The Development of an NETL DAC Reactor: Optimization of Direct Air Capture (DAC) Reactor Configuration Using Artificial Intelligence (AI) Inverse Engineering Techniques

Justin Weber, Jarret Riley, Steven Rowan, Ronald Breault
US Department of Energy, National Energy Technology Laboratory, Pittsburgh PA /Morgantown WV

Research & Innovation Center

NATIONAL ENERGY TECHNOLOGY LABORATORY

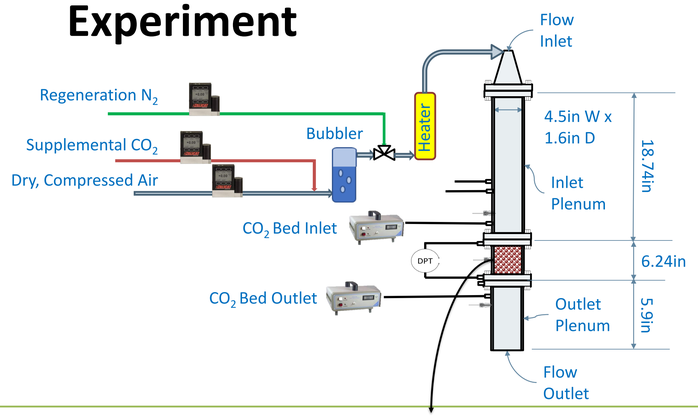
Goal

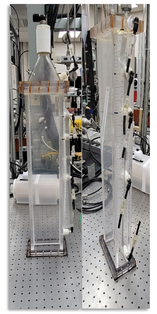
Use generative design techniques to optimize direct air capture (DAC) material packing configurations. Fan power requirements are a significant operation cost, can we use innovative structures to reduce pressure drop while maintaining capture rates?

Objective

$$\max \frac{\frac{CO_{2,in} - CO_{2,out}}{CO_{2,in}} * 100}{\Delta P}$$

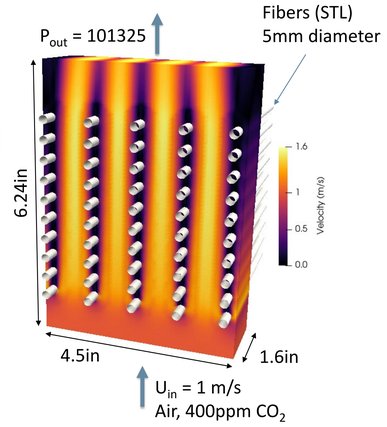
Experiment





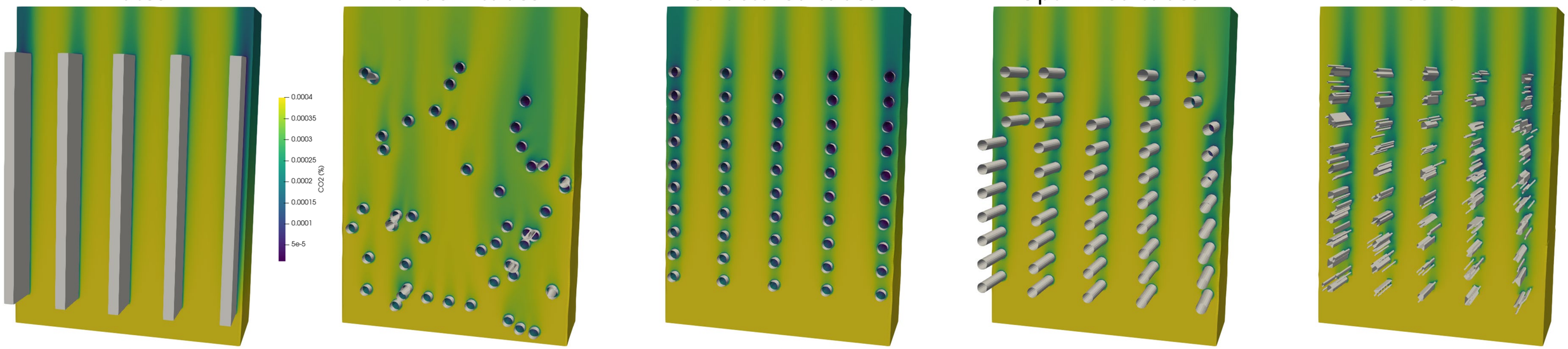
CFD model

Solver: simpleFoam (steady state)
Mesh: 210k cells
Turbulence: kOmegaSST
Runtime: 4 Cores, meshes in 20s, runs in 3.5 minutes



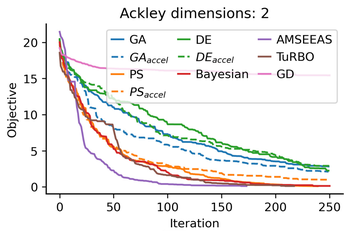
What's the best configuration?

Algorithmic



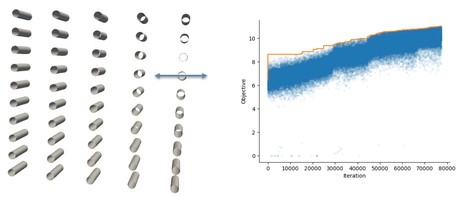
Algorithms

- Genetic algorithm (GA)
- Particle swarm (PS)
- Differential evolution (DE)
- Bayesian optimization
- TuRBO
- AMSEEAS
- Gradient Descent (GD)



GA with lateral spacing

5 x 10 tube array, tubes move in the lateral (x) direction



GA with binary level set

112 x 104 binary array

STL file