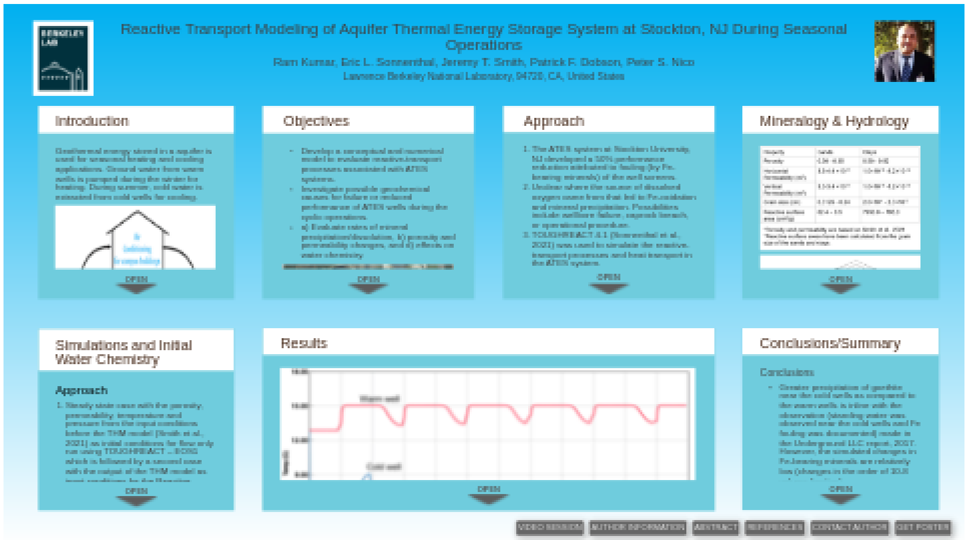
Reactive Transport Modeling of Aquifer Thermal Energy Storage System at Stockton, NJ During Seasonal Operations



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Ram Kumar, Eric L. Sonnenthal, Jeremy T. Smith, Patrick F. Dobson, Peter S. Nico

Lawrence Berkeley National Laboratory, 94720, CA, United States

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Conclusions

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INTRODUCTION

Geothermal energy stored in a aquifer is used for seasonal heating and cooling applications. Ground water from warm wells is pumped during the winter for heating. During summer, cold water is extracted from cold wells for cooling.

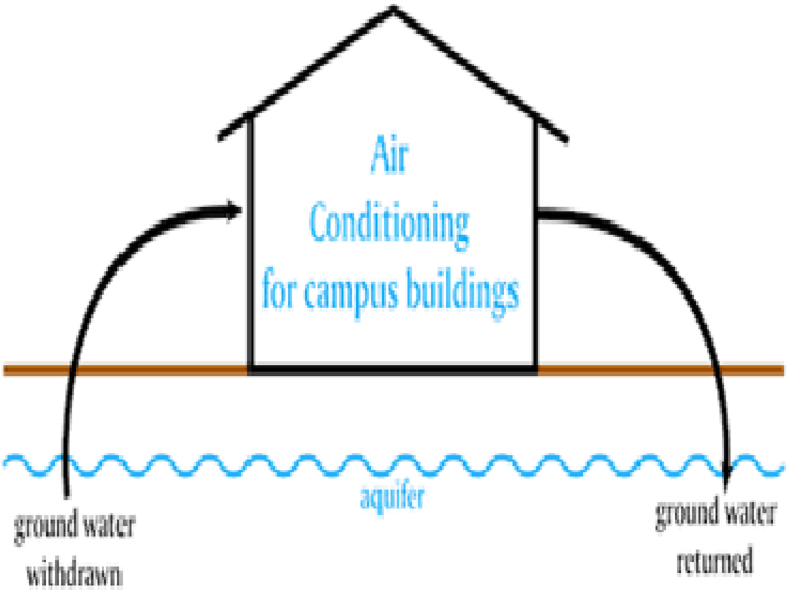


Fig 1. Aquifer Thermal Energy Storage system at Stockton University. https://stockton.edu/facilities-construction/energy-climate.html

Motivation

- Performance reduction due to well failure or clogging of wells is often observed.
- Possible causes of mineral precipitation (e.g., iron-bearing minerals) need to be identified.
- Predictive models of reactive-transport processes associated with the failure of ATES system are lacking.

OBJECTIVES

- Develop a conceptual and numerical model to evaluate reactive-transport processes associated with ATES systems.
- Investigate possible geochemical causes for failure or reduced performance of ATES wells during the cyclic operations.
- a) Evaluate rates of mineral precipitation/dissolution, b) porosity and permeability changes, and d) effects on water chemistry.

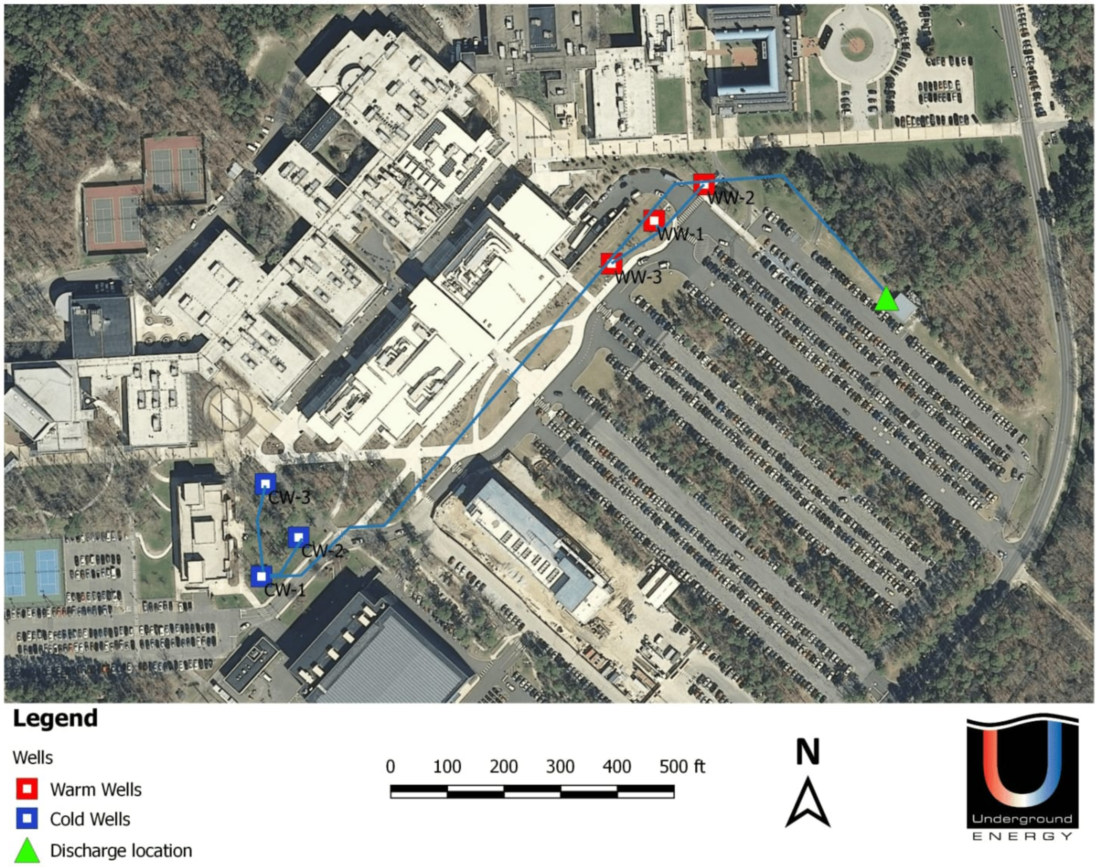


Fig 2. Cold and warm wells at Stockton University, NJ; source: Underground Energy, LLC (2017)

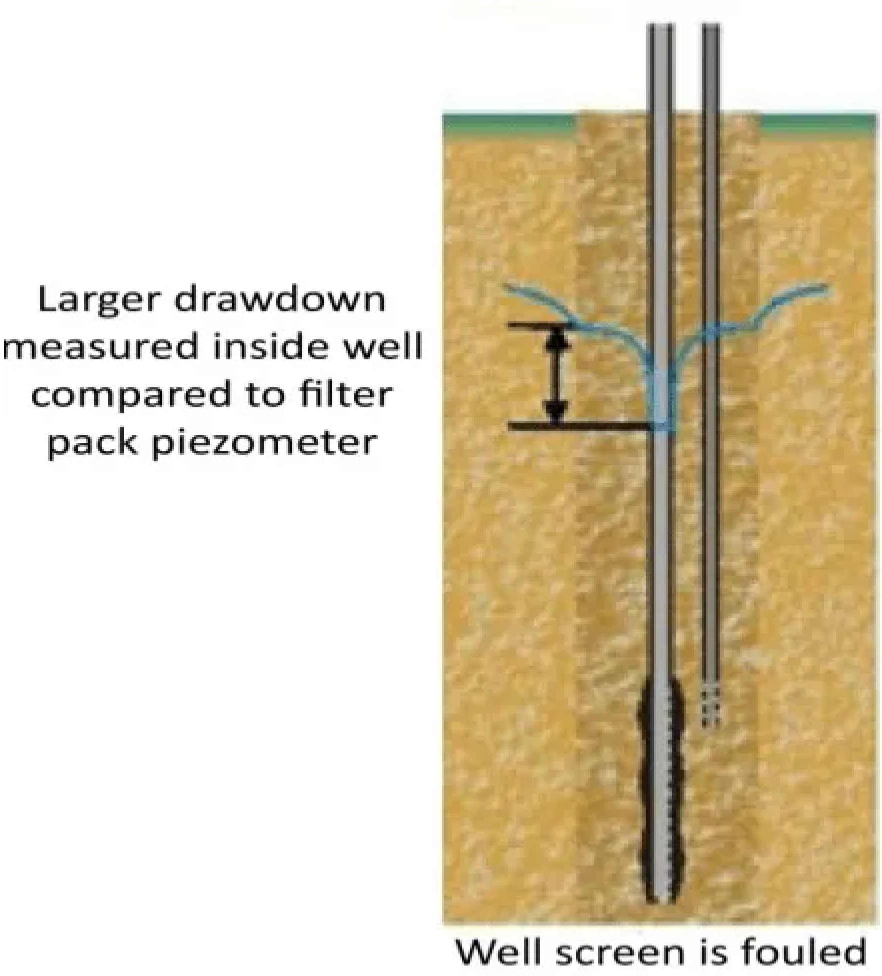


Fig 3. Schematic of fouling at well screen

APPROACH

1. The ATES system at Stockton University, NJ developed a 50% performance reduction attributed to fouling (by Fe-bearing minerals) of the well screens.
2. Unclear where the source of dissolved oxygen came from that led to Fe-oxidation and mineral precipitation. Possibilities include wellbore failure, caprock breach, or operational procedure.
3. TOUGHREACT 4.1 (Sonnenthal et al., 2021) was used to simulate the reactive-transport processes and heat transport in the ATES system.
4. The numerical grid and hydrologic properties are based on Smith et al. (2021) who evaluated the ATES system using thermal-hydrological-mechanical (THM) model. This study takes the initial hydrologic properties and the geomechanically-modified permeability field from Smith et al. (2021) as inputs to the reactive-transport model.

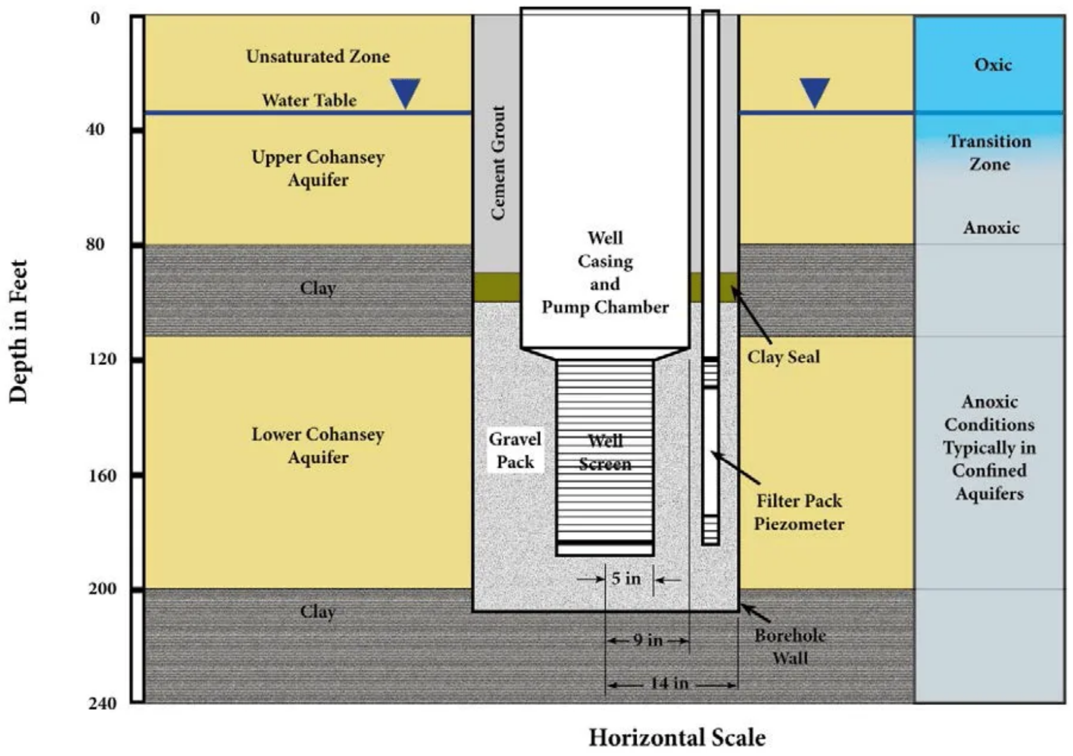


Fig 4. Hydrogeologic units and well schematic (Underground Energy LLC report, 2017)

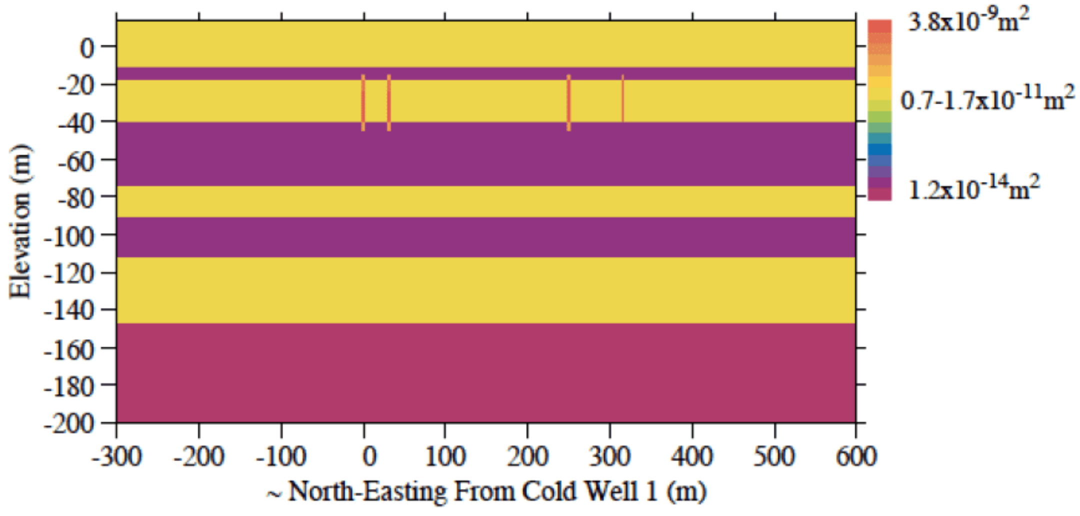


Fig 5. Cross-section of vertical permeability field, elevation in meters (Smith et al., 2021)

MINERALOGY & HYDROLOGY

Property	Sands	Clays
Porosity	0.30 - 0.35	0.50 - 0.52
Horizontal Permeability (m^2)	$3.6\text{-}4.4 \times 10^{-11}$	$1.0\times10^{-16}\text{-}1.2\times10^{-14}$
Vertical Permeability (m^2)	$3.3\text{-}3.4 \times 10^{-11}$	$1.0\times10^{-16}\text{-}1.2\times10^{-14}$
Grain size (cm)	0.0125 - 0.24	2.0×10^{-4} - 2.0×10^{-3}
Reactive surface area (cm^2/g)	62.4 – 6.5	7950.0 – 795.0

*Porosity and permeability are based on Smith et al., 2021
*Reactive surface areas have been calculated from the grain size of the sands and clays.

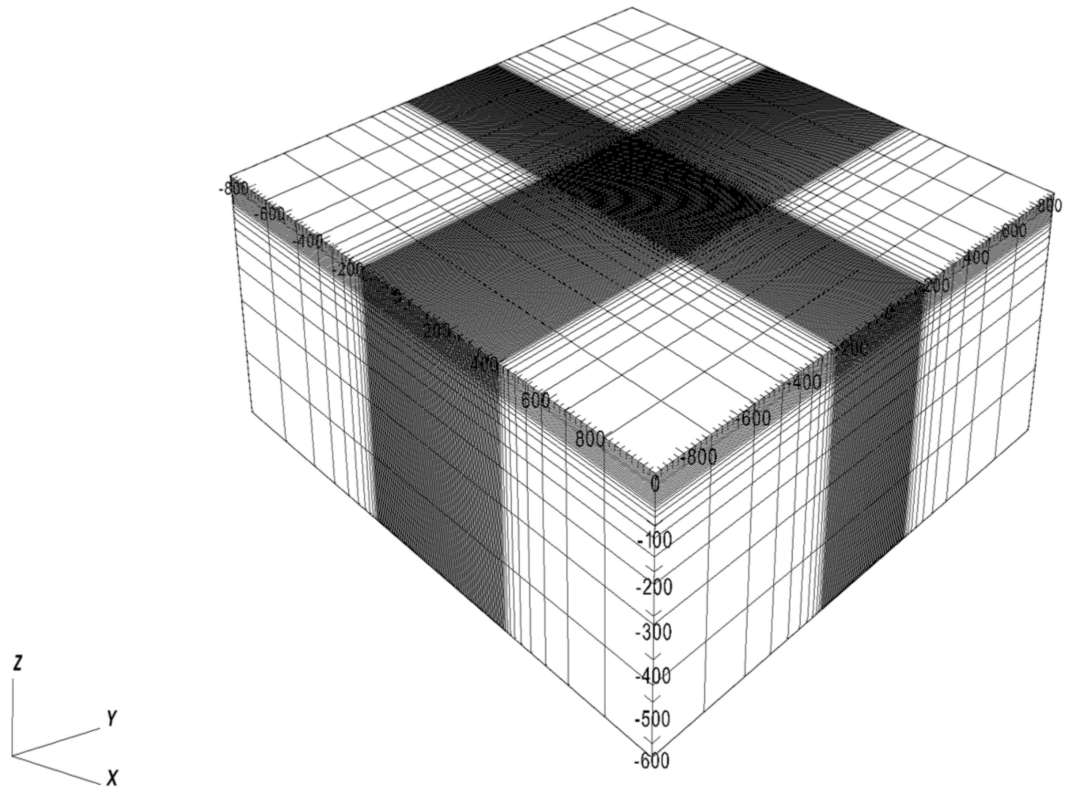
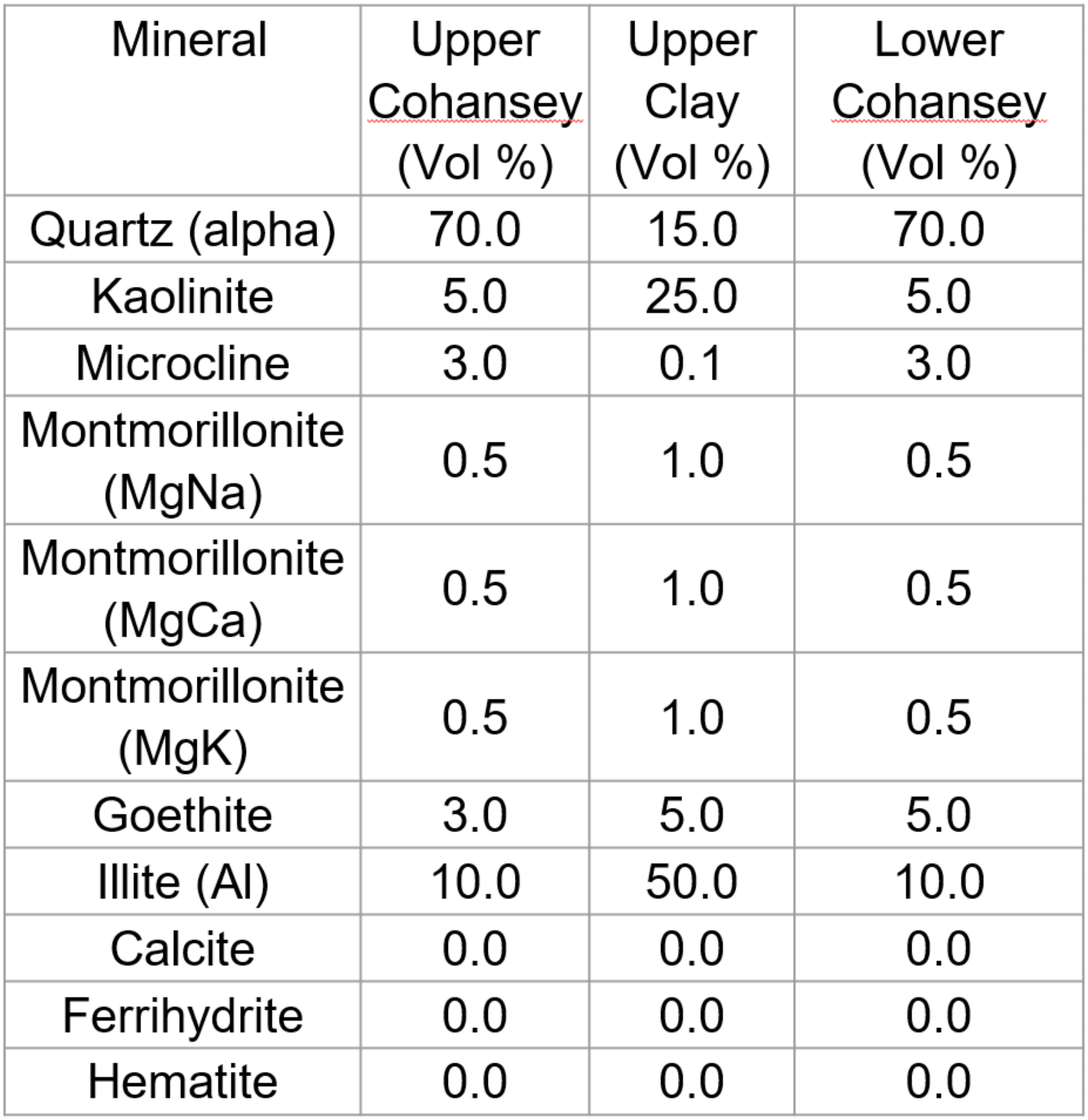


Fig. 6. Numerical 3-D Grid

Table 1: Mineralogy



Mineral	Upper Cohansey (Vol %)	Upper Clay (Vol %)	Lower Cohansey (Vol %)
Quartz (alpha)	70.0	15.0	70.0
Kaolinite	5.0	25.0	5.0
Microcline	3.0	0.1	3.0
Montmorillonite (MgNa)	0.5	1.0	0.5
Montmorillonite (MgCa)	0.5	1.0	0.5
Montmorillonite (MgK)	0.5	1.0	0.5
Goethite	3.0	5.0	5.0
Illite (Al)	10.0	50.0	10.0
Calcite	0.0	0.0	0.0
Ferrihydrite	0.0	0.0	0.0
Hematite	0.0	0.0	0.0

Mineralogy is based on Ishphording, 1970

SIMULATIONS AND INITIAL WATER CHEMISTRY

Approach

1. Steady state case with the porosity, permeability, temperature and pressure from the input conditions before the THM model (Smith et al., 2021) as initial conditions for flow only run using TOUGHREACT – EOS1 which is followed by a second case with the output of the THM model as input conditions for the Reactive-Transport (RT) model.

2. Reactive transport models (no injection/production) were built on the both the scenarios to get the chemical steady state of the ATES system. No-flux boundary conditions are used for the steady state cases.

3. Flow-only cases with the injection/production (large volume side boundaries) cycle were run based on the hydrologic properties obtained in the runs of approach (1).

4. Reactive transport models with the injection production cycle were run based on the outputs from the runs of approach (2) as input conditions.

Cases

1. Base-case (no geomechanical effects on permeability from the THM simulations), initial condition same as the THM model by Smith et al., 2021.
2. Perturbed case (modified hydrologic properties (porosity/permeability) from the THM model.
3. Perturbed case when injection water is saturated with atmospheric oxygen (presented in this poster).

Table 2: Initial Water Chemistry

Species (Total)	Concentration (mg/l)
Dissolved Oxygen	5.8
Calcium	0.78
Iron	0.43
Magnesium	1.6
Manganese	0.02
Sodium	4.5
Potassium	1.0
Chloride	9.5
Alkalinity as $CaCO_3$	1.4
Nitrate-N	1.9
Sulphate	1.9
Aluminium	5.1*
Dissolved Silica	9.2*
pH	5.1

IF Technology, 2005. Sample collected on March 20 and Sept 4, 2003 at 12.7 °C. *Aluminium is estimated by equilibrating the water with Kaolinite. Dissolved Silica is measured by USGS (Owens et al., 1988)

RESULTS

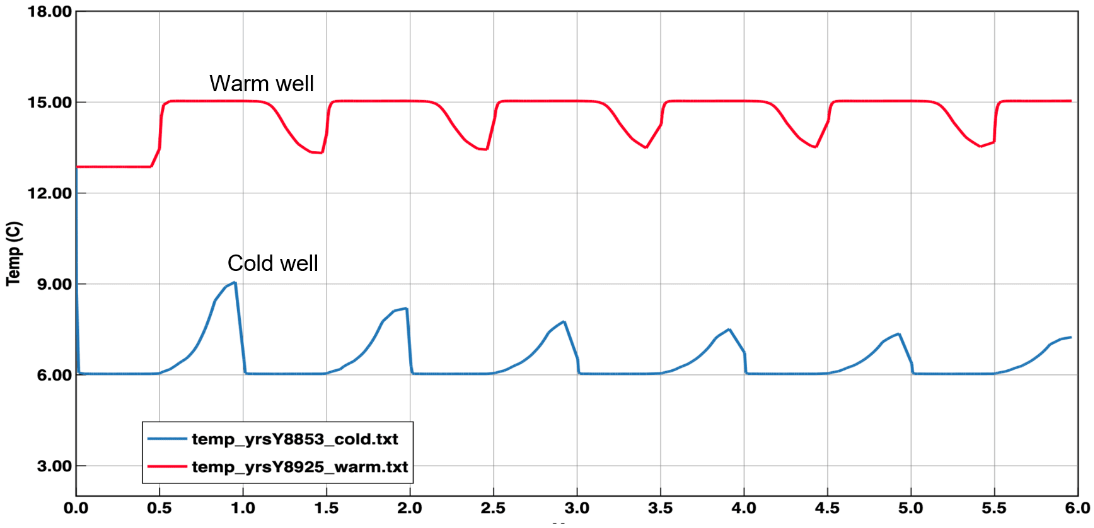
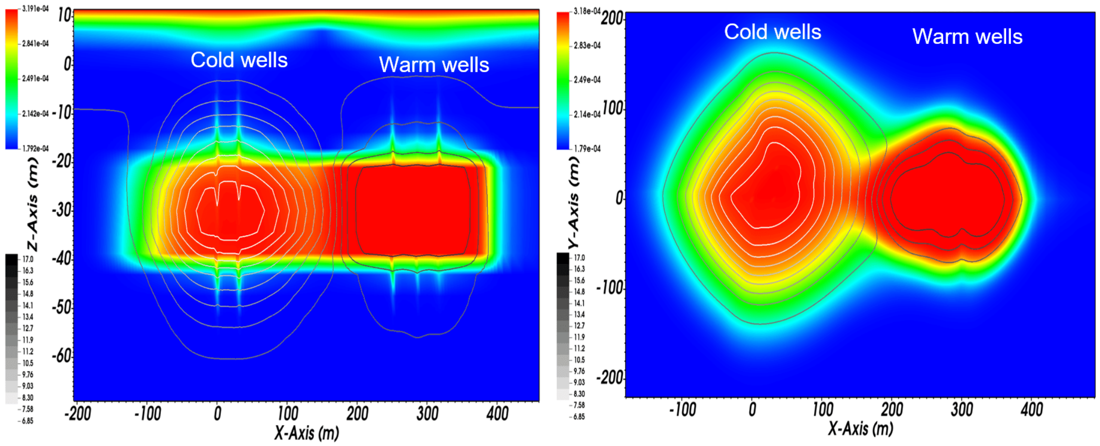


Fig. 7: Temperature after 6 years



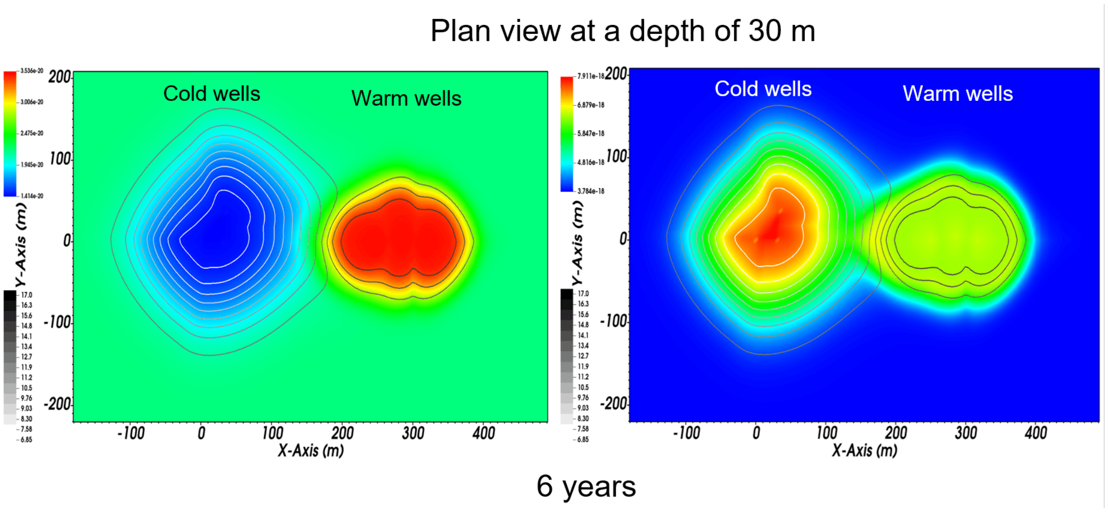
East-west cross section

6 years

Plan view at a depth of 30 m

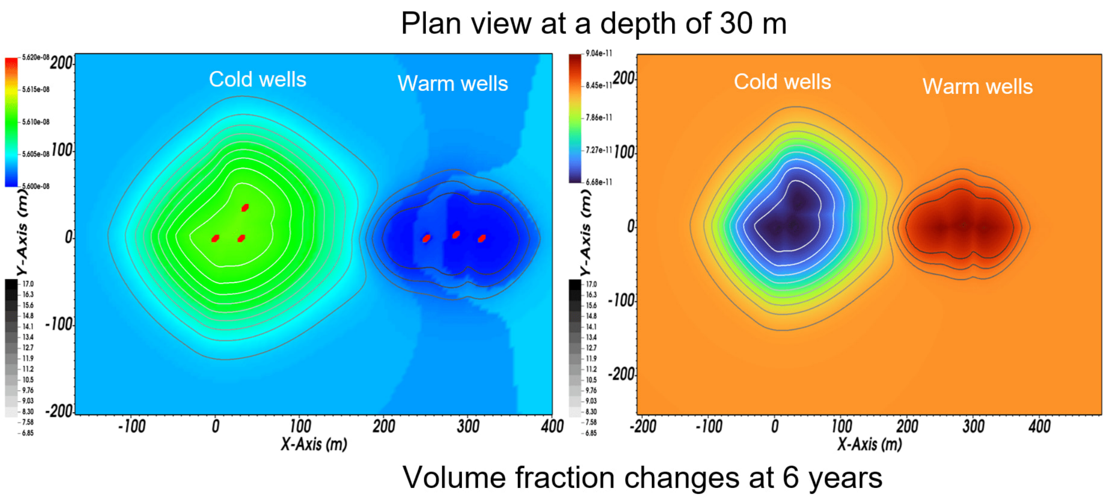
6 years

Fig. 8: Dissolved Oxygen and Temperature


Plan view at a depth of 30 m

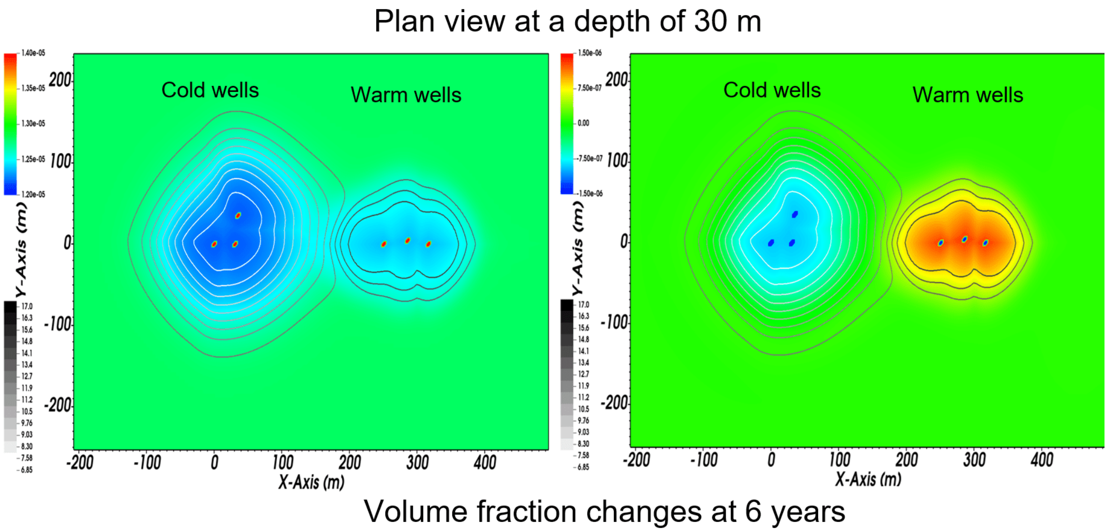
6 years

Fig. 9: Fe^{2+} and Fe^{3+} Concentrations


Plan view at a depth of 30 m

Volume fraction changes at 6 years

Fig. 10: Goethite and Hematite


Plan view at a depth of 30 m

Volume fraction changes at 6 years

Fig. 11: Kaolinite and Illite

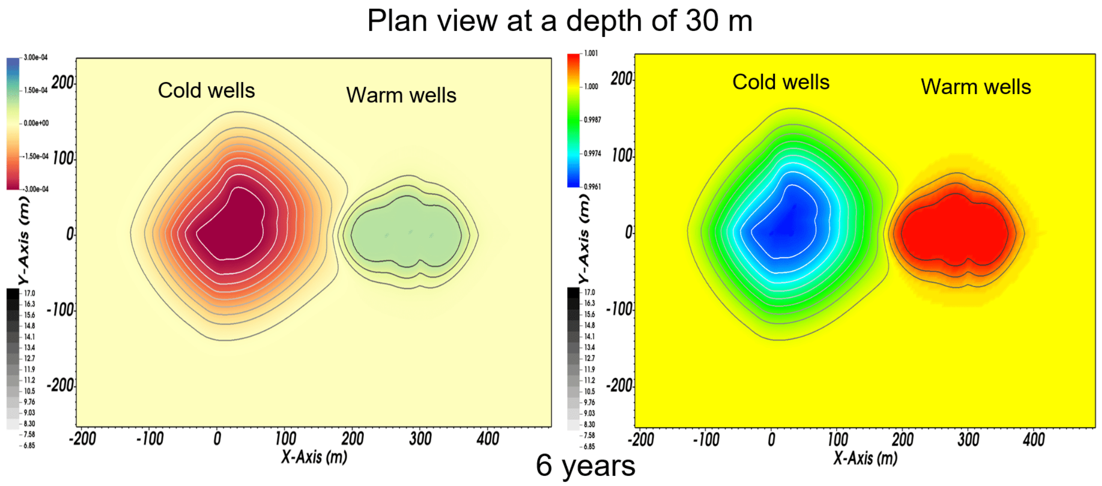


Fig. 12: Porosity Changes and Permeability Ratio (Kz/Kz0)

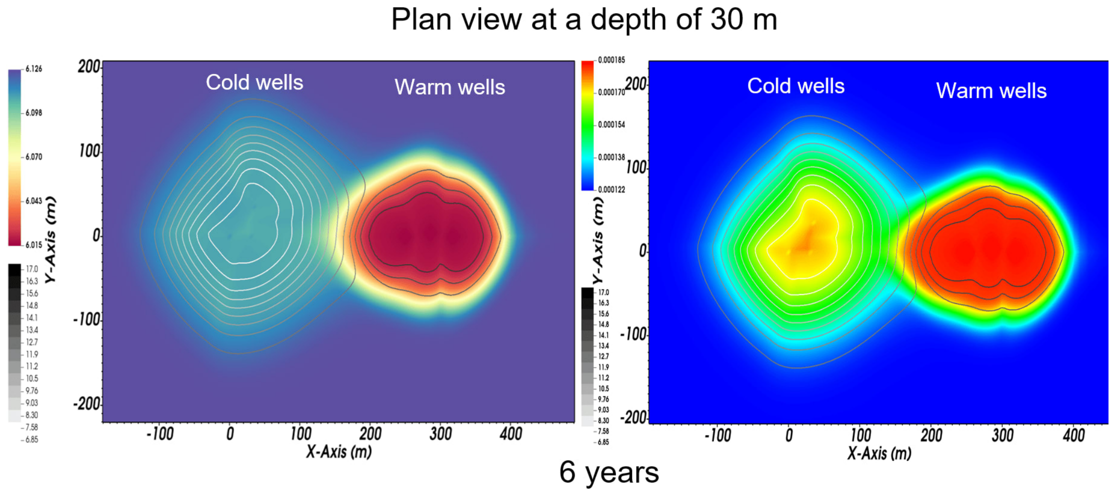


Fig. 13: pH and total Potassium

CONCLUSIONS/SUMMARY

Conclusions

- Greater precipitation of goethite near the cold wells as compared to the warm wells is inline with the observation (standing water was observed near the cold wells and Fe fouling was documented) made in the Underground LLC report, 2017. However, the simulated changes in Fe-bearing minerals are relatively low (changes in the order of 10-8 volume fraction).
- Precipitation of kaolinite is highest among the minerals. Also, it is precipitating more near the cold wells as compared to the warm wells.
- Illite shows dissolution near the cold wells and precipitation near the warm wells.
- There is a net decrease in the porosity near the cold wells and increase near the warm wells. The changes in mineralogy are not the only factor responsible for the porosity change. The pore compression near the cold wells and pore expansion near the warm wells due to temperature and pressure conditions can also be accounted (order of 10-5) for the changes in porosity.

Limitations/Recommendations

- Gridding near the wells needs to be refined (to a mm-scale) to quantify the iron hydroxide precipitation on the well screen.
- Although the mineralogy for the model is based on the USGS data for the Cohansey formation, it needs to be further refined from the characterization of rocks at the ATES site.
- Initial water chemistry should be measured seasonally, and effects of groundwater flow evaluated.

AUTHOR INFORMATION

Ram Kumar, Eric L. Sonnenthal, Jeremy T. Smith, Patrick F. Dobson, Peter S. Nico

Lawrence Berkeley National Laboratory

Email: ramkumar@lbl.gov

ABSTRACT

Understanding the hydrogeochemical processes associated with Aquifer Thermal Energy Storage (ATES) operations can improve functioning of the wells and overall performance of the ATES system. The cause of premature failure of ATES wells due to mineralogical changes has not been studied quantitatively and requires evaluation of coupled geochemical reactions, transport processes, and potential hydrological changes. In this study, the objective is to develop a predictive model to evaluate reactive-transport processes associated with ATES systems. The specific goals are a) evaluate rates of mineral precipitation/dissolution, b) porosity and permeability changes, and d) effects on water chemistry.

The reactive-transport code TOUGHREACT was used to model the seasonal heating and cooling operations at the ATES site. The numerical model evaluates the hydrogeochemical changes during the 6 years of seasonal operation for the perturbed system (geomechanical effects on permeability) when injection water is saturated with atmospheric oxygen. The results show greater precipitation of goethite near the cold wells as compared to the warm wells. However, the simulated changes in Fe-bearing minerals are relatively low (changes in the order of 10^{-8} volume fraction). Kaolinite shows highest precipitation among the minerals. Also, it is precipitating more near the cold wells as compared to the warm wells. Illite shows dissolution near the cold wells and precipitation near the warm wells. There is a net decrease in the porosity near the cold wells and increase near the warm wells. The changes in mineralogy are not the only factor responsible for the porosity change. The pore compression near the cold wells and pore expansion near the warm wells due to temperature and pressure conditions can also be accounted (order of 10^{-5}) for the changes in porosity. The study presents a detailed analysis of the hydrogeochemical processes and modeling methodology which can be used for ATES system design and long-term performance optimization. For the future work, the gridding near the wells needs to be more refined (to a mm-scale) to quantify the iron hydroxide precipitation on the well screen.

REFERENCES

1. Smith, T., Sonnenthal, E., Dobson, P., Nico, P., & Worthington, M. Thermal-Hydrological-Mechanical Modeling of Stockton University Reservoir Cooling System. Proceedings, 46th Workshop on Geothermal Reservoir Engineering, Stanford University, Stanford, California, February 15-17, 2021.

2. Underground Energy, LLC. Aquifer Thermal Energy Storage (ATES) System Evaluation, Stockton University (New Jersey), July 2017. UE Project No. STO.2016.01.

3. Isphording, W. C., Petrology, stratigraphy, and re-definition of the Kirkwood Formation (Miocene) of New Jersey. Journal of Sedimentary Research 1970, 40 (3), 986-997.

4. Sonnenthal, E.; Spycher, N.; Xu, T.; Zheng, L., TOUGHREACT V4.1-OMP reference manual: a parallel simulation program for non-isothermal multiphase geochemical reactive transport. University of California, Berkeley 2021