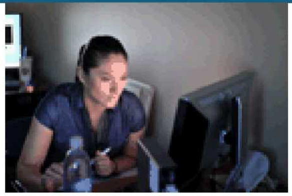
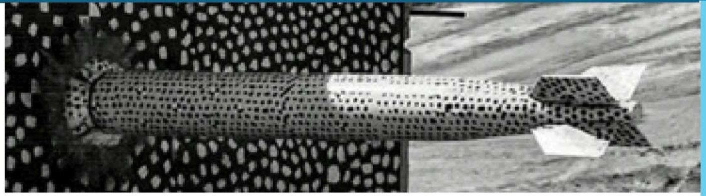
SAND2020-5594C

Parameter Sensitivity in Subsurface Gas Transport Calculations





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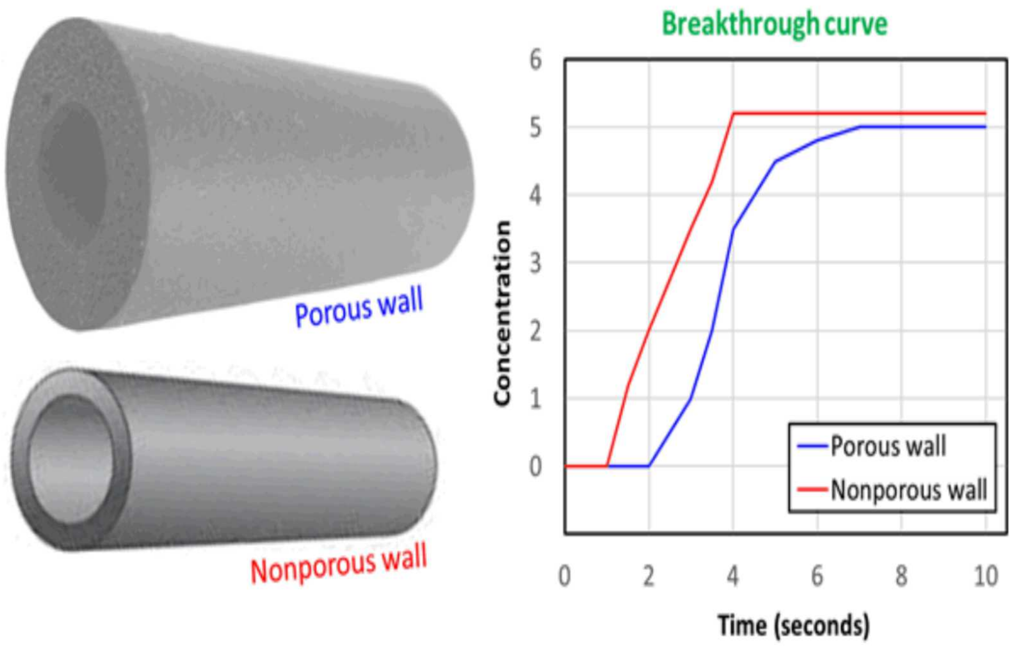
Outline

- Project Introduction
  - Purpose
  - Planned Work
    - Modeling: Molecular Dynamics and Reactive Transport
    - Experimental
- Reactive Transport Modeling Results
  - Field-scale Model
  - Parameter Sensitivity
- Continued Work



Molecular-scale properties such as porosity directly impact gas transport rates.

For example, gas transport via a more porous pathway could lead to delayed breakthrough as gas is lost to the porous host rock.

Introduction

Subsurface explosions may result in the production of gases that can be detected at the surface

Interactions between the gases and host rocks impact the rate of gas transport, e.g.:

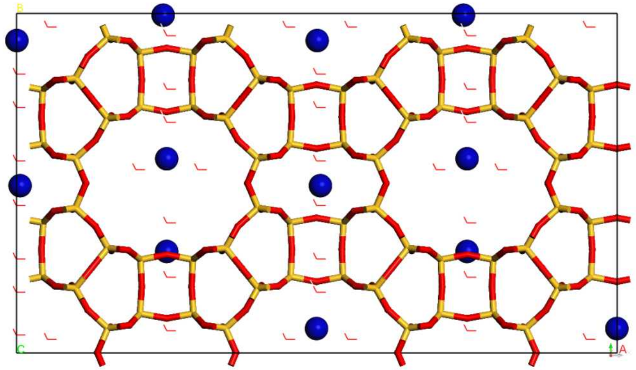
- Porosity
- Permeability
- Diffusion
- Gas-Surface Adsorption

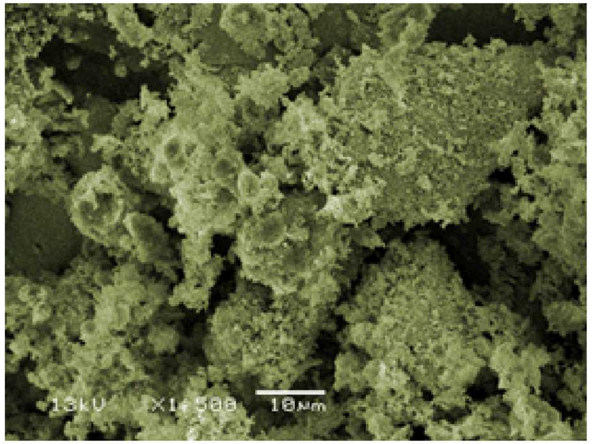
These properties and processes are impacted by molecular-level phenomena

A new project at SNL investigates the effect of host rock and gas properties on adsorption and transport, experimentally and with modeling for a variety of host rocks

Varied crystal structures, pore structures, and adsorption behavior among host rocks impact subsurface gas transport rates

Mordenite (zeolitic mineral)





SEM image of clinoptilolite showing microstructure
https://www.kmizeolite.com/technical-data/

Planned Work

Modeling

Molecular Dynamics (MD)/Grand Canonical Monte Carlo (GCMC)

- Atomic-scale simulations of gas adsorption in pores of varying sizes

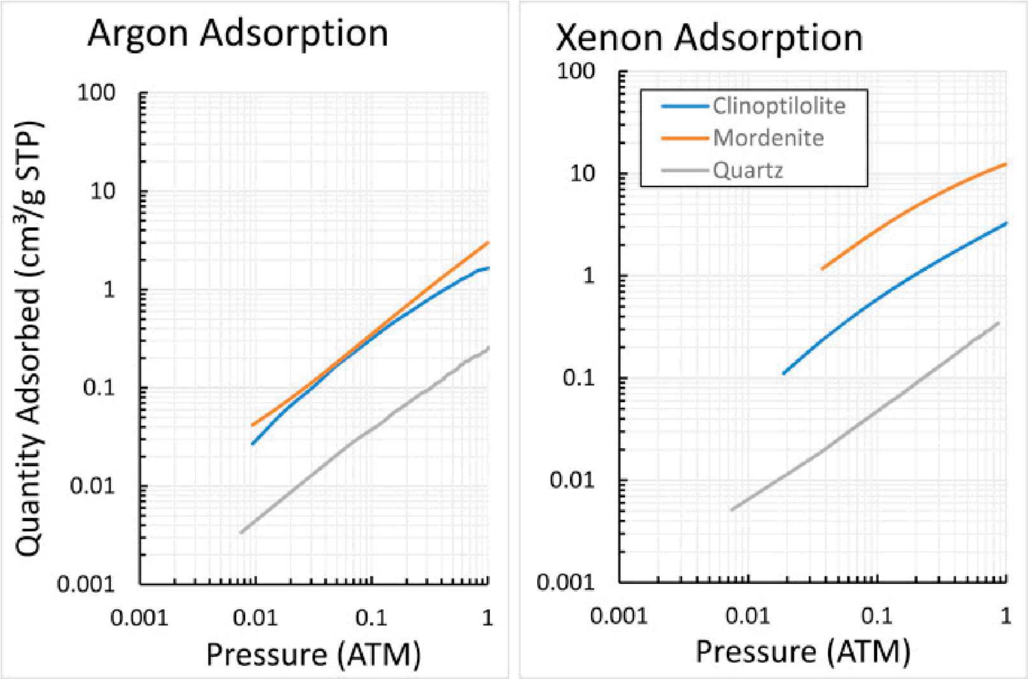
Reactive Transport

- Lab-scale simulations to complement experimental work
- Field-scale simulations will eventually extend information gained by experiments and MD modeling to interpretation under real-life conditions
- **Field-scale simulations presented here are part of an preliminary study to set up the general framework to accommodate MD and experimental data, as well as provide a parameter sensitivity analysis framework**

Experimental

Adsorption and diffusion properties of noble gases in representative mineral phases will be determined in the laboratory

See talk by Guangping Xu in this session



Feldman, J., et al., (2020) Journal of Environmental Radioactivity, 220–221, 106279

Reactive Transport Modeling – Model Setup

Field-scale model domain of 50m x 250m

Two-dimensional model

Run using PFLOTRAN, SNL's open-source reactive transport code

Single vertical column of "fracture" material
- 10^{-3}m wide, extending to surface along axis of symmetry

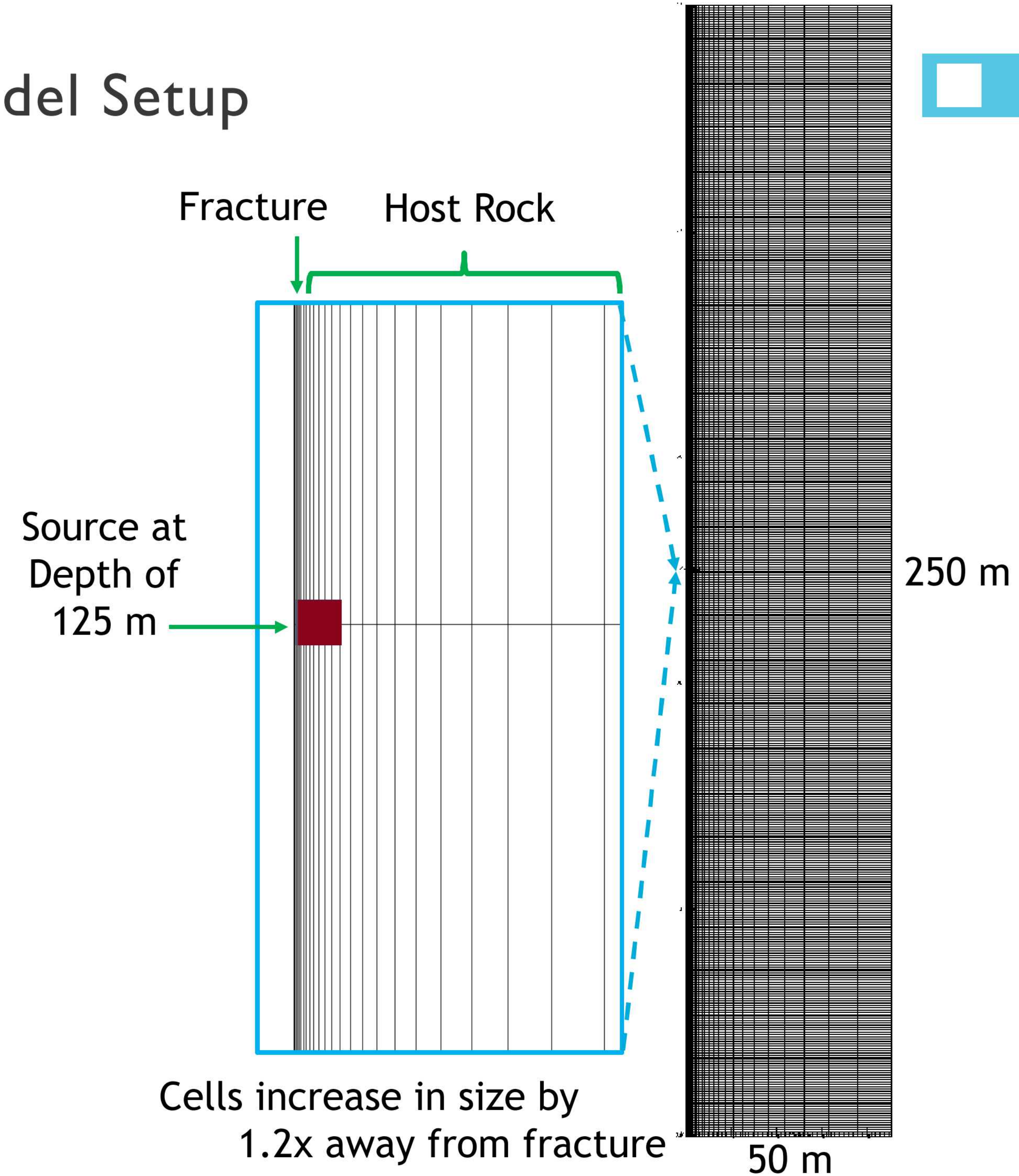
Remaining 49 columns are "host rock" material

Total of 25,000 cells (50 x 500)

Gas source modeled by high initial pressure in a region of 1m x 1m at a depth of 125m

Simulation time of 20 days

Argon is assumed transport gas
- Half-life of 35 days



Reactive Transport Modeling – Parameter Distributions

Eight parameters varied across 100 simulations

- Fracture and host rock properties
  - Porosity and permeability
- Gas diffusion coefficient (argon)
- Matrix partition coefficient
- Gas source properties
  - Temperature and pressure

Permeabilities sampled across log-uniform distributions

Other parameters sampled randomly across uniform distributions

Parameter distributions based roughly on literature values, with some broadening to account for uncertainty in this initial study

Parameter	Units	Distribution Type	Min.	Max.	Range
Temperature	C	Uniform	20	50	30
Pressure	Pa	Uniform	1.03E+05	2.06E+06	1.95E+06
Gas Diffusion Coefficient	cm^2/s	Uniform	0.05	1	0.95
Partition Coefficient	kg/m^3	Uniform	0	100	100
Fracture Porosity	-	Uniform	0.9	0.99	0.09
Fracture Permeability	m^2	Loguniform	-14	-10	4
Matrix Porosity	-	Uniform	0.1	0.5	0.4
Matrix Permeability	m^2	Loguniform	-20	-15	5

Reactive Transport Modeling – Breakthrough Timing Results

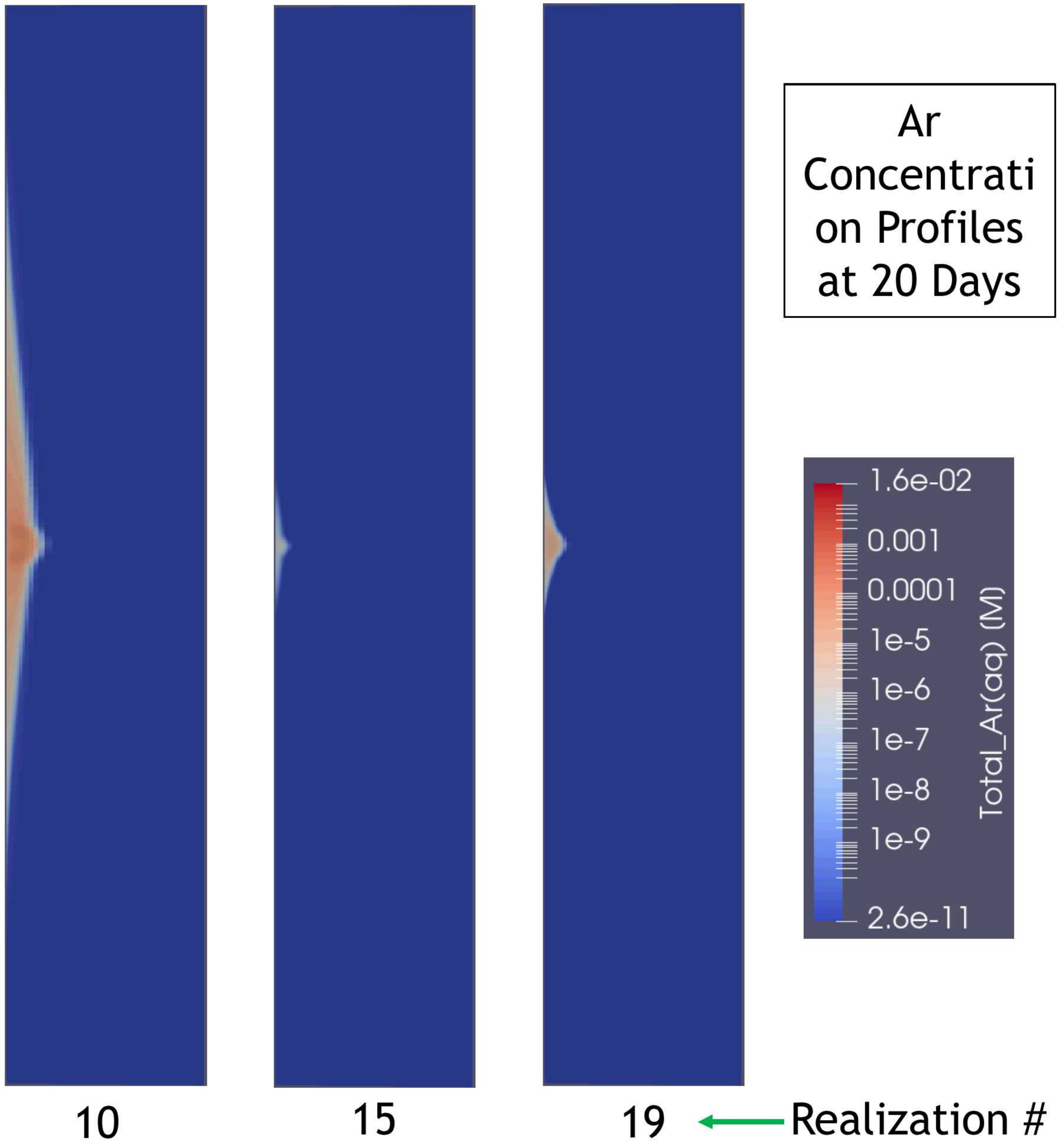
100 realizations of sampled parameters were investigated

Concentration of Ar at the surface is computed over time

A variety of output concentration profiles across the modeling domain are observed due to parameter sampling

- With eight parameters being varied, it is difficult to pinpoint a single parameter that is driving the observed differences – it is likely due to impacts from various parameters.
- A parameter sensitivity study that covers the results from a large number of simulations will provide insight.

Realization	Temp. (C)	Press. (Pa)	Gas Diffusion Coefficient (cm^2/s)	Partition Coefficient (kg/m^3)	Fracture Porosity	Fracture Perm. (m^2)	Matrix Porosity	Matrix Perm. (m^2)
10	25	1.3E+06	0.22	9.74	0.98	9.0E-14	0.18	5.3E-20
15	38	5.9E+05	0.36	9.41	0.94	6.6E-14	0.20	7.9E-17
19	36	1.8E+06	0.83	75.96	0.90	1.1E-12	0.31	1.2E-20

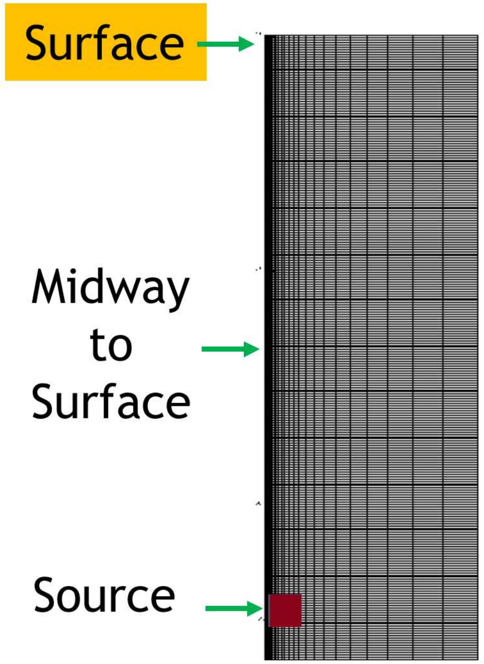


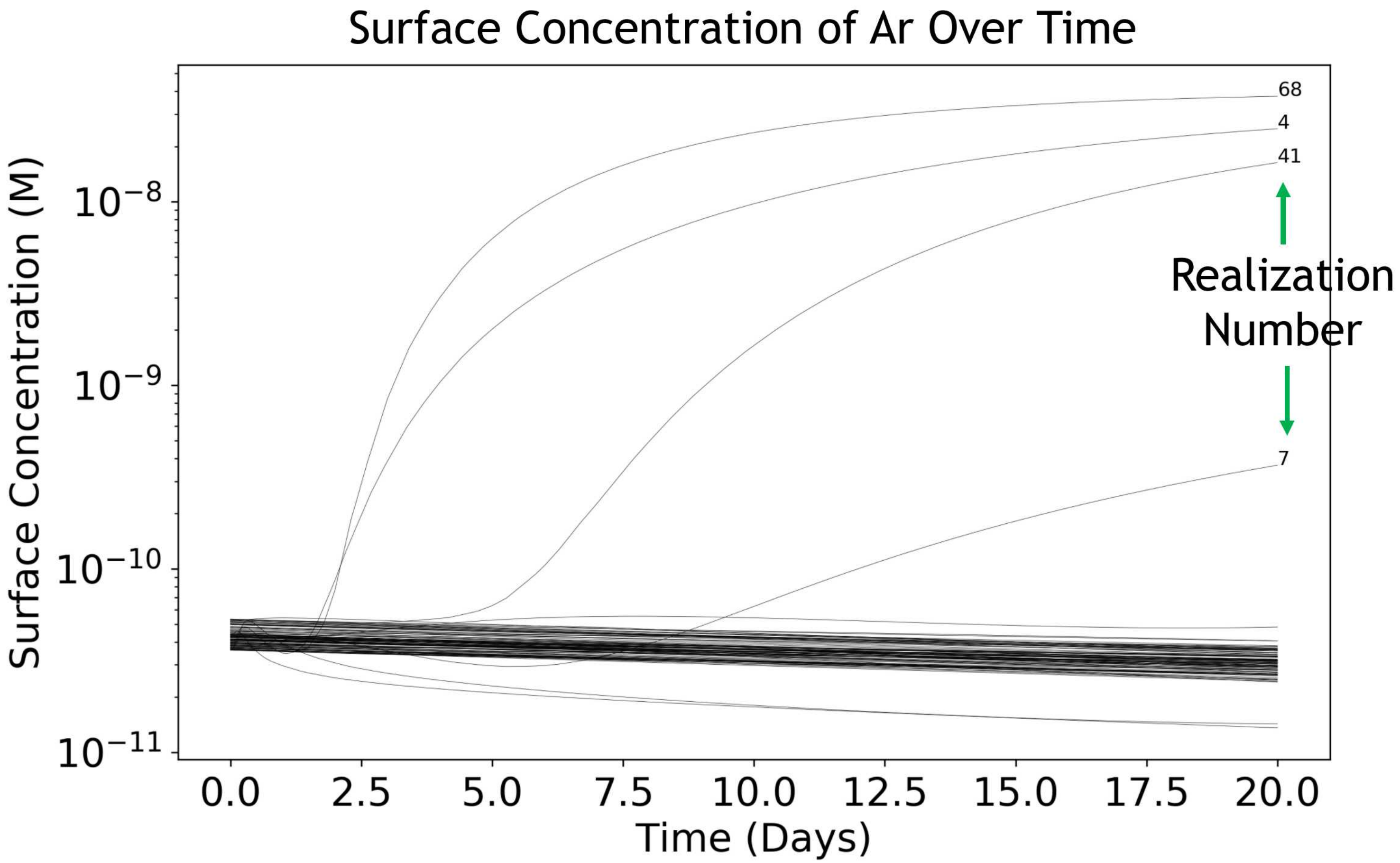
Reactive Transport Modeling – Breakthrough Timing Results

Few realizations result in breakthrough of Ar to the surface due to various factors:

- Combinations of sampled parameters
- Radioactive decay (Ar-37 half life of 35 d)
- Lack of time
- Diffusion into host rock

Realization	Temp. (C)	Press. (Pa)	Gas Diffusion Coefficient (cm^2/s)	Partition Coefficient (kg/m^3)	Fracture Porosity	Fracture Perm. (m^2)	Matrix Porosity	Matrix Perm. (m^2)
4	50	1.9E+06	0.58	41.01	0.97	4.9E-11	0.28	3.1E-18
41	22	1.8E+06	0.60	16.03	0.94	1.8E-11	0.28	2.9E-17
68	50	1.6E+06	0.54	0.64	0.95	2.5E-11	0.47	2.1E-17

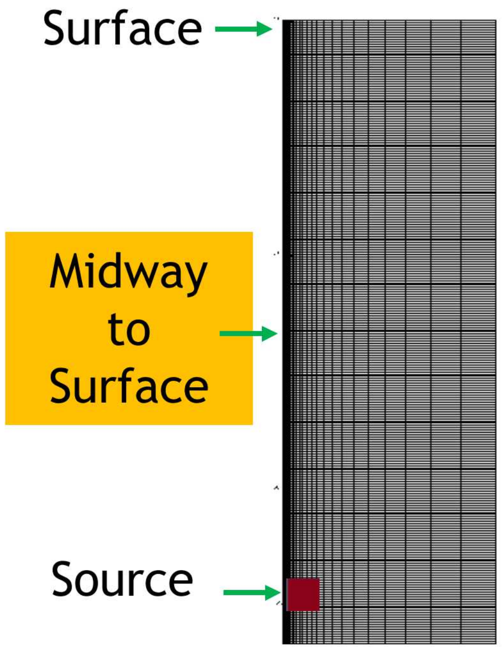


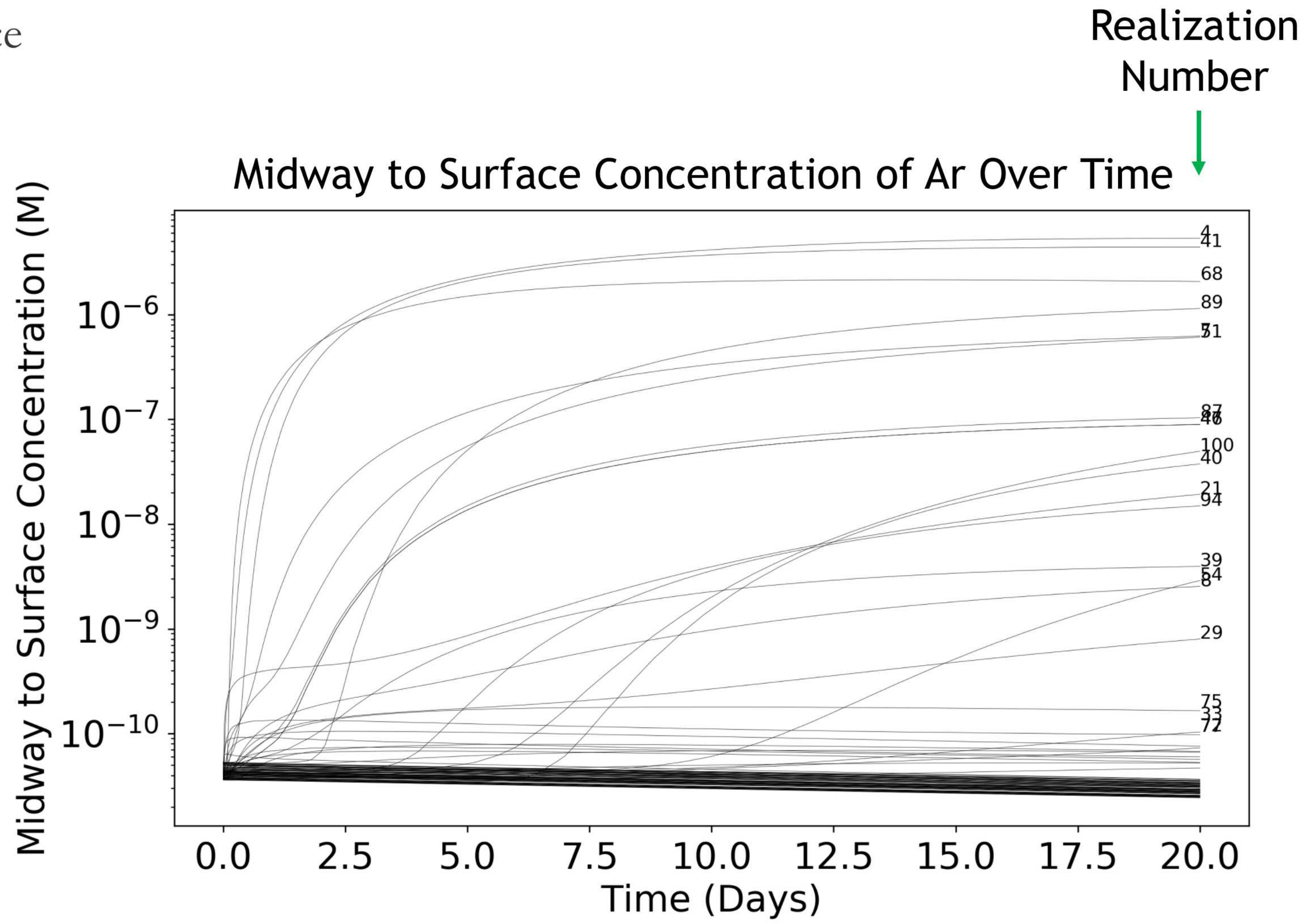


Reactive Transport Modeling – Breakthrough Timing Results

Looking at the concentration histories at the midway point between the source and surface indicate that:

- Some transport to the surface is continuing
- Insufficient time has passed to breakthrough to the surface

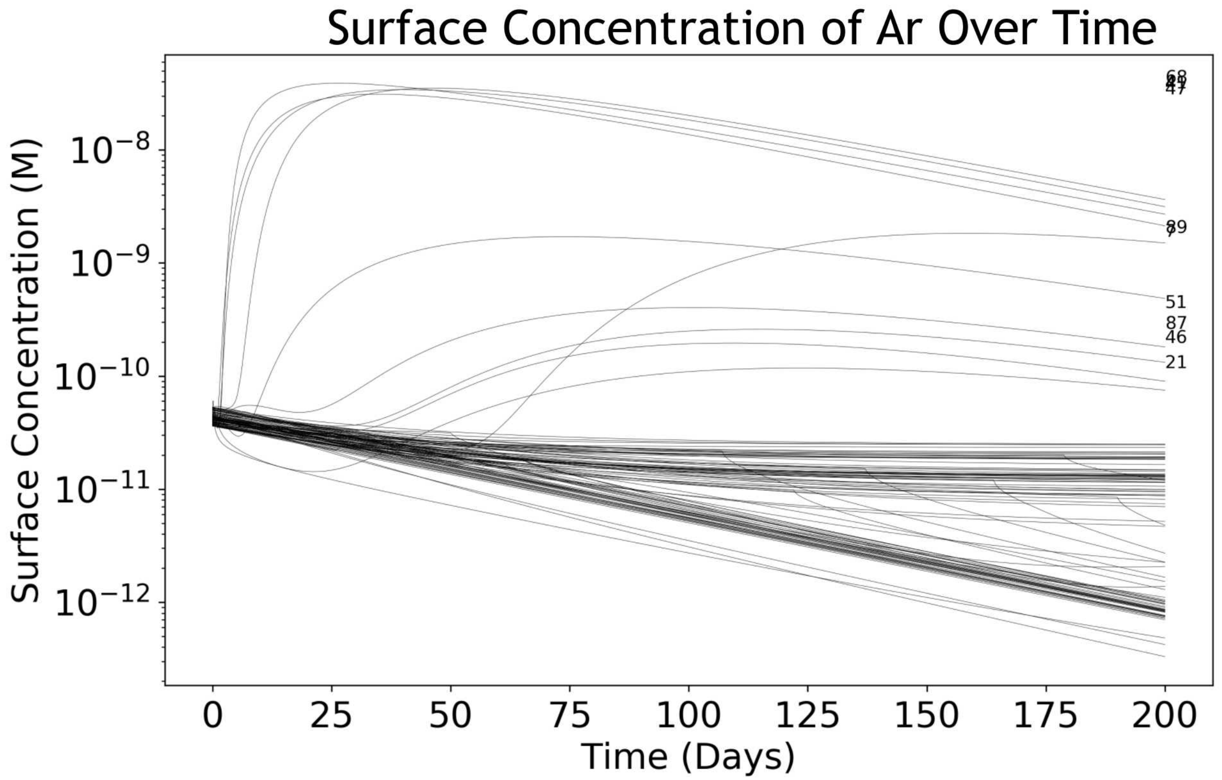


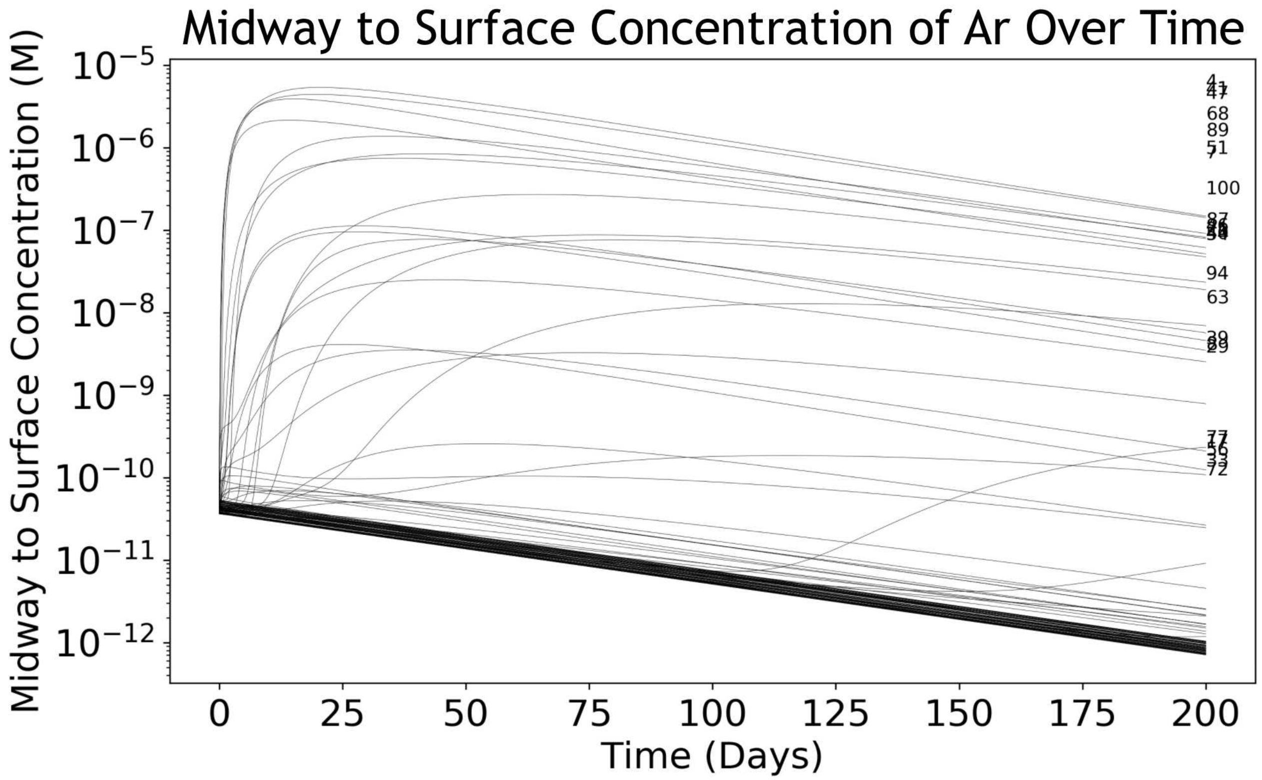


Reactive Transport Modeling – Breakthrough Timing Results

Extending simulations out to 200 days indicates:

- Some realizations (i.e., combinations of sampled parameters) show later breakthrough than 20 days
- Setting an appropriate minimum concentration to define "breakthrough" will be important for the follow-on parameter sensitivity study





Reactive Transport Modeling – Sensitivity to Input Parameters

With the preliminary breakthrough timing results in hand, a sensitivity study is now feasible

However, for a meaningful sensitivity study, attention will be paid to:

- The appropriate concentration/breakthrough definition (based on detection sensitivity)
- Appropriate statistics (i.e., a sufficient number of breakthroughs) in order to derive clearer correlations between sampled parameter values and observed breakthrough times
  - This may include redefining parameter distribution limits; e.g., higher initial pressures

Continued work will also consider the impacts on breakthrough times due to:

- Barometric pumping—variable pressure at surface has been shown to shorten transport time
- Properties of a more complex fracture network
- Incorporation of molecular dynamics-derived adsorption isotherms

Conclusions

As part of a project that considers experimental and modeling approaches to subsurface gas transport, reactive transport modeling calculations have been investigated

A framework has been set up to run many variations on input parameters using parameter sampling

- Ultimately, this will aid in a parameter sensitivity study that will all focus on the most influential parameters
- Preliminary results point to the importance of defining a breakthrough concentration, as well as evaluating parameter sensitivity with a limited number of observed breakthroughs

Future work will consider added complexity in the transport model

Questions?

Acknowledgements:

Guangping Xu, SNL experimentalist and team member

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