Advancing In Situ Mining Simulations: A JupyterLab Framework for Reactive Transport Modeling and Environmental Impact Analysis

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Enhancing In Situ Mining with Reactive Transport

Estimates **total metal recovery**

Optimizes well field operations and lixiviant formulation

Assesses feasibility of **site restoration** alternatives
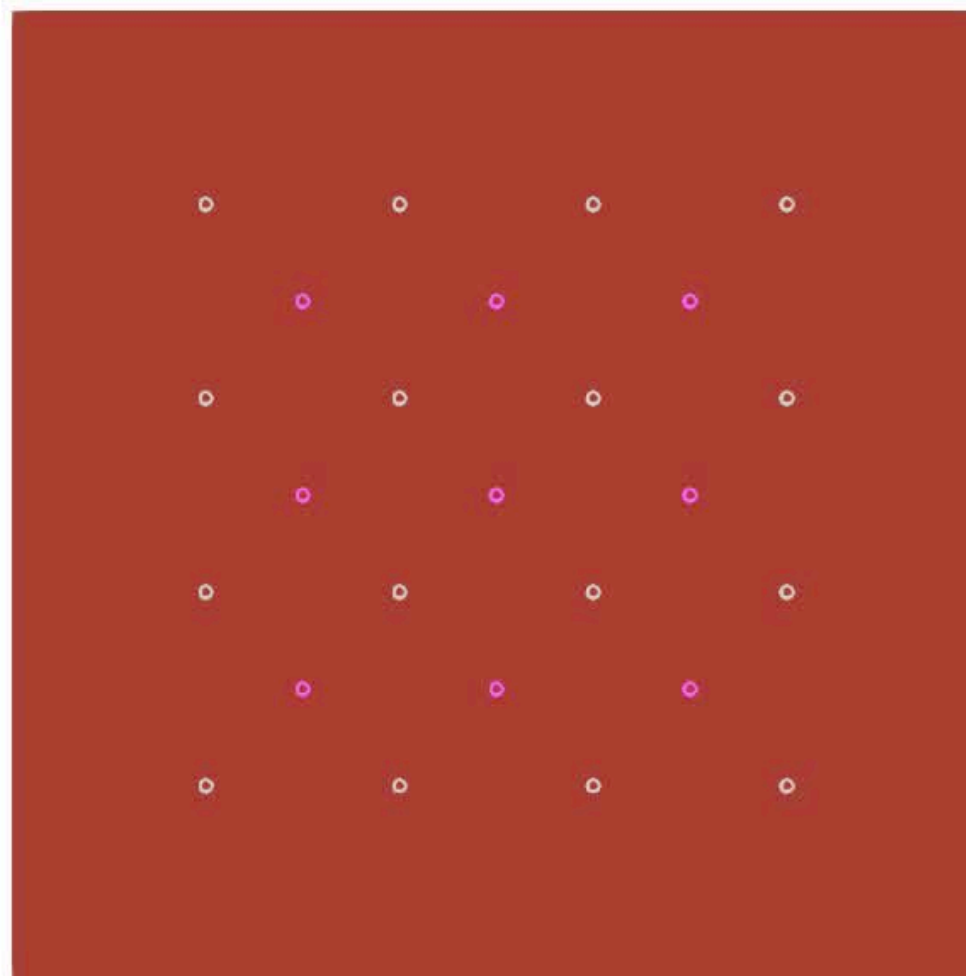
Builds **scientific intuition** on reacting flow dynamics

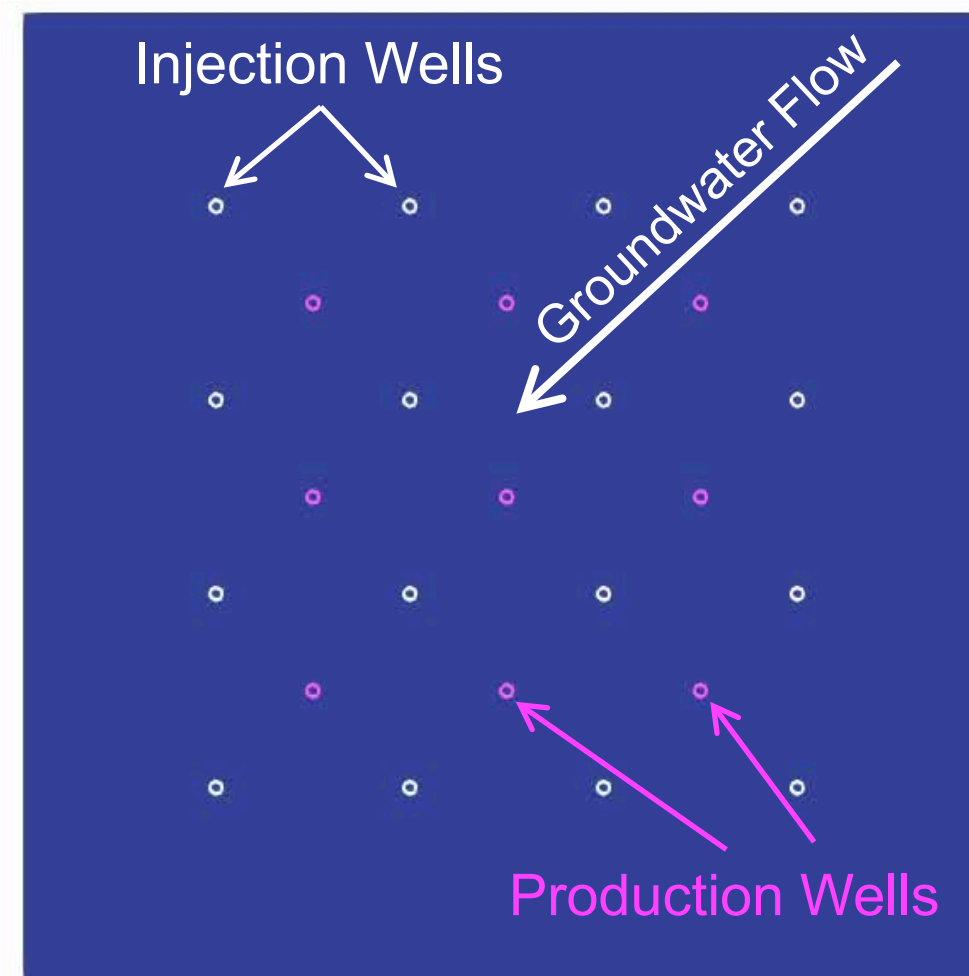# Reactive Transport Enables Cost-Effective Analysis of Well Configurations

Time: 0.000 y

Chrysocolla Mineral

Mineral Volume Fraction (m^3 mineral/m^3 bulk)
2.2e-03 0.003 0.004 5.2e-03

Sulfuric Acid Lixiviant

Injection Wells

Groundwater Flow

Production Wells

Lixiviant Concentration (mole/Liter)
5.0e-04 0.1 0.2 2.6e-01

Hammond et al., 2025

Reactive Transport Enables Cost-Effective Analysis of Well Configurations

Time: 3.000 y

Excursions result in loss of profit
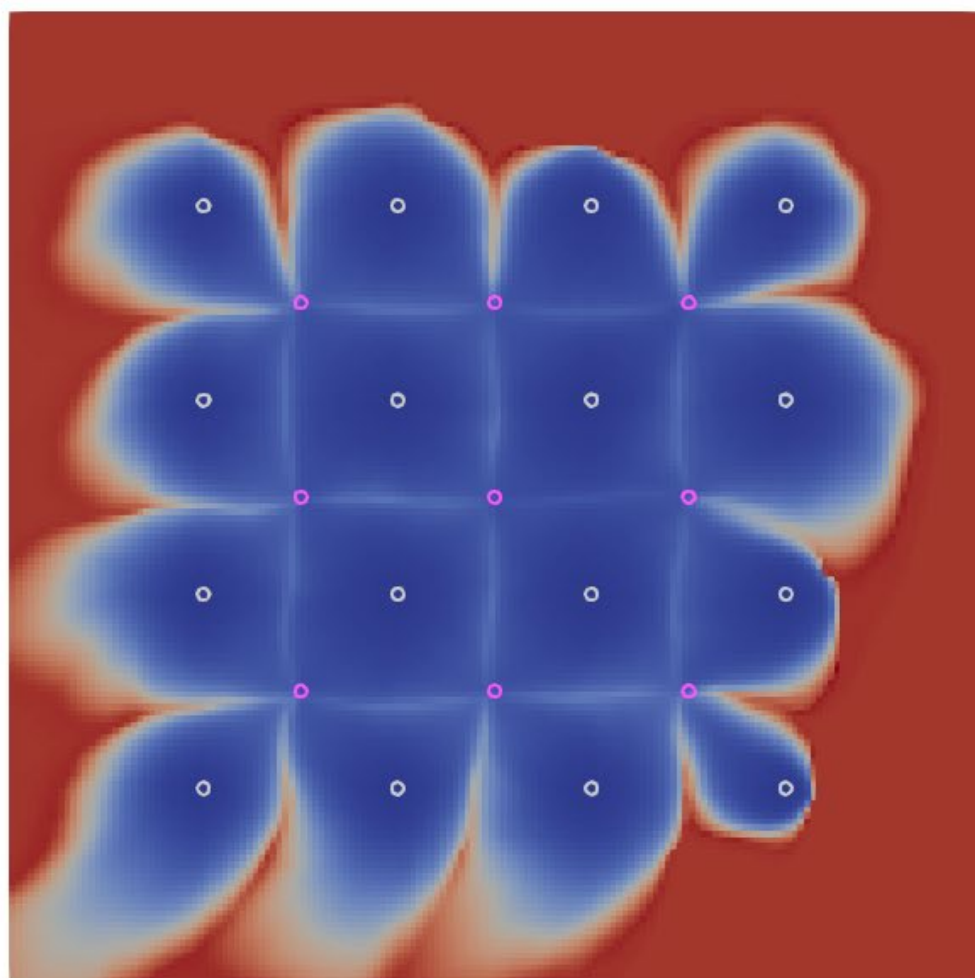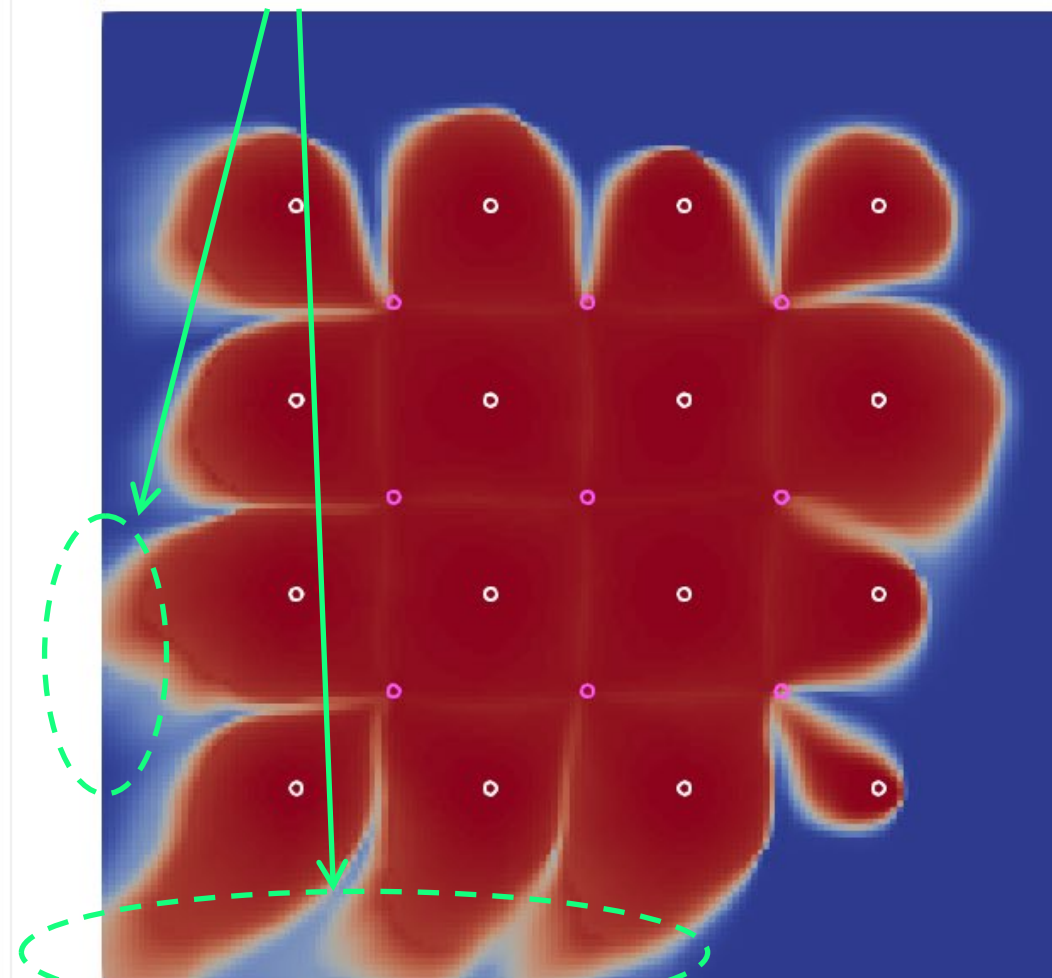
2.2e-03 0.003   0.004   5.2e-03
Mineral Volume Fraction (m^3 mineral/m^3 bulk)

5.0e-04   0.1   0.2   2.6e-01
Lixiviant Concentration (mole/Liter)

Hammond et al., 2025

Reactive Transport Enables Cost-Effective Analysis of Well Configurations

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Time: 0.000 y

Reactive Transport Guides Lixiviant Redistribution to Reduce Excursions
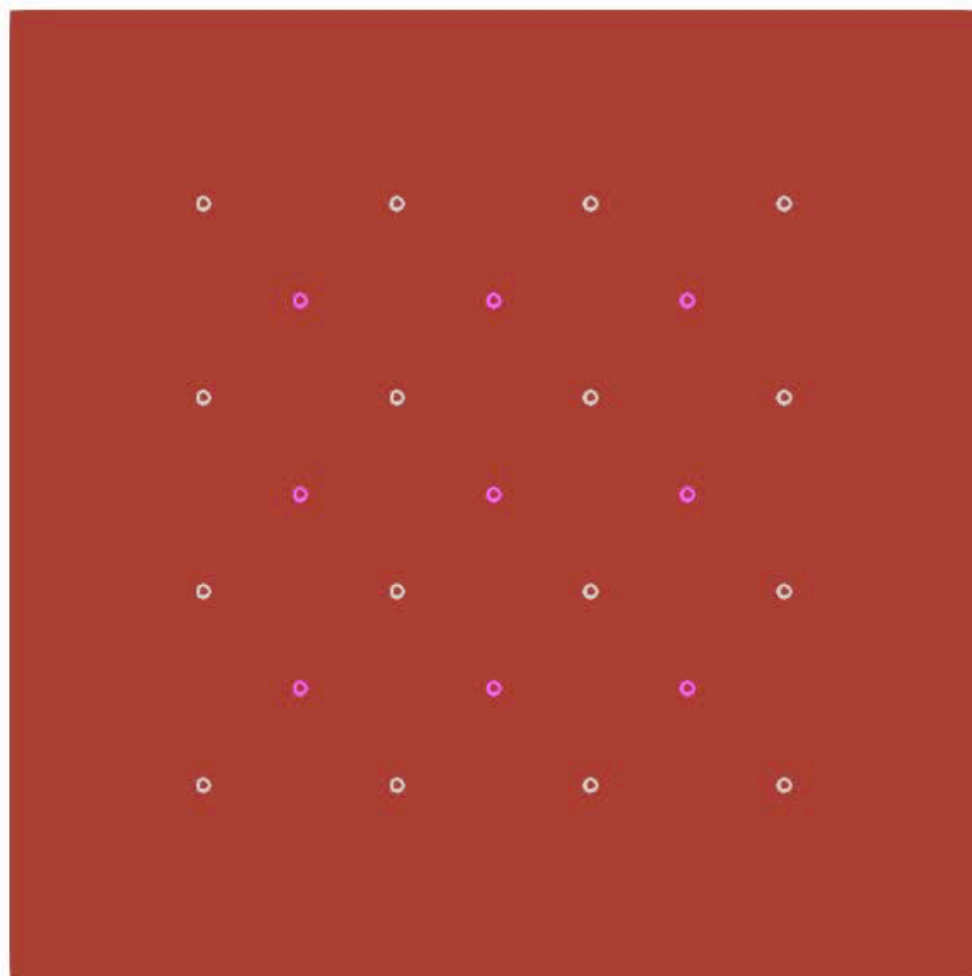
2.2e-03 0.003 0.004 5.3e-03
Mineral Volume Fraction (m^3 mineral/m^3 bulk)

5.0e-04 0.1 0.2 2.6e-01
Lixiviant Concentration (mole/Liter)

Hammond et al., 2025
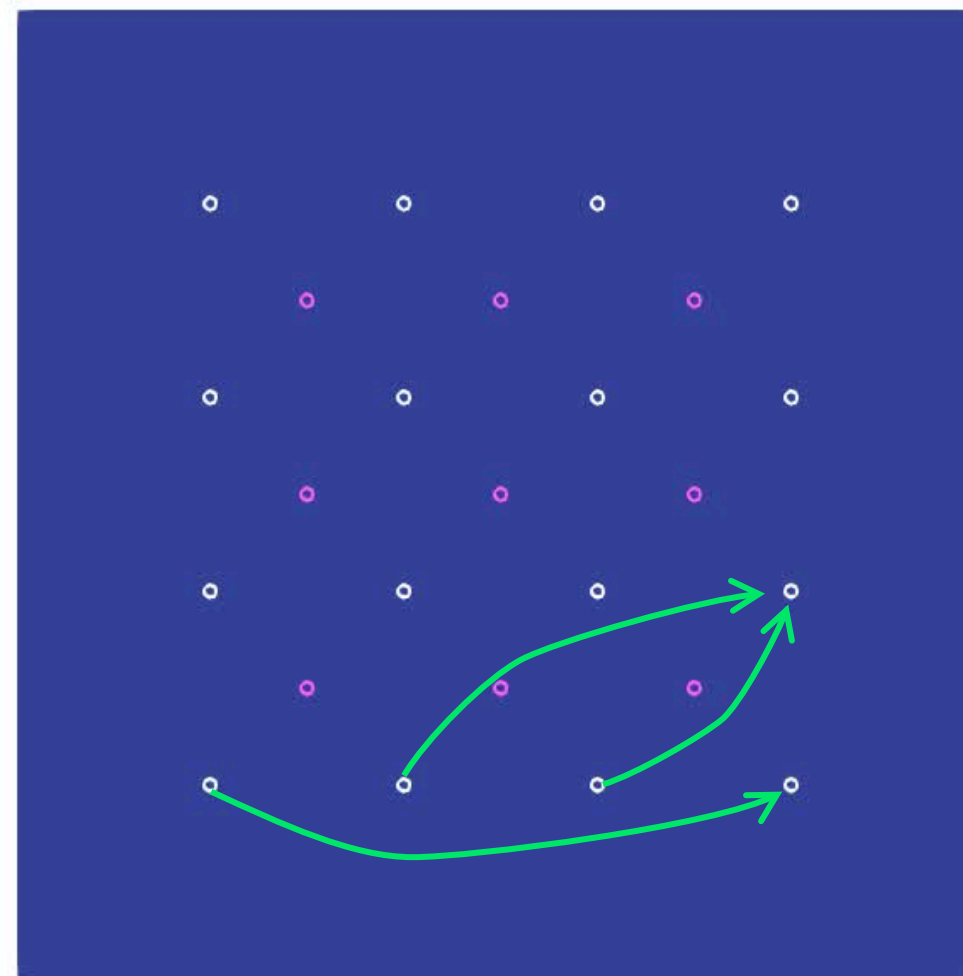
Insights from Collaboration in ISR Operations

- Well Spacing: ISR operations typically follow predefined well spacing.

- Critical Data Collection: Hydrology and mineralogy should be prioritized.

- Reactive Transport Modeling Challenges:
  - Requires a realistic geologic model
    - ✓ Layered horizons with potential vertical flares complicate geological analysis.
    - ✓ Incorporation and spatial interpolation of extensive exploration borehole data (e.g., permeability, porosity, faults).
  - Difficult to infer intermediate initial conditions after prolonged well field operation.
  - Pressure-based injection rates (e.g., adjusting butterfly valves) require a single well model that accounts for all wells simultaneously.
  - Limited resolution and frequency of produced fluid measurements.

Settings | Timing | Domain | Discretization | Material Properties | Regional Flow | Output Settings | **Wells**

Well Layout

Read Well Field | Clear Wells | ☐ Print Unmatched Wells

○ Gridded
○ Custom Coordinates
● Well Field

Well Field Layout

○ Mining Unit, Header House and Horizon
● List of Pumping Wells

Pumping Well Filename: ./data/HH2-3_Flow_Data_All_Wells_geh.csv

	Header House	Horizon	Stratigraphic Unit
Start Date 08/31/2017	☐ HH2-2	☐ UHJ	☑ 120-130
End Date 10/30/2020	☑ HH2-3	☐ MHJ1	☐ 140-150
Final Simulation Time 1157 d	☐ HH2-4	☐ MHJ2	☐ 160-170
		☐ LHJ	

☑ 2M1187 ☐ Override Rate 6846.327869
☑ 2M1188 ☐ Override Rate 3282.346086
☑ 2M1189 ☐ Override Rate 3935.375420
☑ 2M1190 ☐ Override Rate 4881.714835
☐ 2M1191 ☐ Override Rate -13700.4933:
☑ 2M1192 ☑ Override Rate 2000
☑ 2M1193 ☐ Override Rate 6656.089401
☑ 2M1194 ☑ Override Rate -7000
☑ 2M1195 ☐ Override Rate 1506.941320
☑ 2M1196 ☐ Override Rate 8998.418977
☑ 2M1197 ☐ Override Rate -6723.42982:
☑ 2M1210 ☐ Override Rate 9783.859227
☑ 2M1212 ☐ Override Rate -4575.69928:
☑ 2M1213 ☐ Override Rate 8764.049059
☑ 2M1214 ☐ Override Rate 8755.219696
☑ 2M1215 ☐ Override Rate -6560.66728:
☑ 2M1216 ☐ Override Rate 10631.52392
☑ 2M1217 ☐ Override Rate -11193.1277:
☑ 2M1225 ☐ Override Rate 7584.120877
☑ 2M1226 ☐ Override Rate 3390.306506
☑ 2M1227 ☐ Override Rate -10036.1030:
☑ 2M1228 ☐ Override Rate 11711.76614

Well Field

Legend:
- ● Injection Wells
- ● Production Wells
- ○ Override Injection Wells
- ○ Override Production Wells
- ● Inactive Wells

Y [ft]

595600
595400
595200
595000
594800
594600

2M1295
2M1187 2M1188 2M1192 2M1195
2M1191 2M1197
2M1194
2M1189 2M1190 2M1193 2M1196
2M1217 2M1215 2M1212
2M1216 2M1214 2M1213 2M1210
2M1227 2M1309
2M1225 2M1226 2M1308 2M1310
2M1228 2M1229A
2M1313 2M1312
2M1253
2M1314

X [ft]
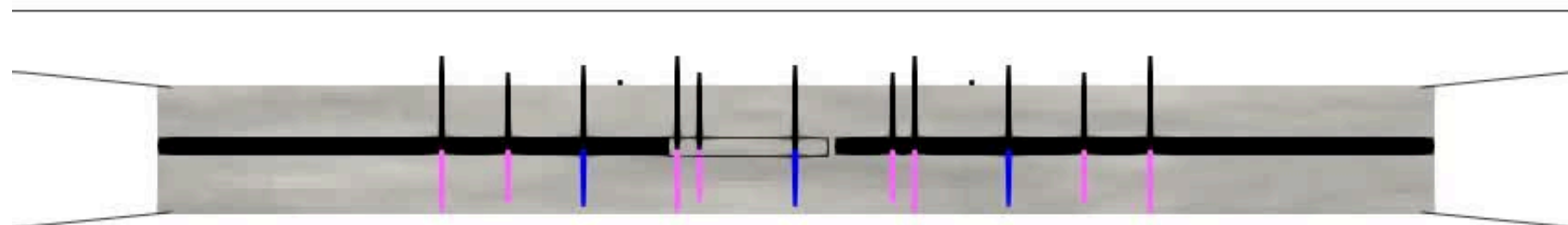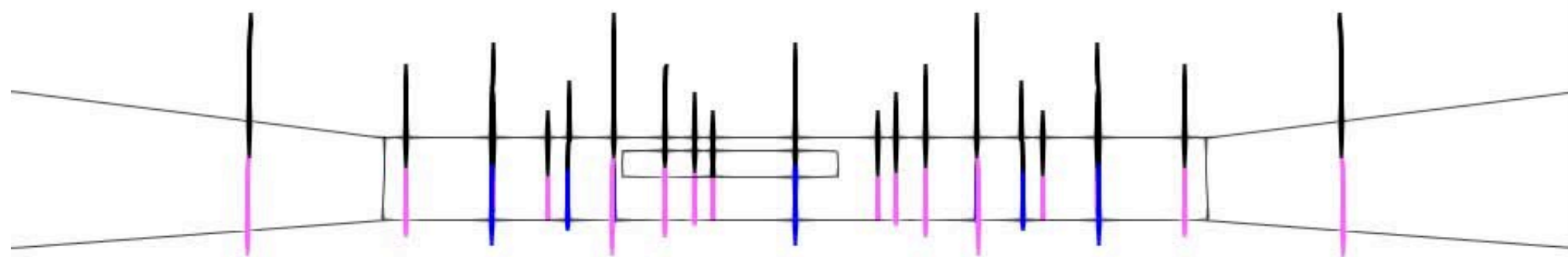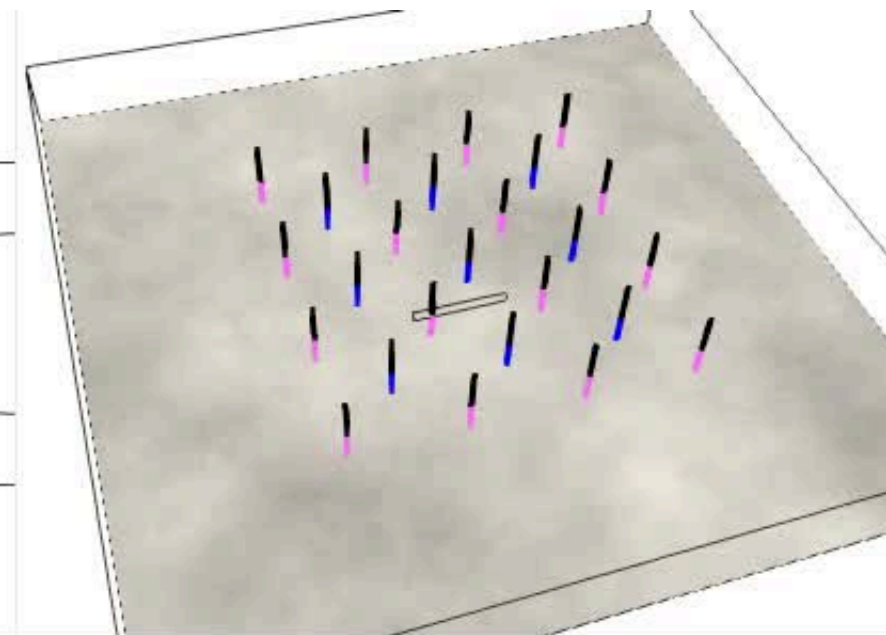2.2080 2.2082 2.2084 2.2086 2.2088 2.2090 2.2092
1e6

Live Demo

Reactive Transport Enables 3D Visualization of Leakage within Well Field Operations

Time: 0.00 d

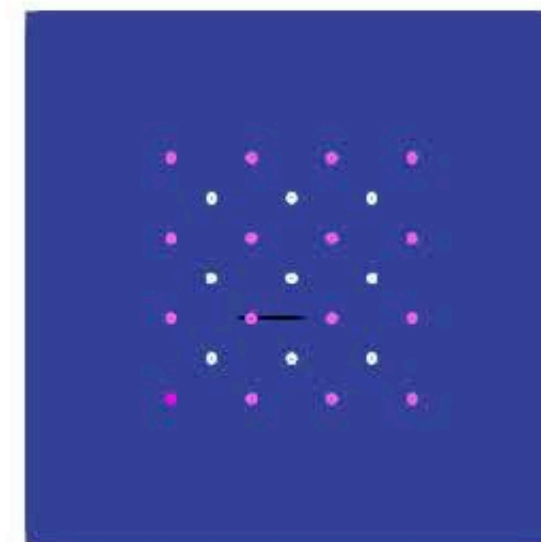1.0e-17 1.0e-11
Intrinsic Permeability (m^2)

1.0e-10 0.0005 1.0e-03
Tracer Concentration

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Thank you