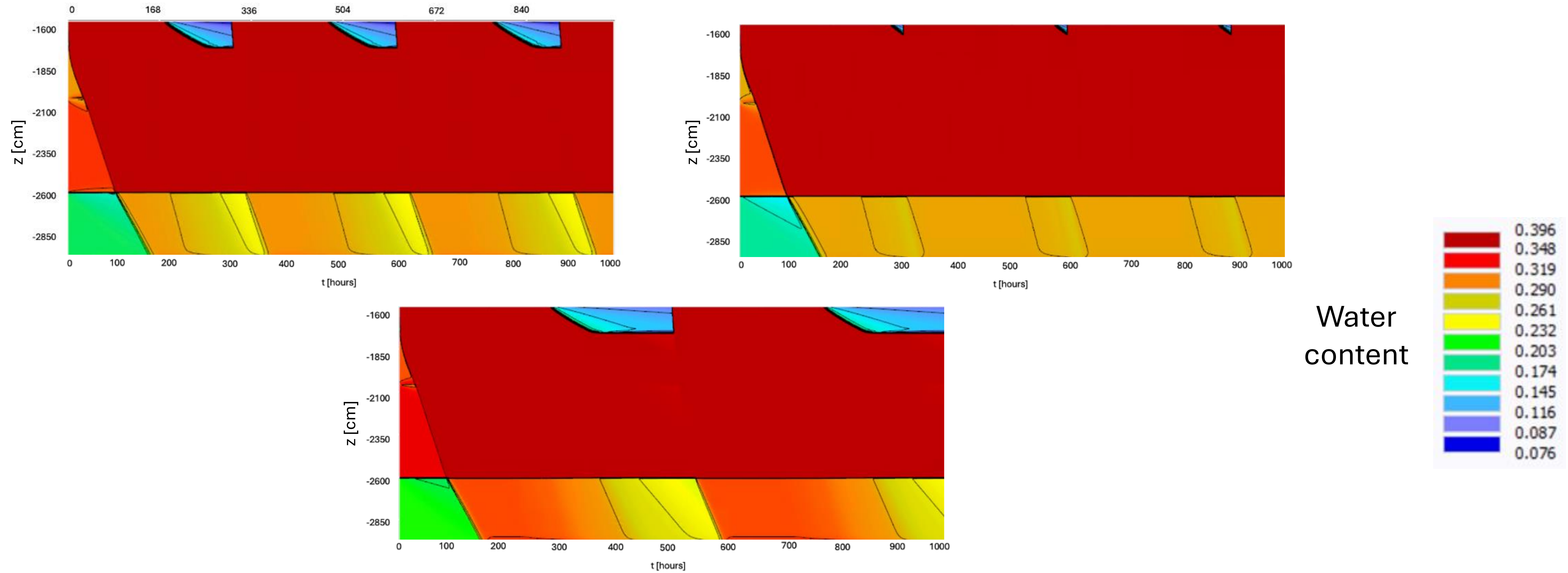
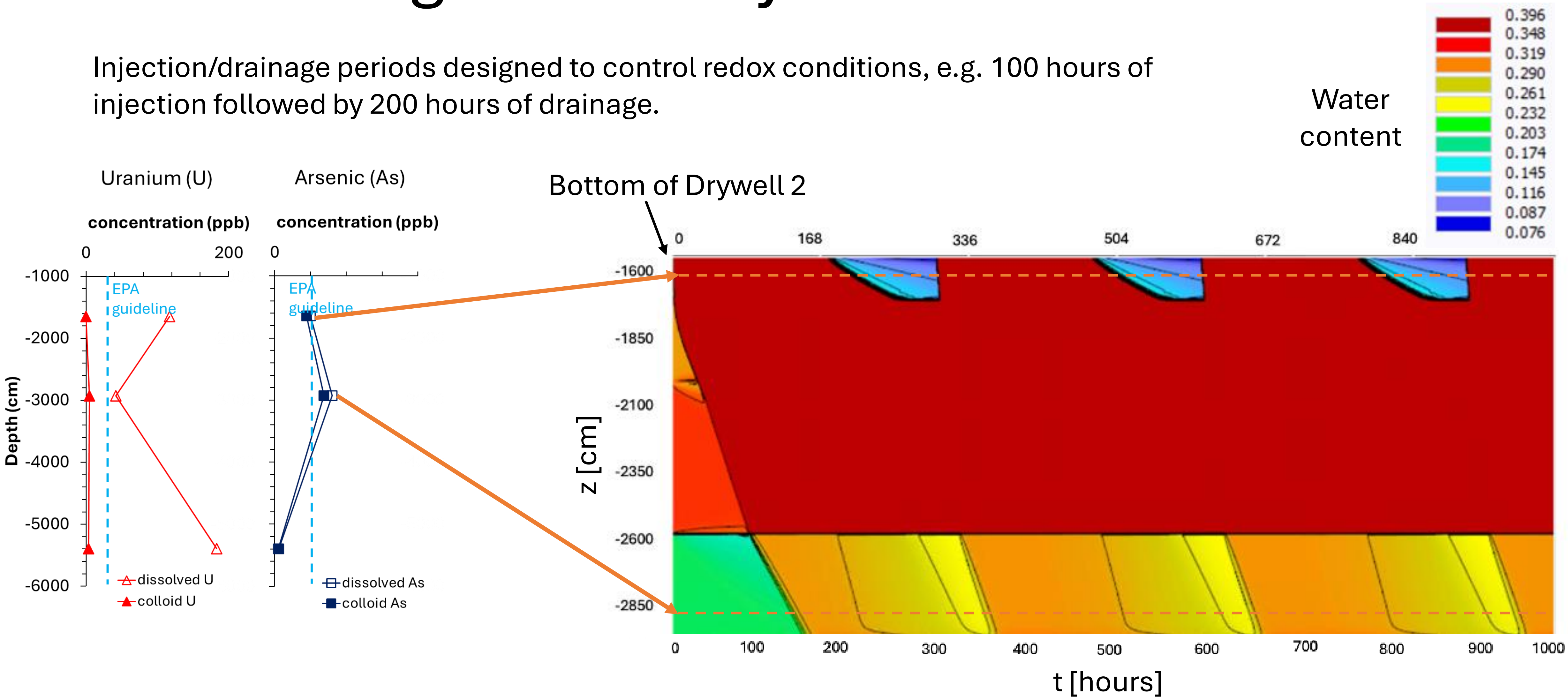


Contour plots of water content from 16 meters (bottom of drywell 2) to 30 meters of depth in time, obtained modeling, in Hydrus 1D, 100 hours of injection followed by 200 hours of drainage over a period of 1000 hours (top left), 200 hours of injection followed by 100 hours of drainage (top right), and 200 hours of injection followed by 300 hours of drainage (bottom).

Can we engineer the system?

Injection/drainage periods designed to control redox conditions, e.g. 100 hours of injection followed by 200 hours of drainage.

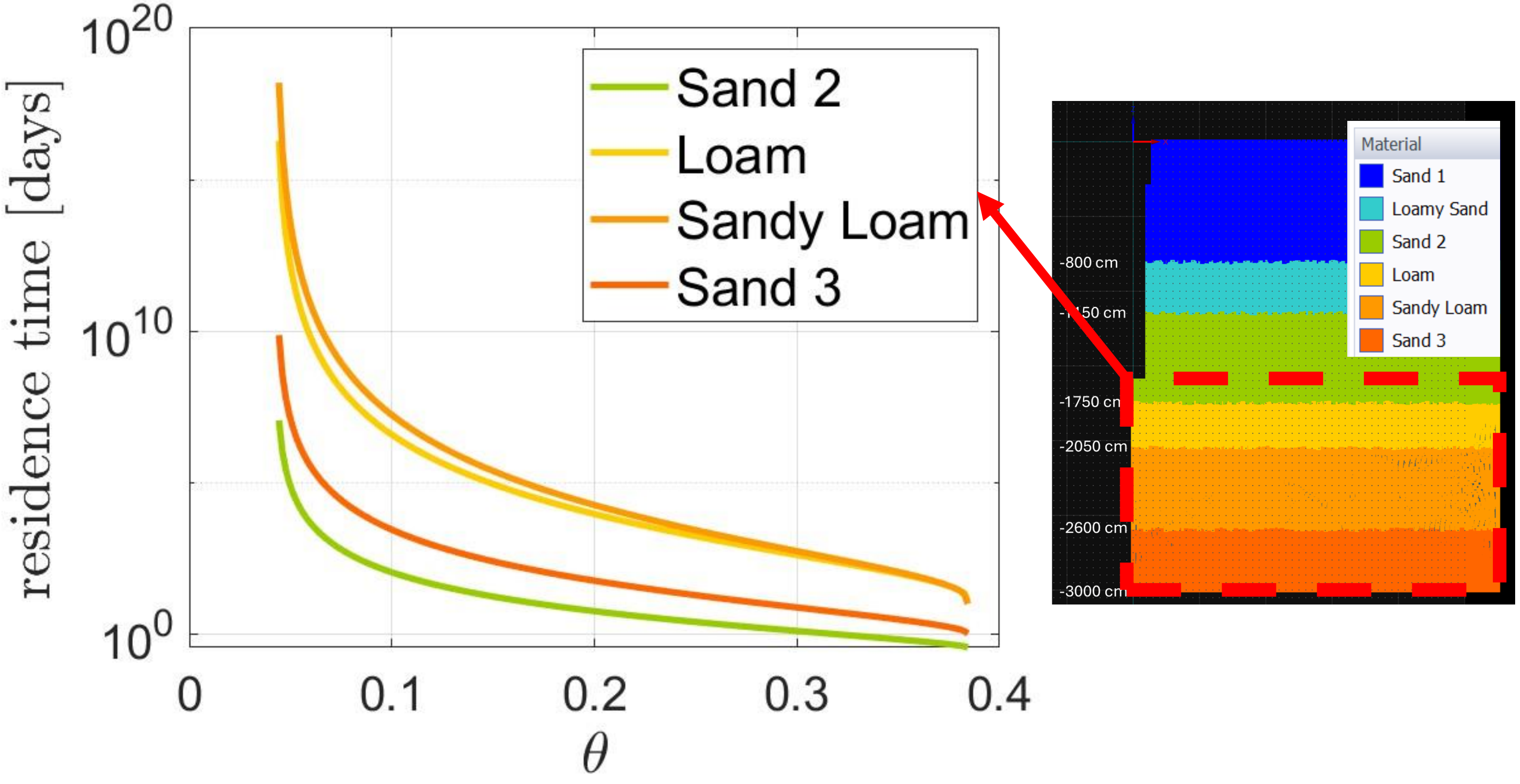


Right image: contour plot of water content from 16 meters (bottom of drywell 2) to 30 meters of depth in time, obtained modeling, in Hydrus 1D, 100 hours of injection followed by 200 hours of drainage, over a period of 1000 hours.

Influencing redox conditions: Residence times

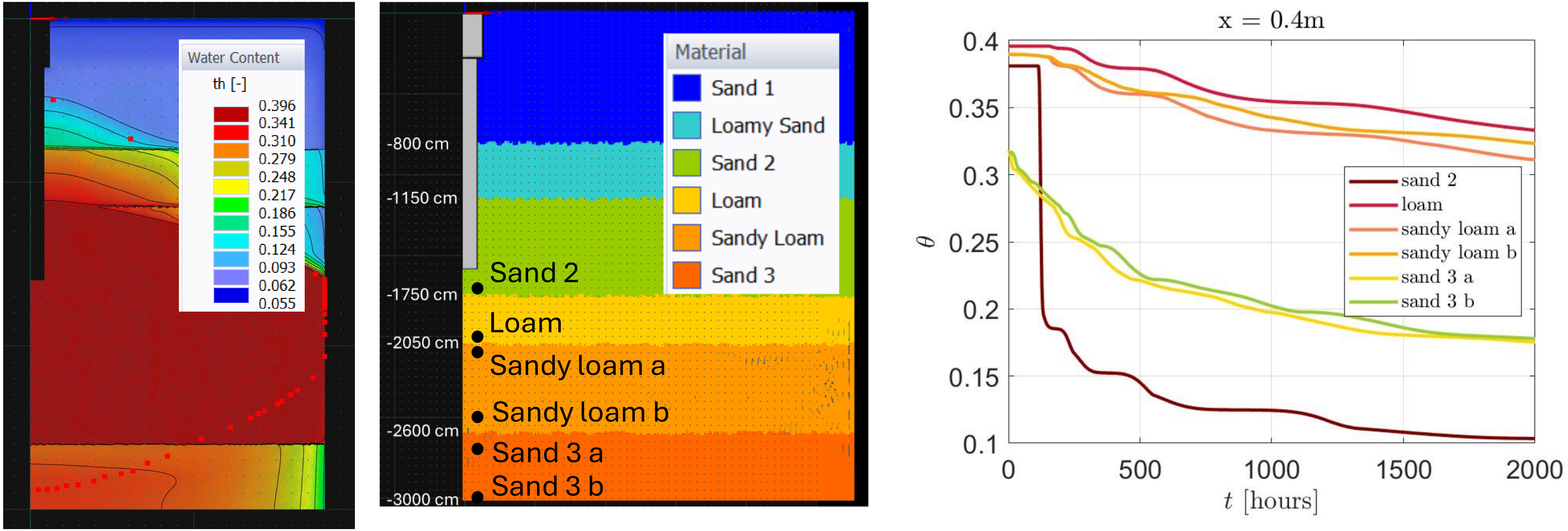
- In all layers, residence time decreases exponentially with water saturation, reaching a variability of orders of magnitude as conditions become drier.

- The Loam and Sandy Loam layers have much longer residence times compared to the other layers. Their position relative to the other layers is thus expected to affect water flow through the domain.



Left: Residence time of water in the four bottom layers as a function of the water content θ. Right: Numerical domain and analyzed layers highlighted in the red box.

Influencing redox conditions: Residence times

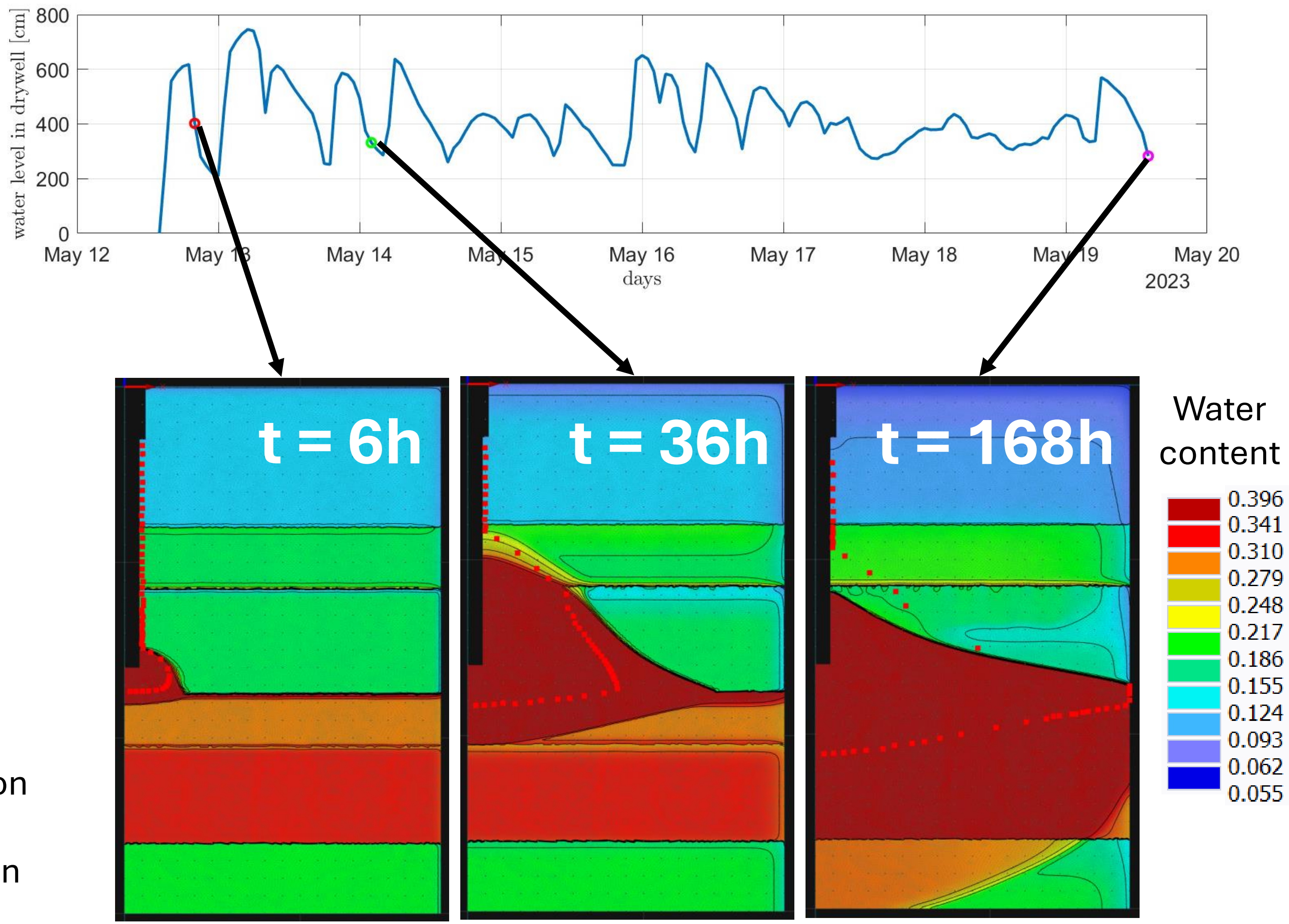


Left: Initial water content in the domain before 2000 hours (~12 weeks) of drainage. Center: Location of the points where the evolution of thw water content in time was observed. Right: Water content in time at six selected locations.

Influencing redox conditions: Water content

- We can see lateral ponding in the Sand 2 layer, which leads to extended retention time.

- The particles in the figure take between 10 and 33 hours to cross the bottom 1.5 meter of the Sand 2 layer. Analytical predictions that do not account for ponding predict a residence time around 9 hours.



Top: Water level in Drywell 2 during a seven-day injection period in 2023. Bottom: Evolution of water content at three different times during water injection. The position at that time of particle tracers (red dots) is also shown.

Influencing redox conditions: O_2 consumption

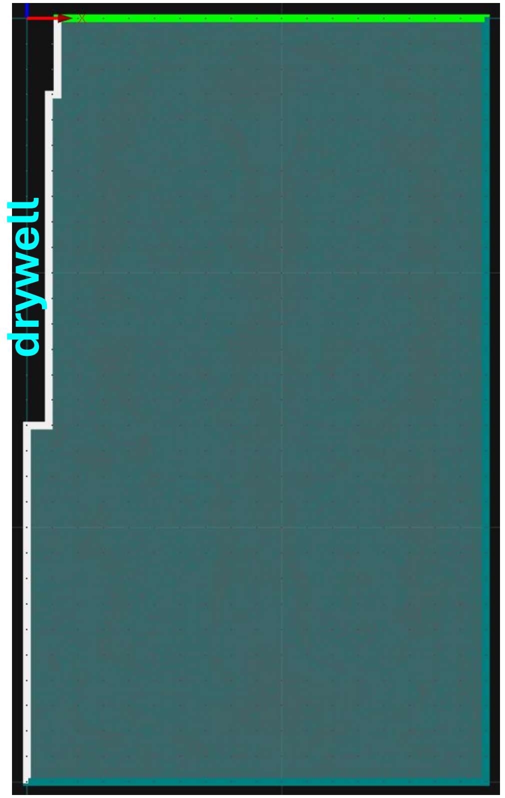
- Challenge: most literature on microbial oxygen consumption focuses on the first 1-2 meters of topsoil
- Studies that looked into ~10-30 meters of depths describe the respiration rate as a zeroth order decay (e.g. Tune, Alison K., et al. "Deep root activity overprints weathering of petrogenic organic carbon in shale." *Earth and Planetary Science Letters* 607 (2023): 118048.)

- We do not know the initial oxygen distribution in the system

O_2 infiltration from the atmosphere with bacterial consumption (NO injection)

Atmospheric boundary

No flux

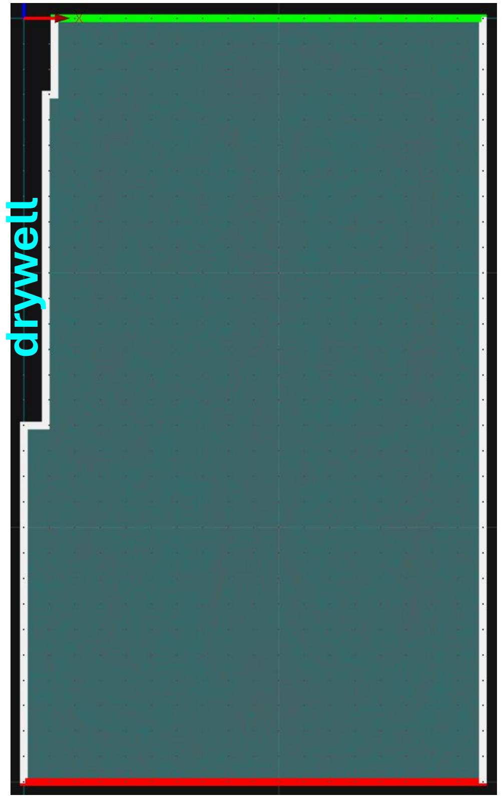


Free drainage

Free drainage

Volatile type

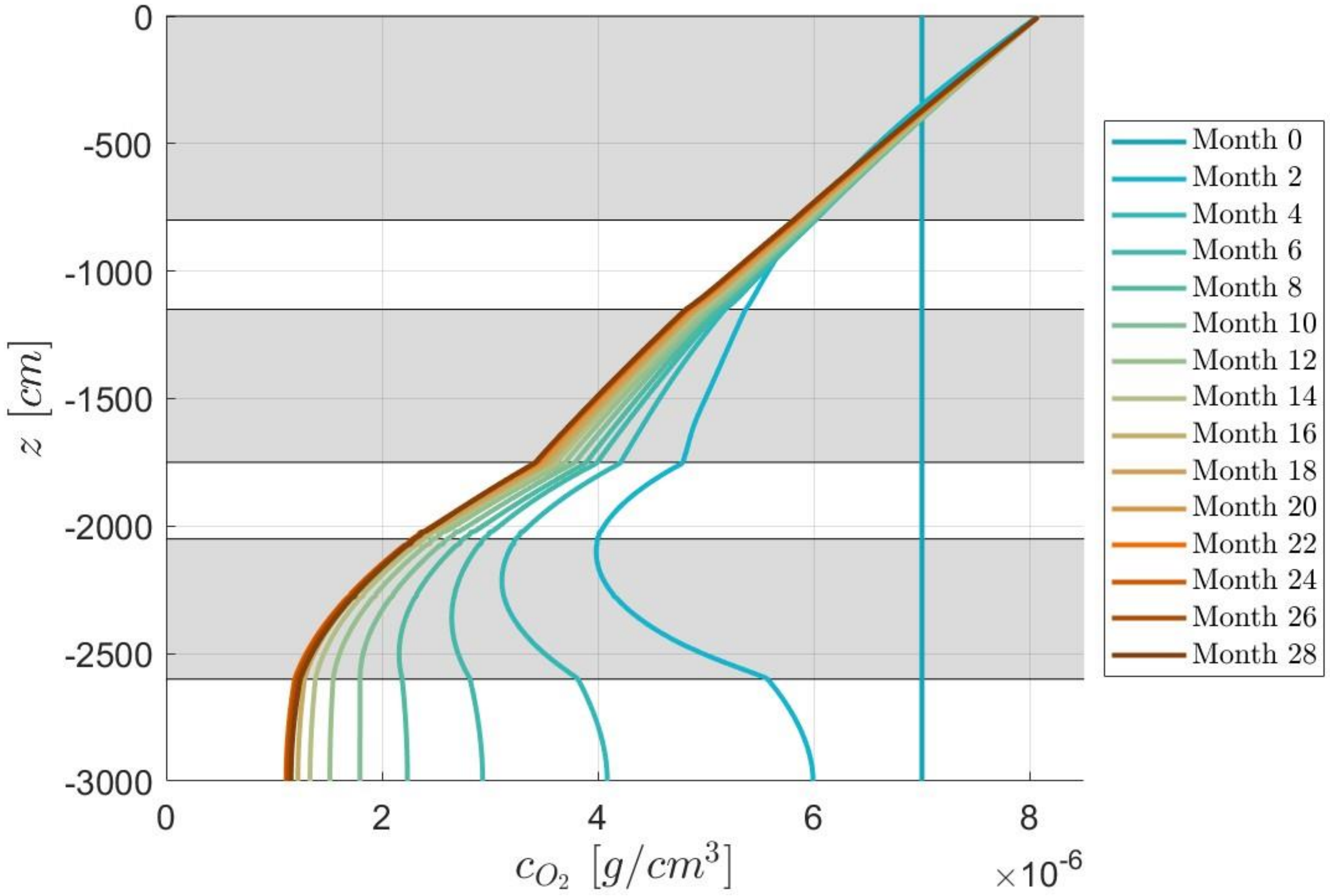
No flux



No flux

Third type

O_2 infiltration from the atmosphere with bacterial consumption (NO injection)



Oxygen concentration in depth. Different lines represent different months (from the initial condition to the distribution after 28 months). Initial concentration set as 7e-6. The decay rate was set as 1.5 g/cm^3/h (zeroth order decay).

Influencing redox conditions: O_2 consumption

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- The decay rate was set as 1.5 g/cm^3/h (zeroth order decay).
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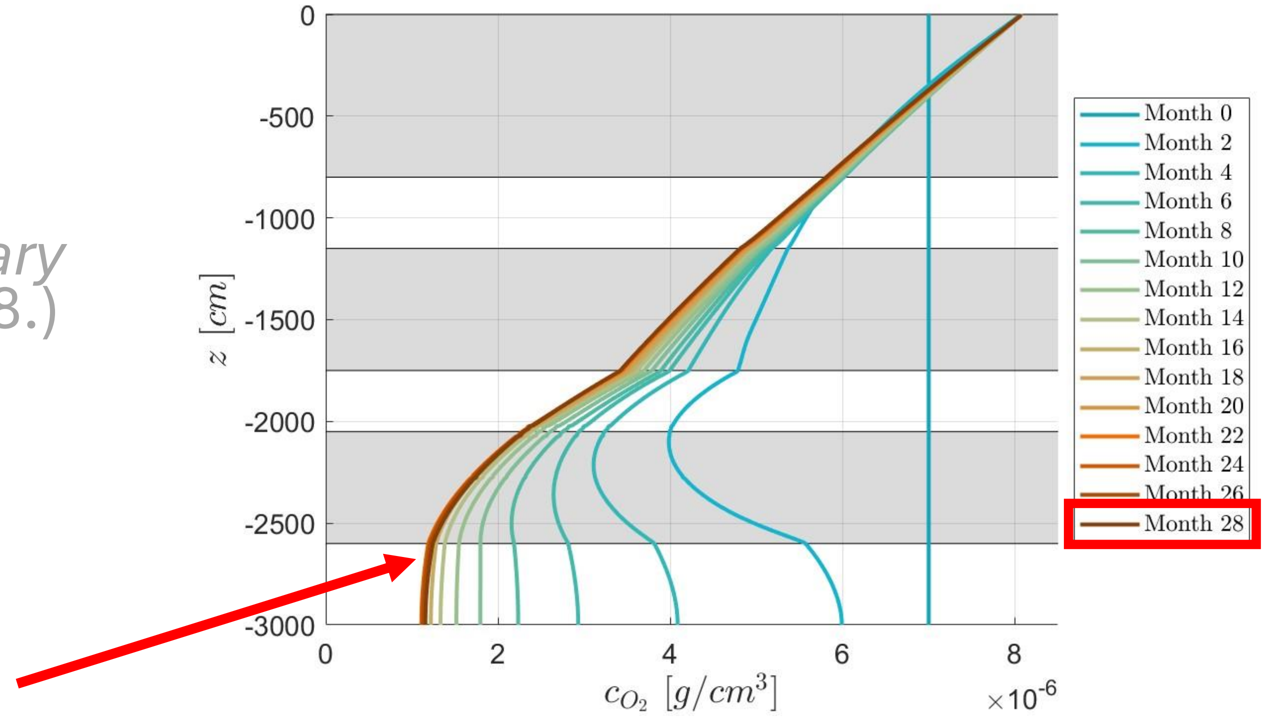
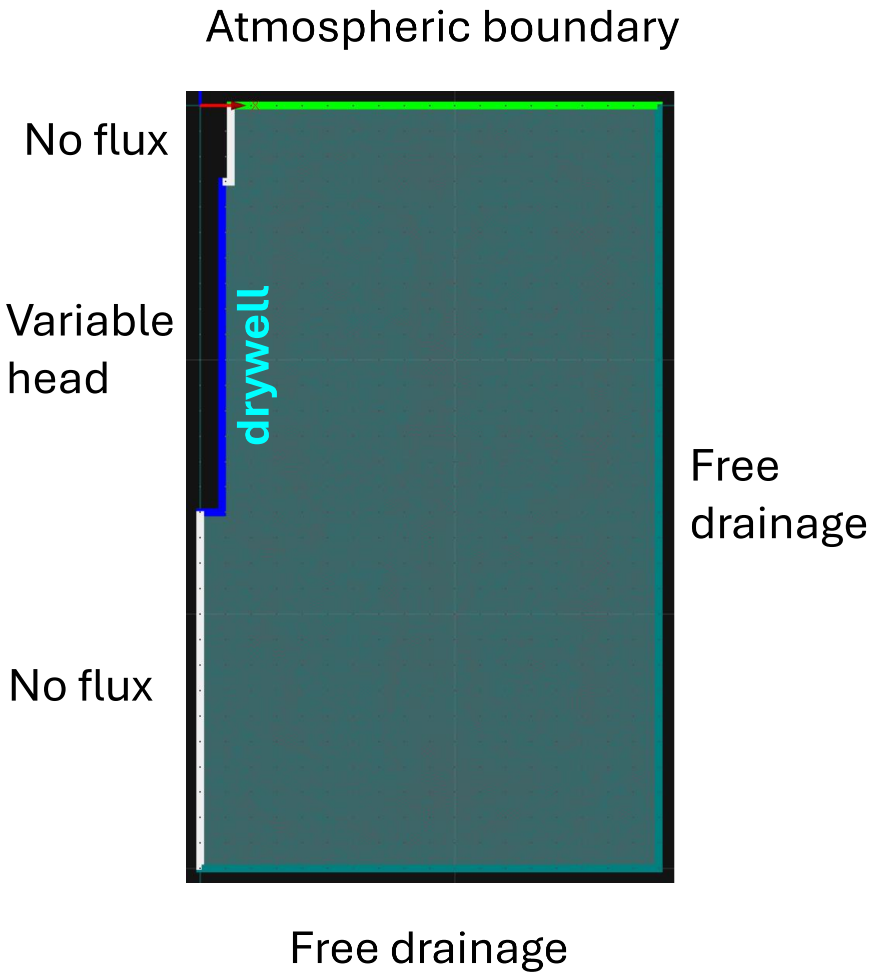
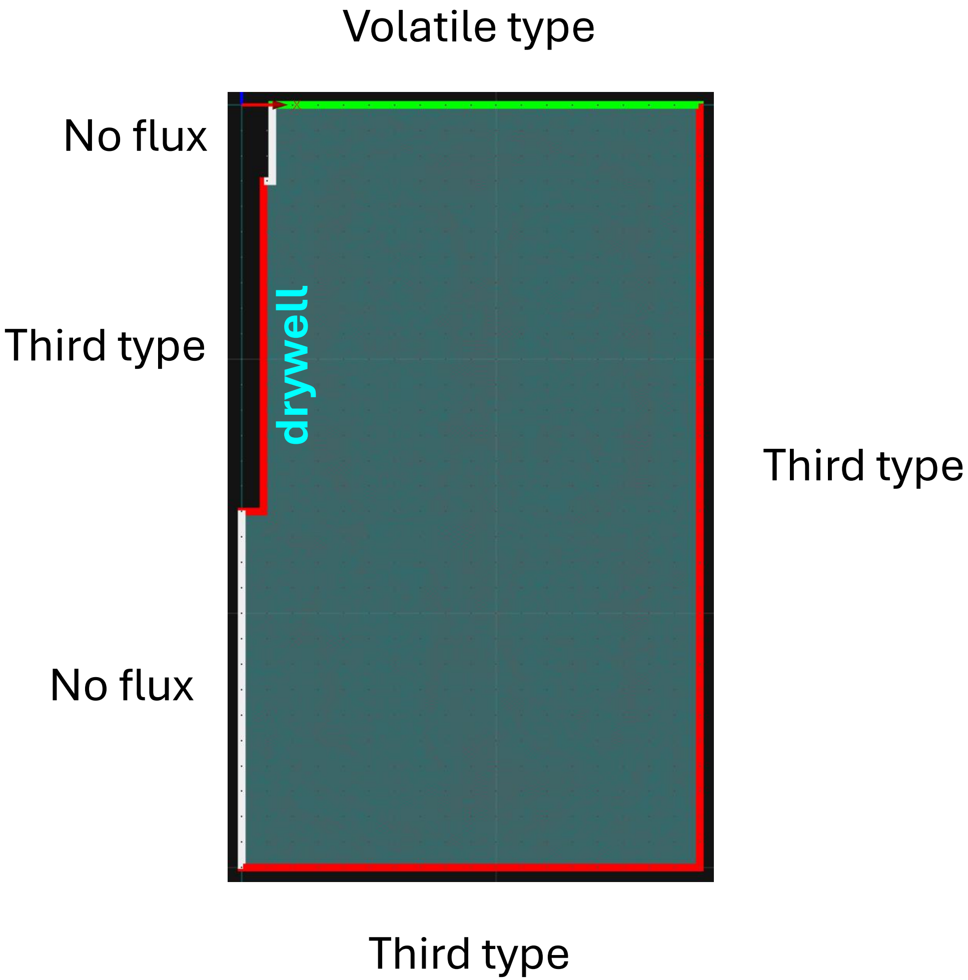


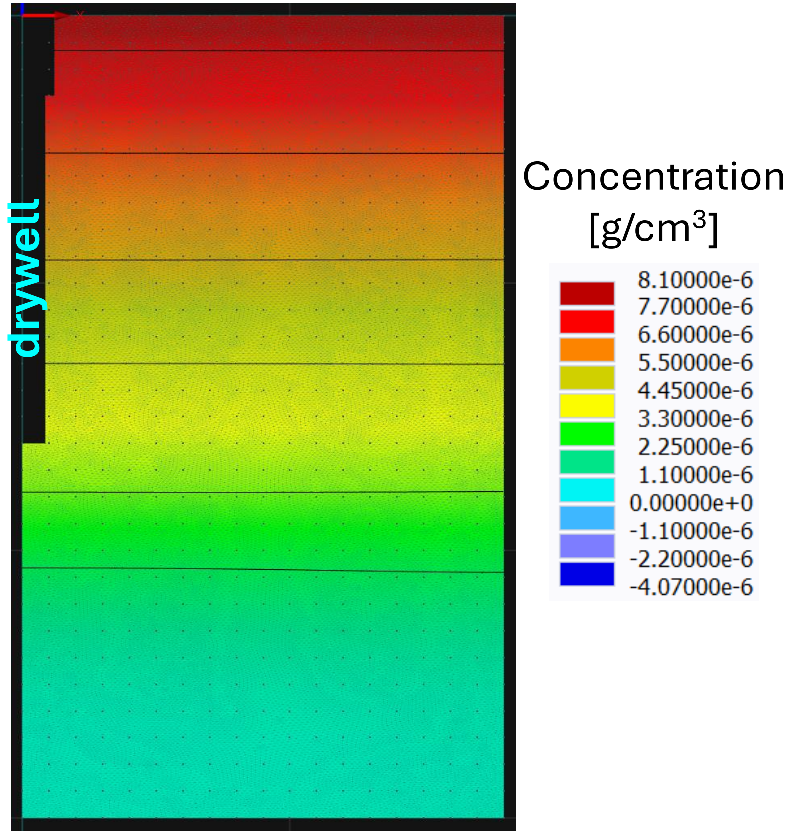
What happens when we are injecting water?





What happens when we are injecting water?

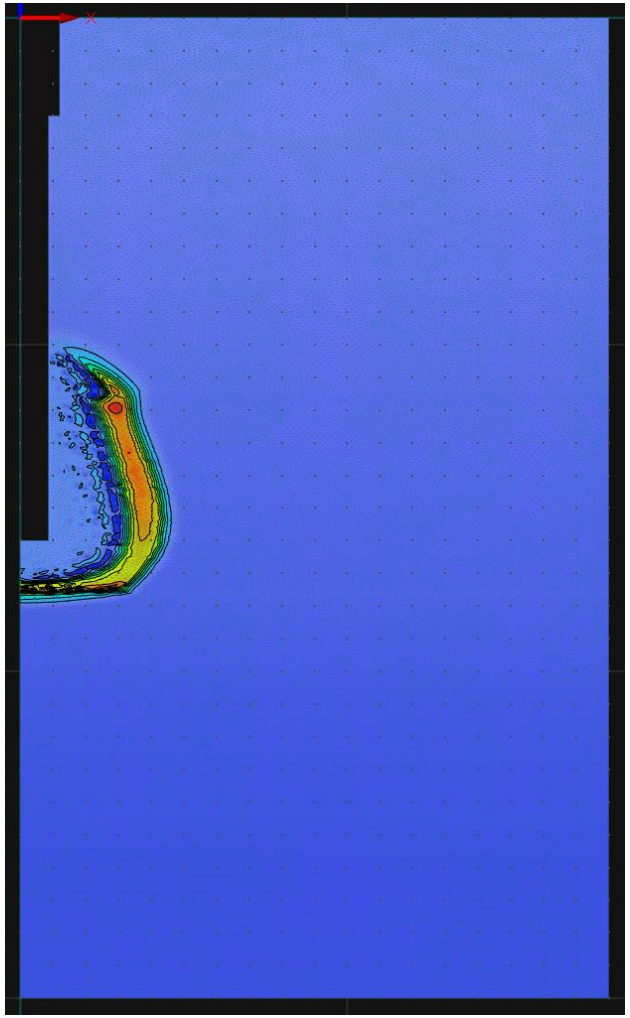
Initial condition for concentration



Injection scheme: 200 hours of injection followed by 300 hours of drainage (~8days/~13days)

How will this injection scheme compare to others (e.g. 100 hours of injection followed by 200 hours of drainage) in terms of changing redox conditions?

Work in progress – stay tuned!



Concentration [g/cm^3]

	1.40842e-4
Dark red	1.26000e-4
Red	1.12000e-4
Orange	9.80000e-5
Olive	8.40000e-5
Yellow	7.00000e-5
Green	5.60000e-5
Teal	4.20000e-5
Cyan	2.80000e-5
Light blue	1.40000e-5
Lavender	0.00000e+0
Blue	-1.89789e-5

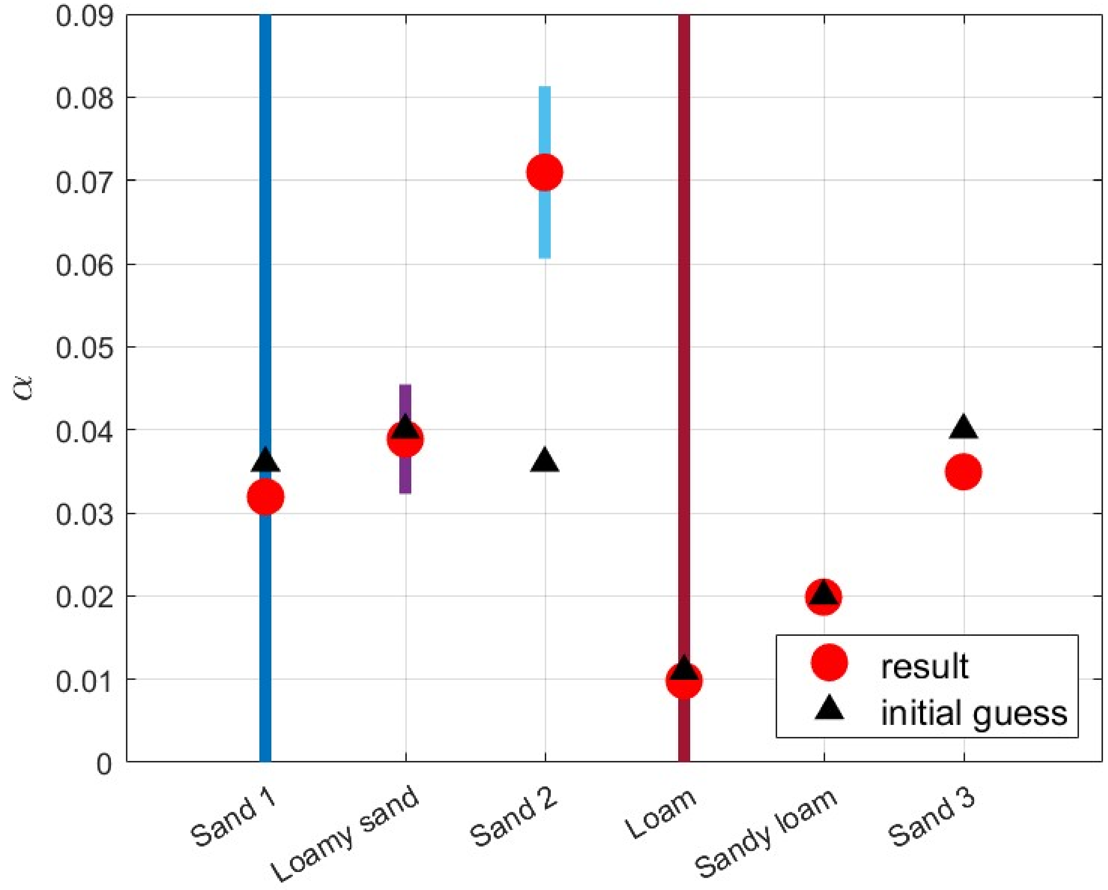
Concentration distribution after 2 hour of injection. The injected water has a constant oxygen concentration of 10^{-5} g/cm^3.

Currently having issues most likely due to numerical instability.

Thank you!

Fitted parameters: alpha

Material	Initial guess	Final estimate	Standard error coeff.
Sand 1	0.036	0.032	1003
Loamy sand	0.04	0.039	0.003
Sand 2	0.036	0.071	0.005
Loam	0.011	0.010	0.26
Sandy loam	0.020	0.020	10^(-17)
Sand 3	0.04	0.035	10^(-17)



Fitted parameters: K_{sat}

Material	Initial guess	Final estimate	Standard error coeff.
Sand 1	31.5	39.8	10^8
Loamy sand	7	13.1	1
Sand 2	21.6	6.8	0.08
Loam	0.587	0.41	3.7
Sandy loam	0.914	0.93	10^(-17)
Sand 3	7	6.4	10^(-17)