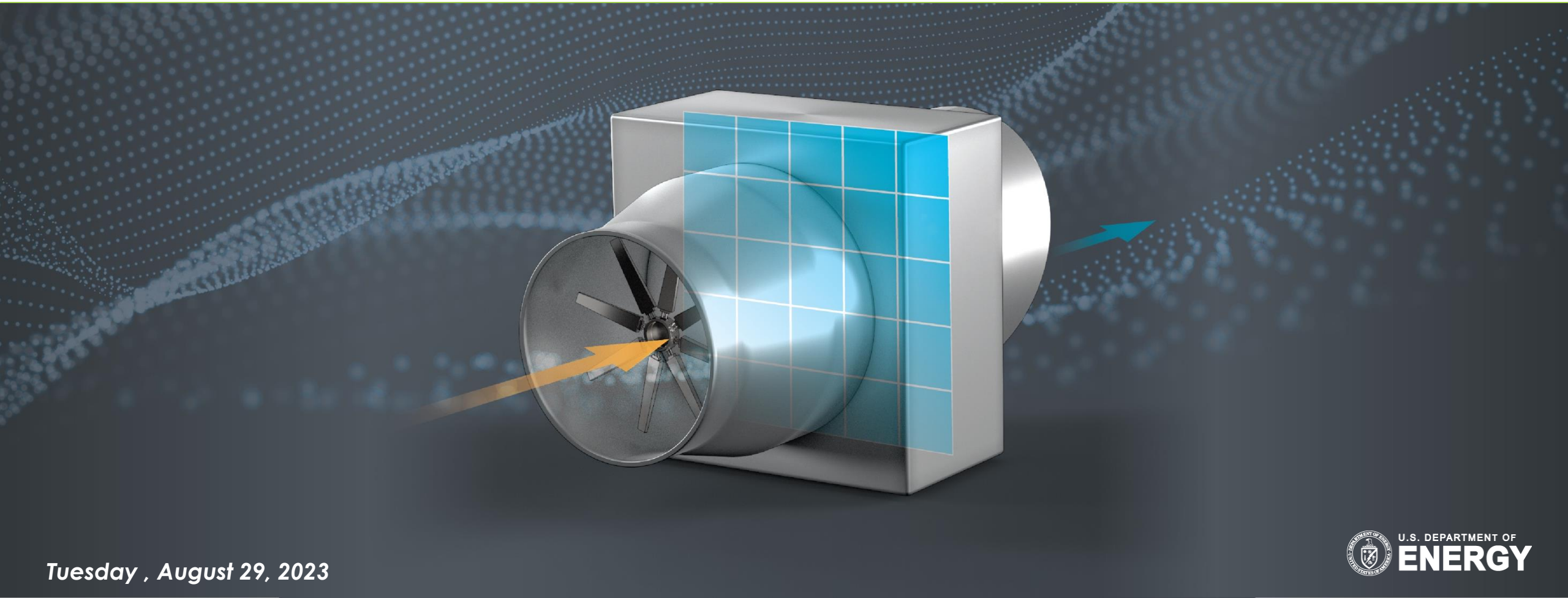
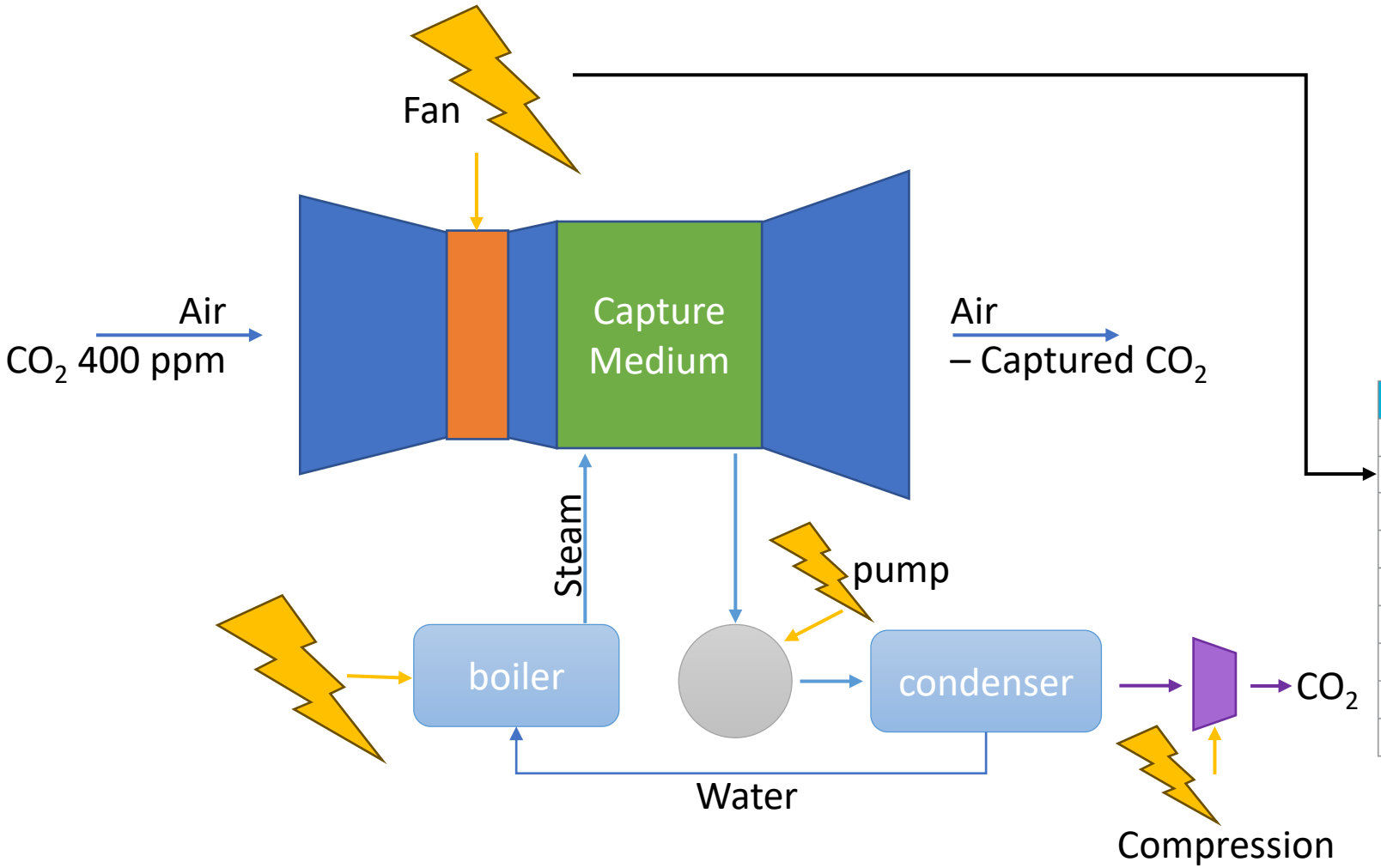
The Development of an NETL DAC Reactor: Optimization of Direct Air Capture (DAC) Reactor Configuration Using Artificial Intelligence (AI) Inverse Engineering Techniques

Justin Weber, Jarrett Riley, Steven Rowan, Ronald Breault



Tuesday , August 29, 2023

Challenge: Reduce the cost of DAC



CASE 0B-EB – ELECTRIC BOILER

Performance Summary	
Total Gross Power, MWe	**0**
DAC Air Fans, kWe	28,800
DAC CO_2 Compression, kWe	1,490
Electric Boiler, kWe	19,510
Balance of Plant, kWe	163
Total Auxiliaries, MWe	**50**
Net Power, MWe	**-50**
DAC CO_2 Removed from Air (Gross), tonnes/yr	100,000
Net CO_2 Removed from Air, tonnes/yr	**100,000**

J. Valentine, A. Zoelle, "Direct Air Capture Case Studies: Sorbent System," National Energy Technology Laboratory, Pittsburgh, PA, July 8, 2022.

Polymers with intrinsic microporosity (PIMs)

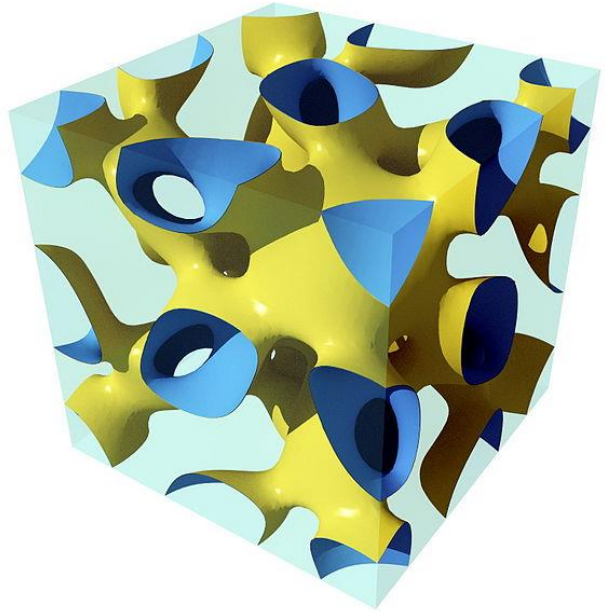
What is the best form factor?

plates

tubes

Mat/felt

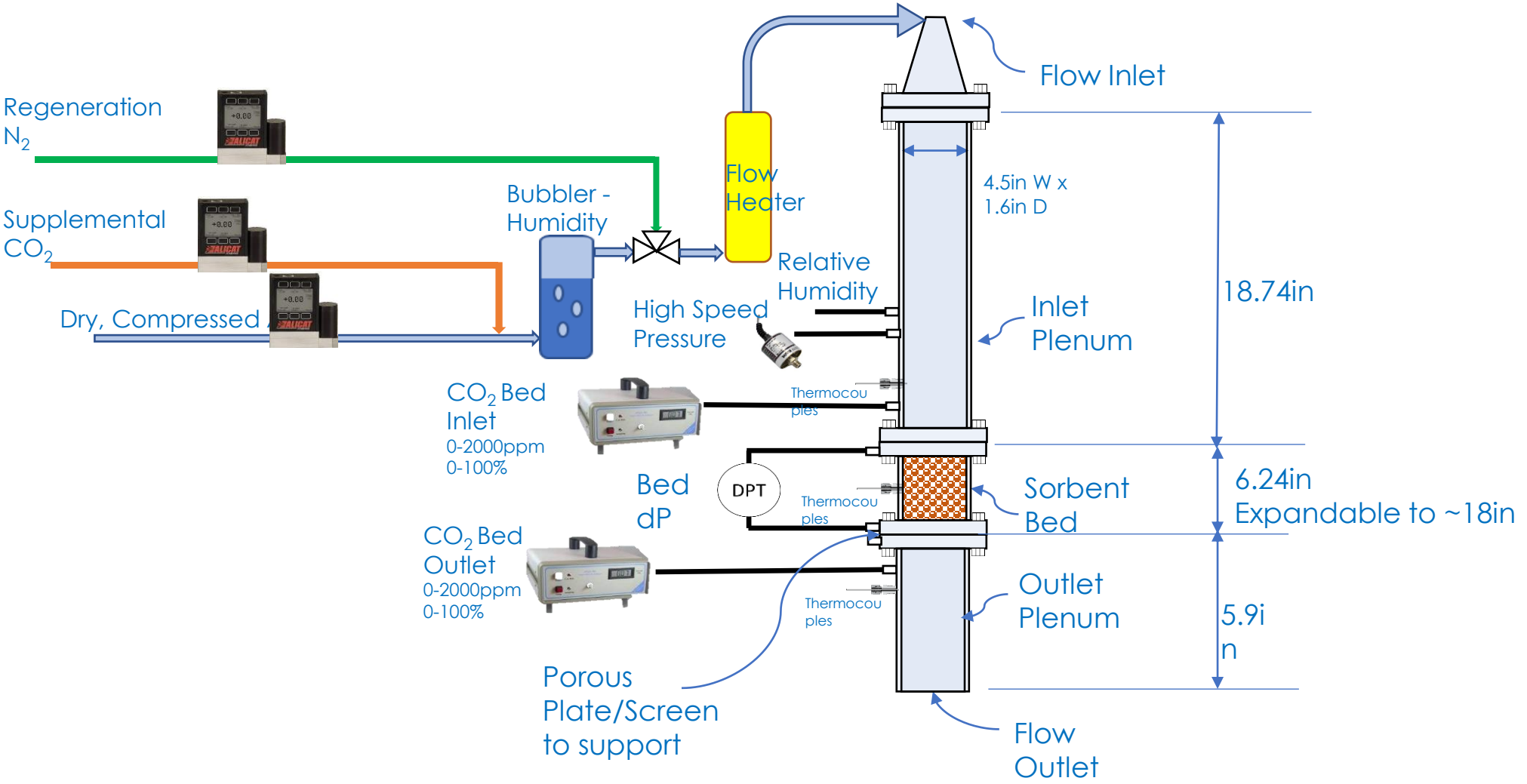
Gyroids



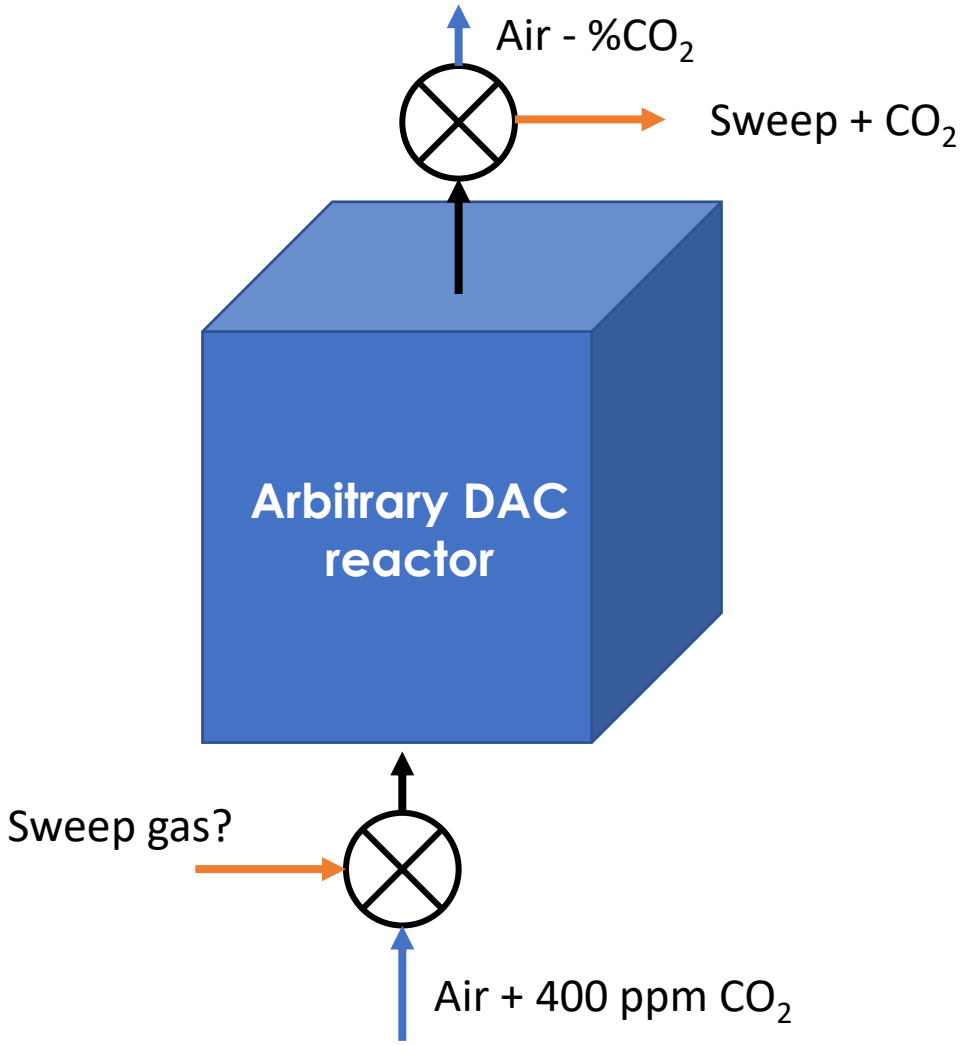
Anders Sandberg, https://commons.wikimedia.org/wiki/File:Lidinoid_surface.jpg

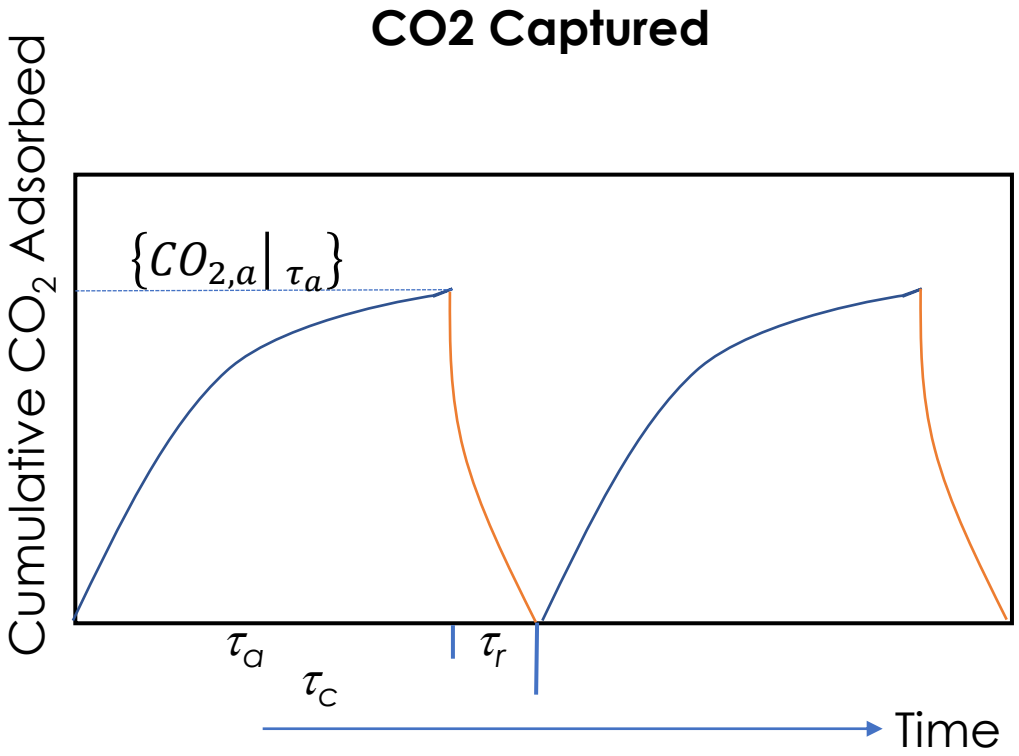
Objective: Maximize: Mass transfer
Minimize: Pressure drop

Lab scale test unit



DAC process





$$CO_{2,D} = \{CO_{2,a}|\ \tau_a\}\, N_{cycles}$$

Generative design (optimization)

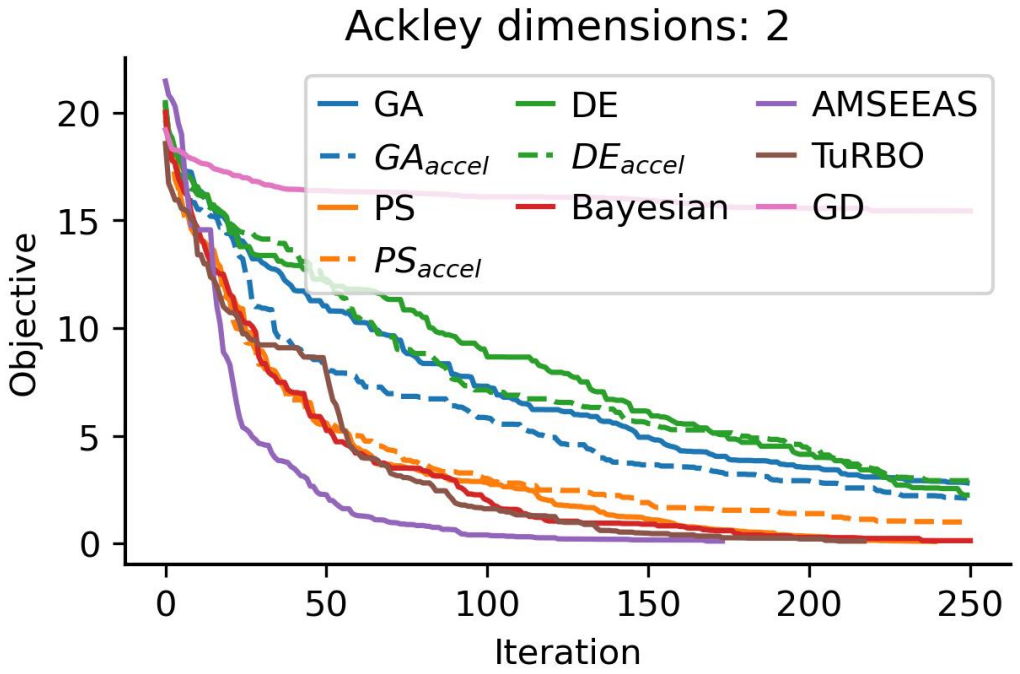
Use AI algorithms with computational models to generate and evaluate multiple design alternatives

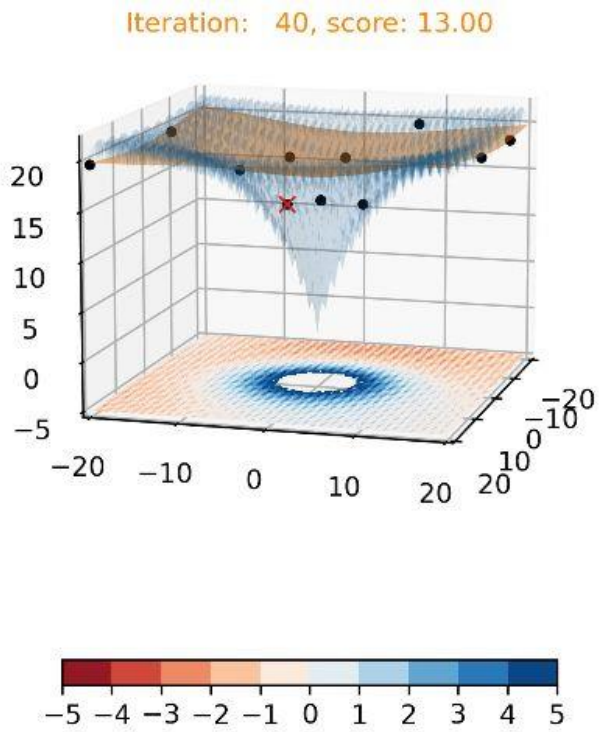
Genetic algorithm (GA)
Particle swarm (PS)
Differential evolution (DE)
Bayesian optimization
TuRBO
AMSEEAS
Gradient Descent (GD)

+

Meta model accelerator

Minimize the number of expensive function calls





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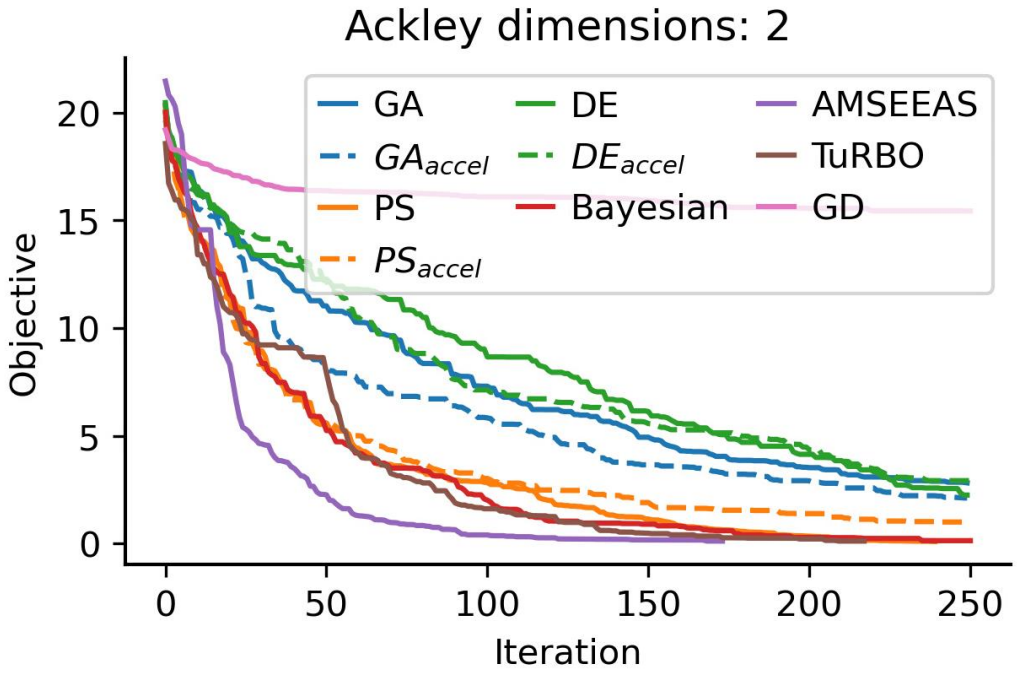
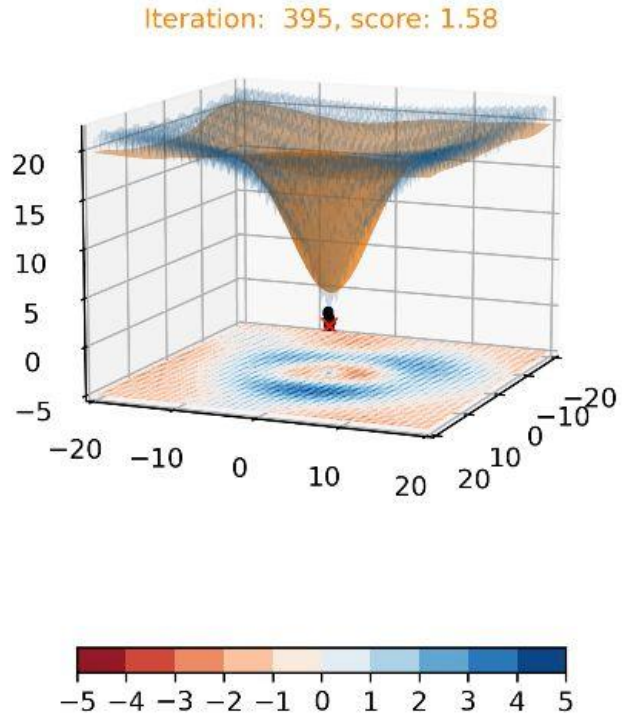
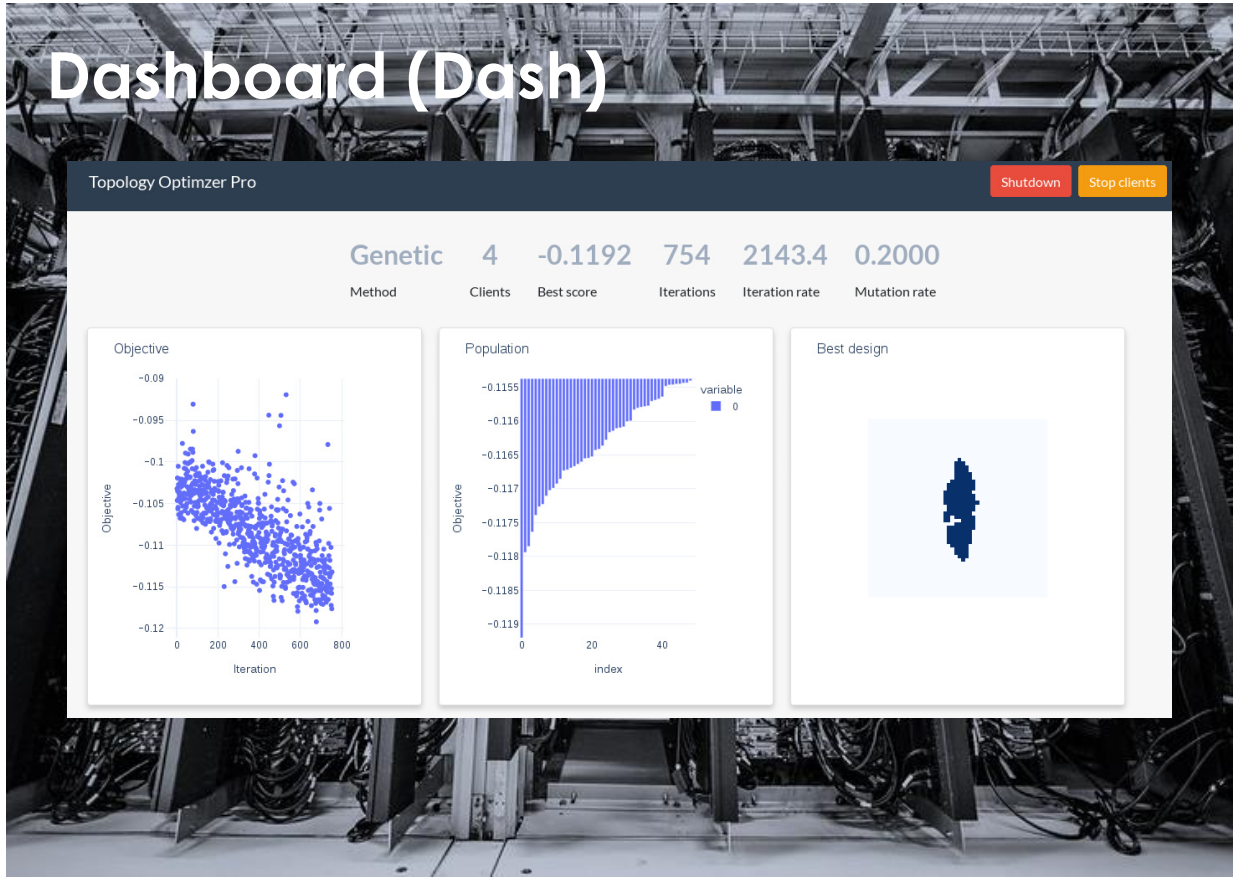
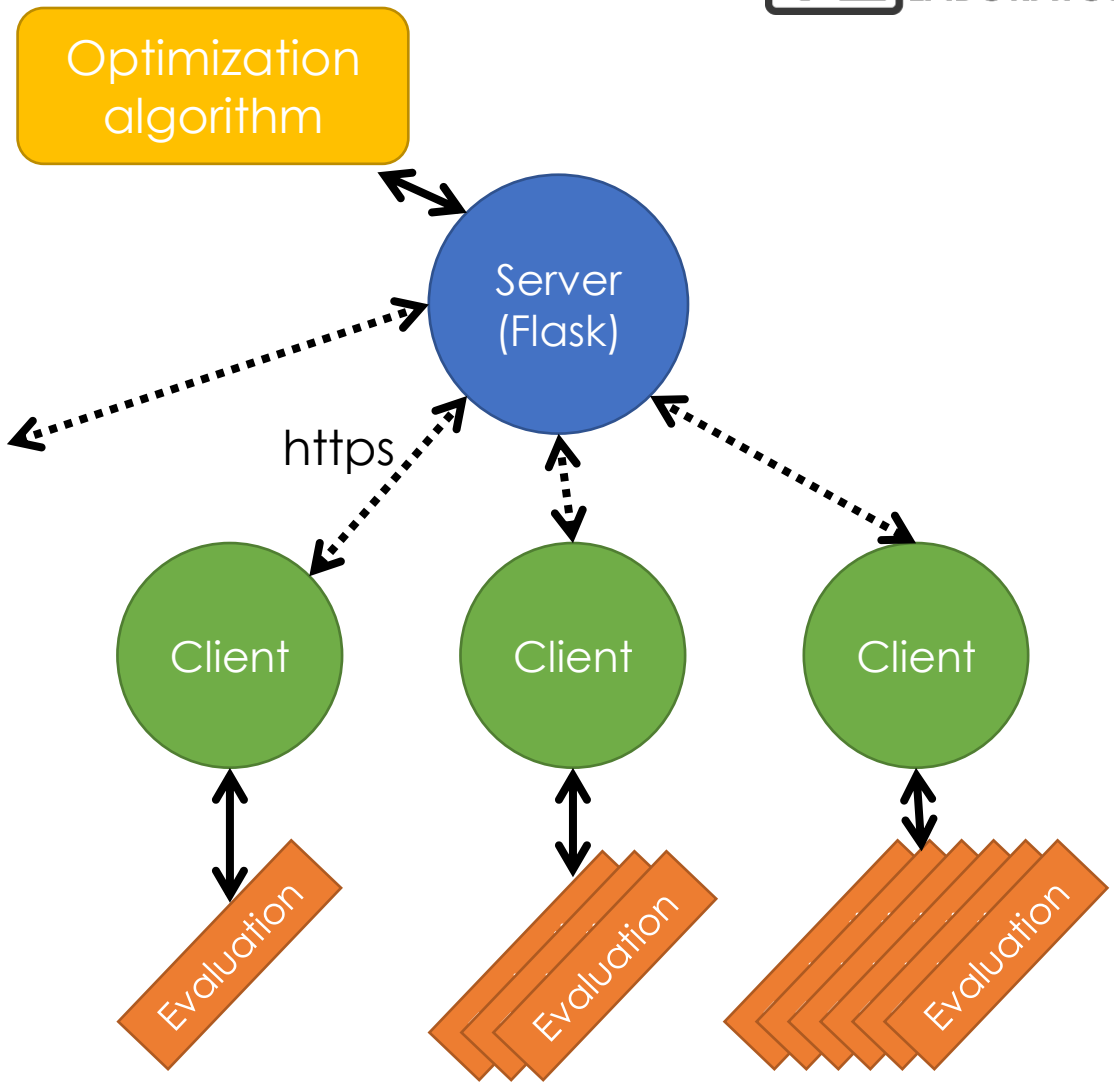




Custom framework for large scale campaigns



- Allows for distributed computing
- Thousands of simultaneous evaluations



Example usage: Aerothermal/heat transfer

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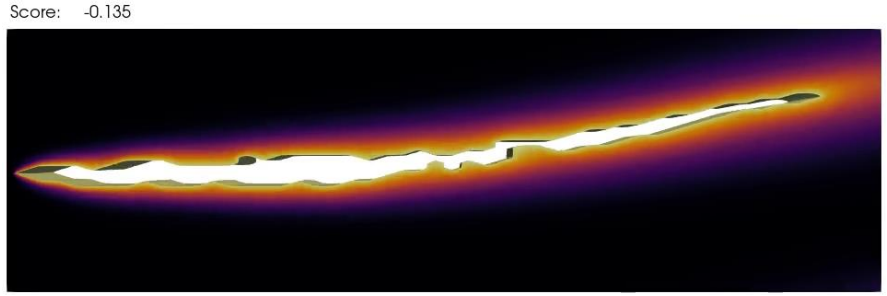
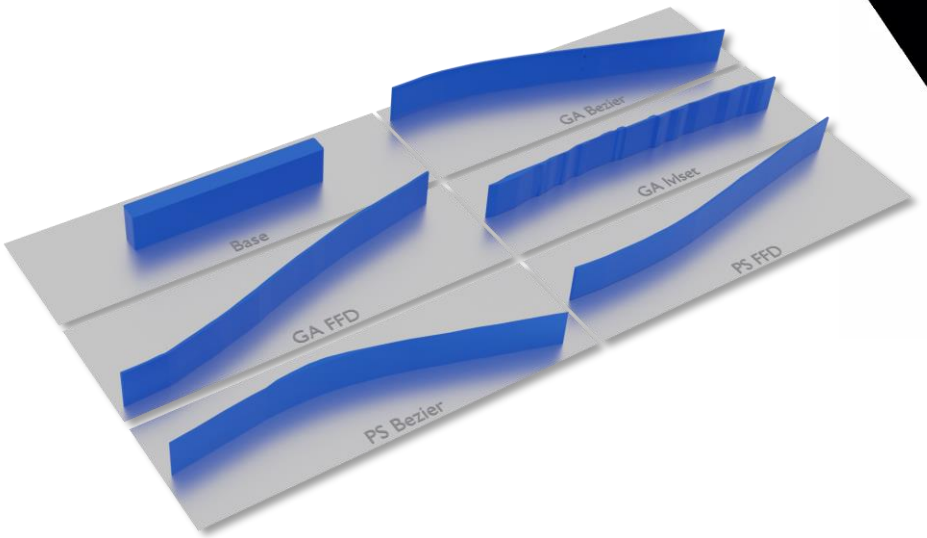
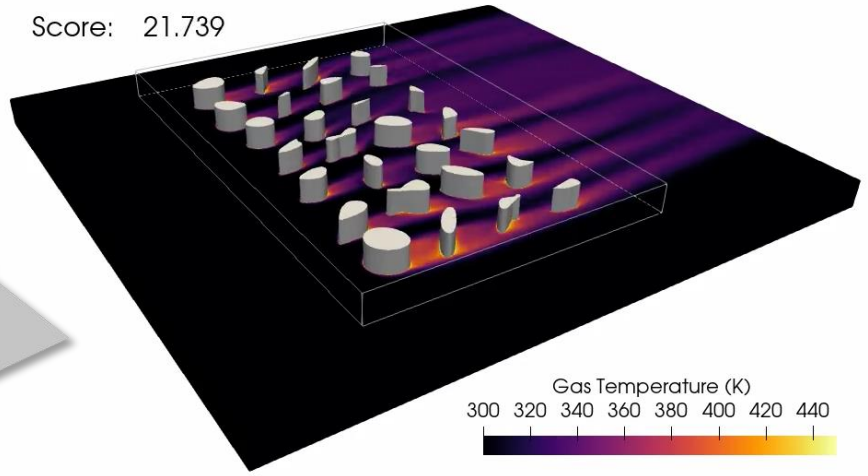
Single pin fin



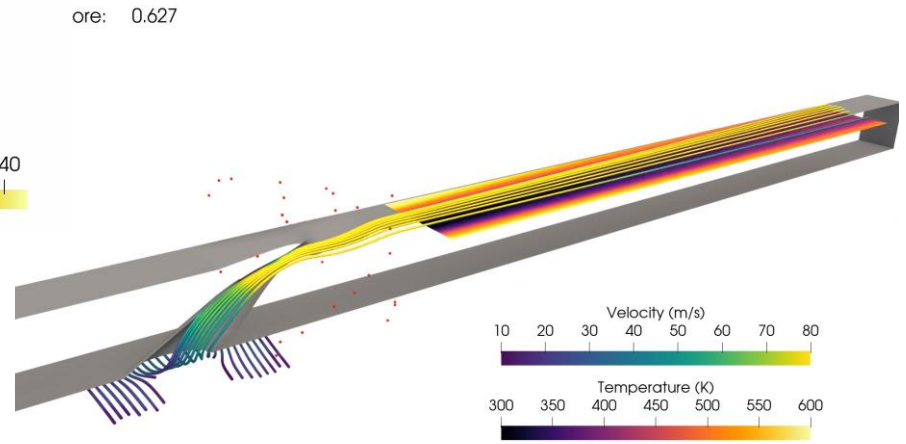


Pin fin array



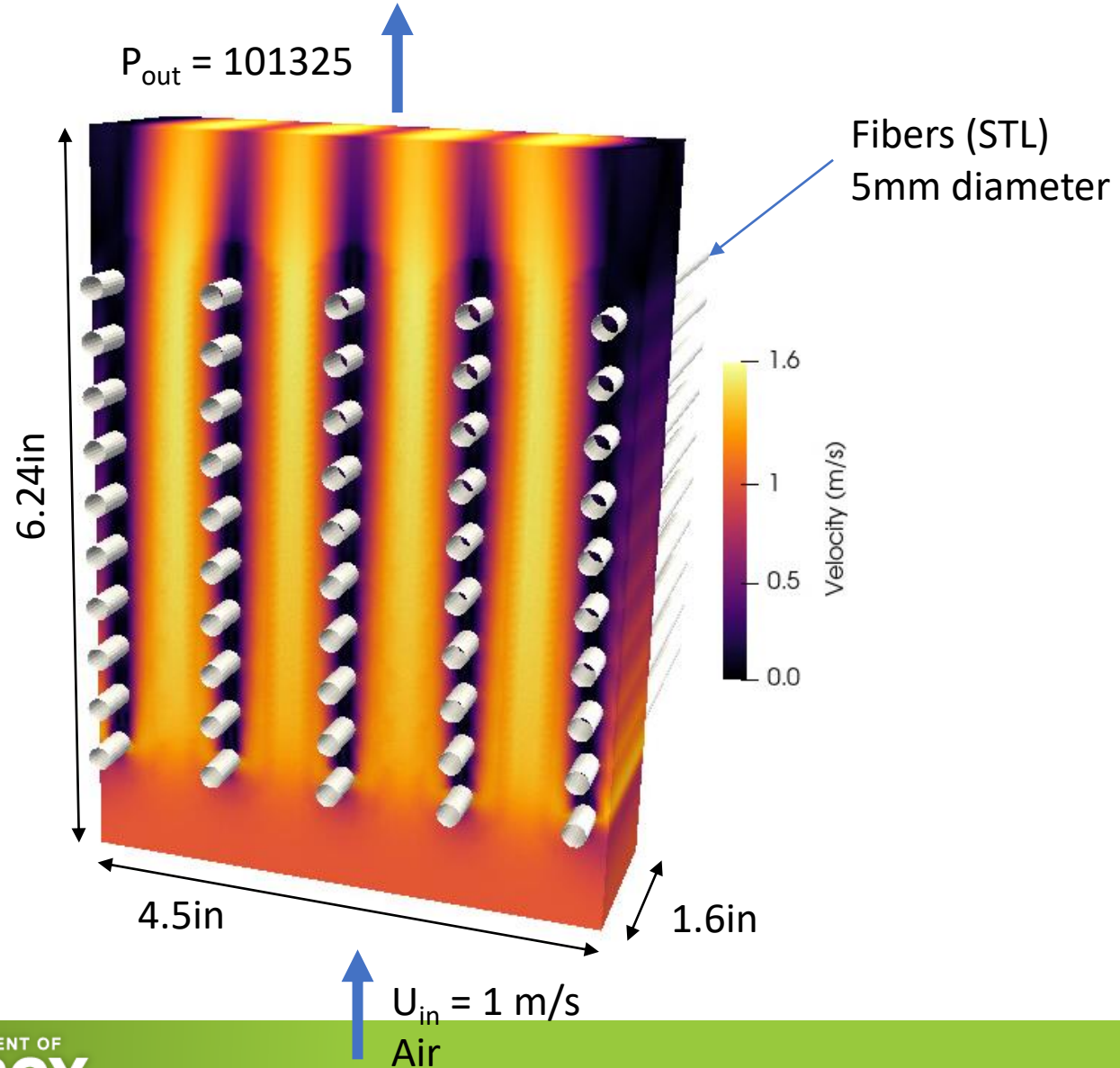
7x4x4x2 = 224 dims

Film cooling



3x3x3x3 = 81 dims

Base OpenFoam model

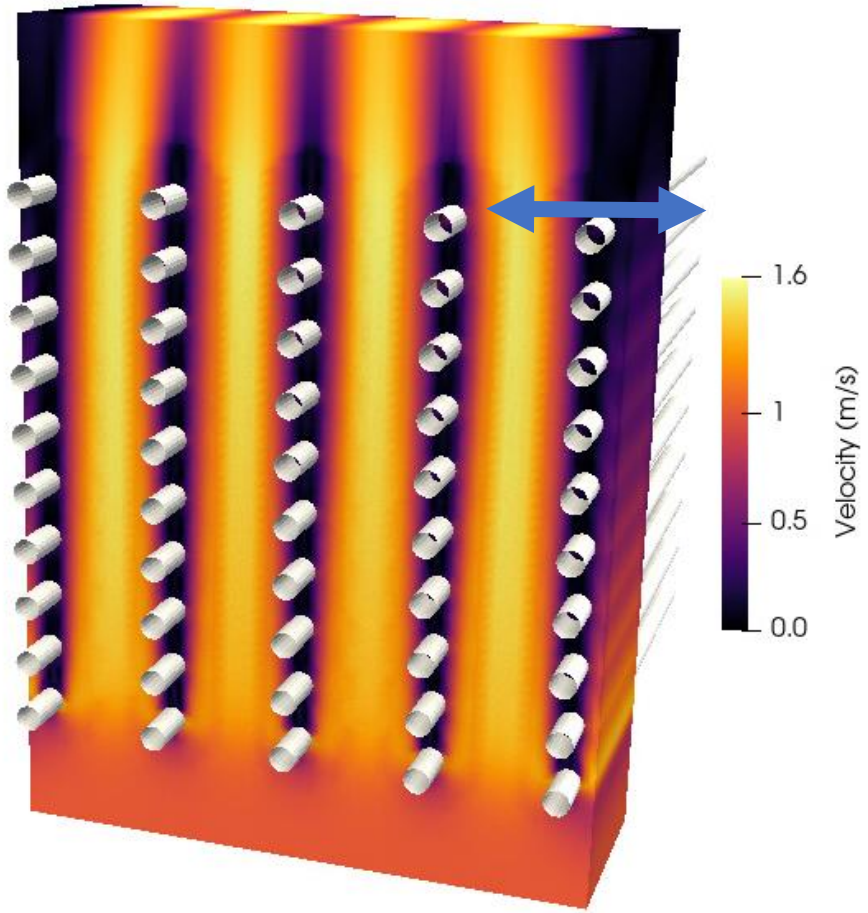


Solver: simpleFoam (steady state)
Mesh: 210k cells
Turbulence: kOmegaSST
Runtime: 4 Cores, meshes in 20s, runs in 3.5 minutes

10 x 5 = 50 dims

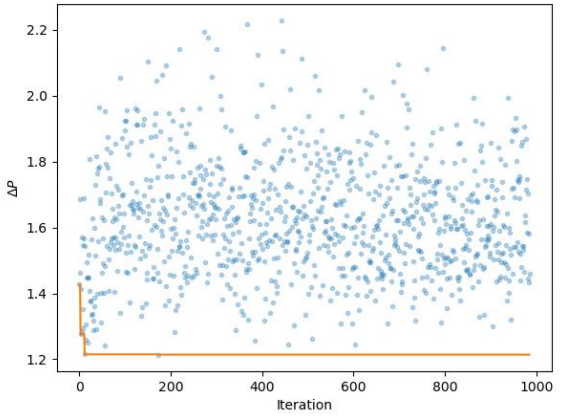
Optimization results: min ΔP

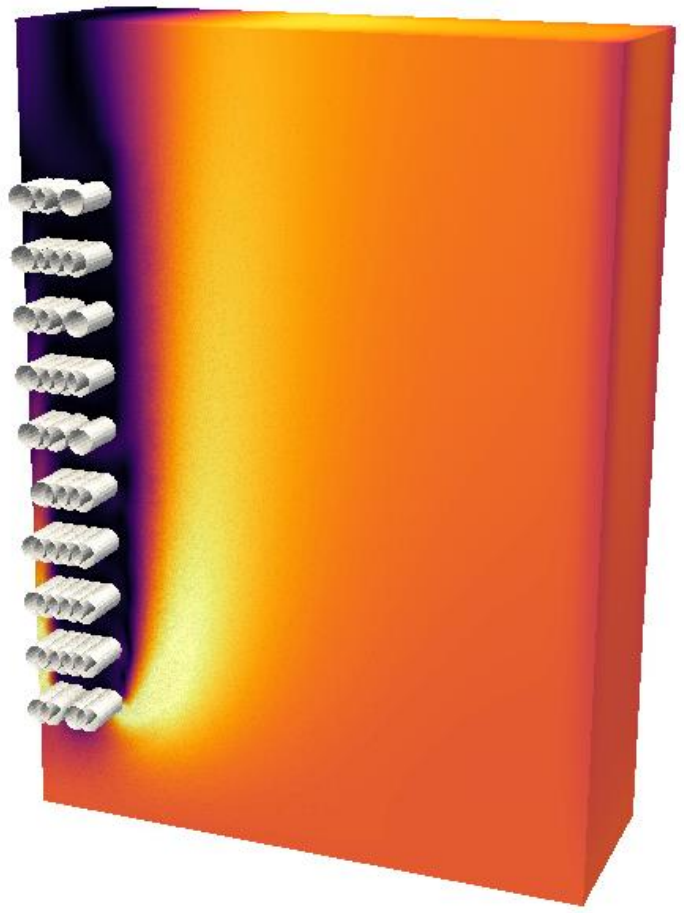
Fixed fiber count, allow the positions to move in the lateral (x) direction



$$\min \Delta P$$

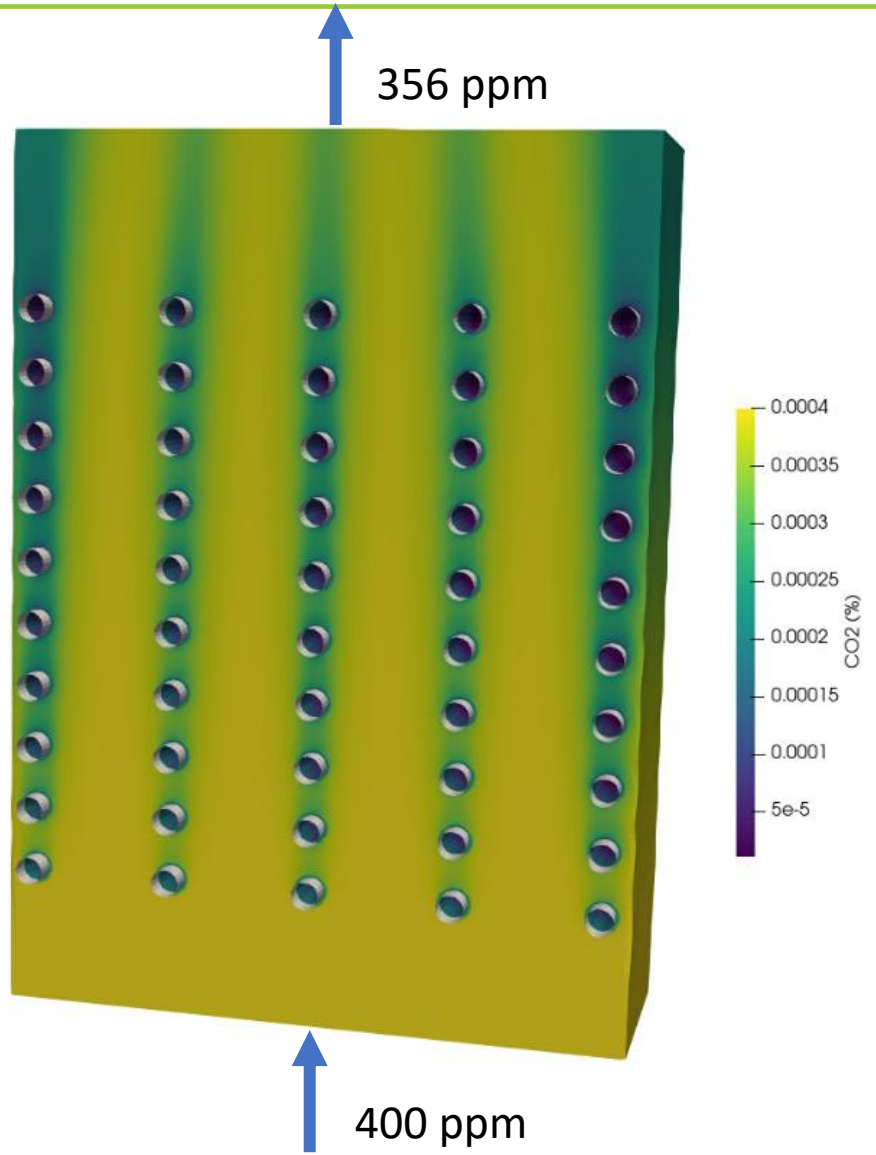
1,000 OpenFoam models





It works! Minimizes pressure drop by condensing all the geometry to one side, not good for surface reactions!

Add Reactions!

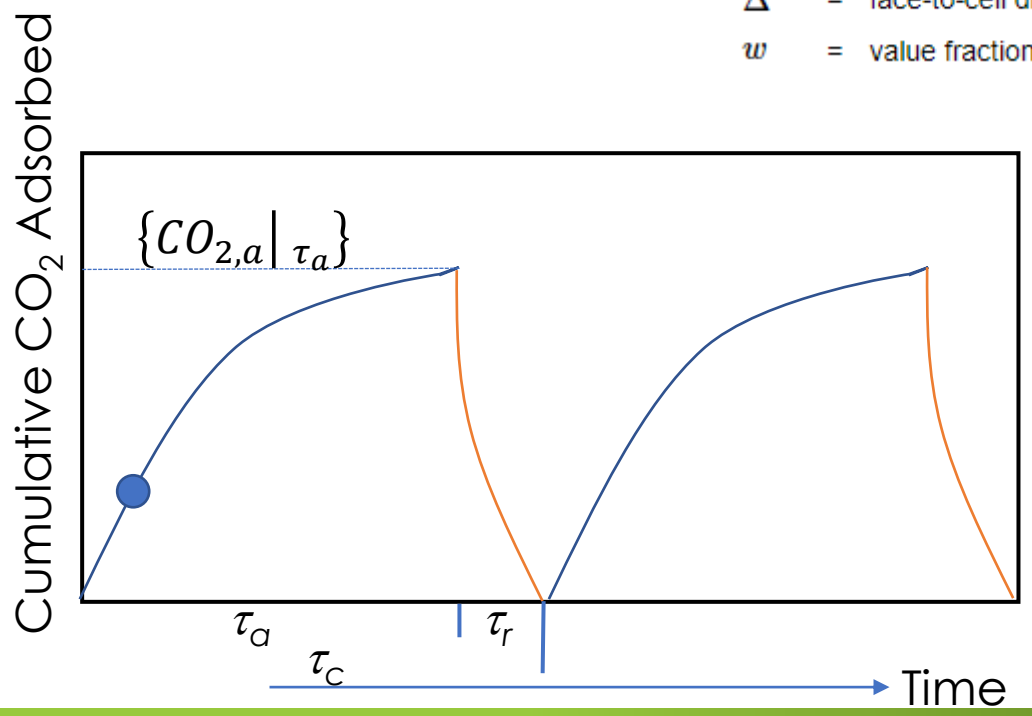


Fake reactions with a “CO2” scalar

Use a “Mixed boundary condition” to mimic absorption

$$\phi_f = w\phi_{ref} + (1-w)\left(\phi_c + \Delta\nabla\phi_{ref}\right)$$

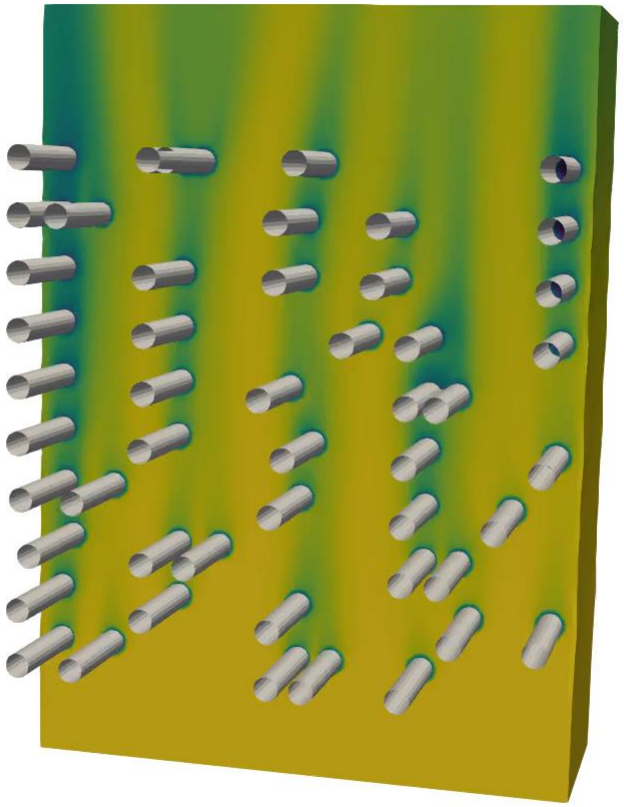
ϕ_f	=	face value
ϕ_c	=	cell value
ϕ_{ref}	=	reference value
Δ	=	face-to-cell distance
w	=	value fraction

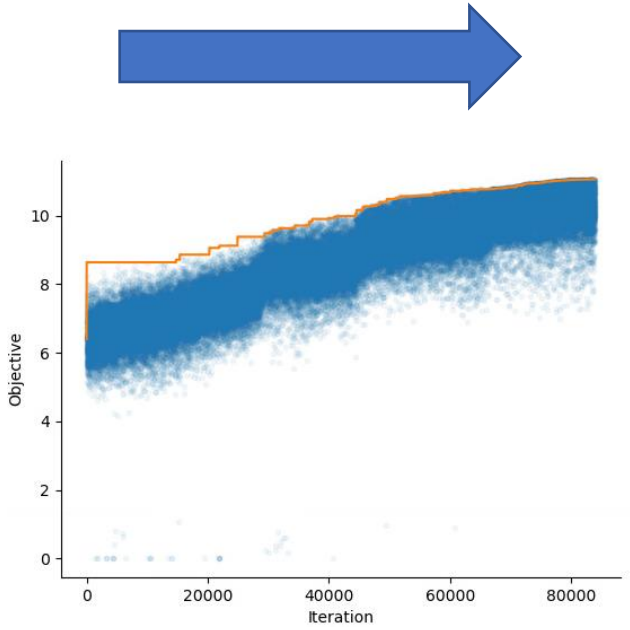


Optimization results: with reactions

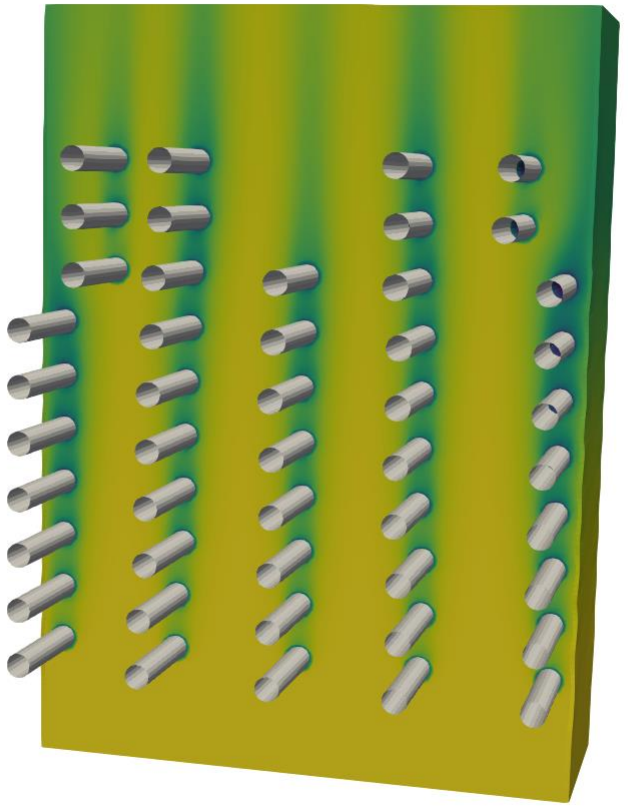
$$\max \frac{\frac{CO_{2,in} - CO_{2,out}}{CO_{2,in}} * 100}{\Delta P}$$

Score: 5.350





Score: 11.058



Binary Level set + GA

112 x 104 binary array

solid

gas

contoured

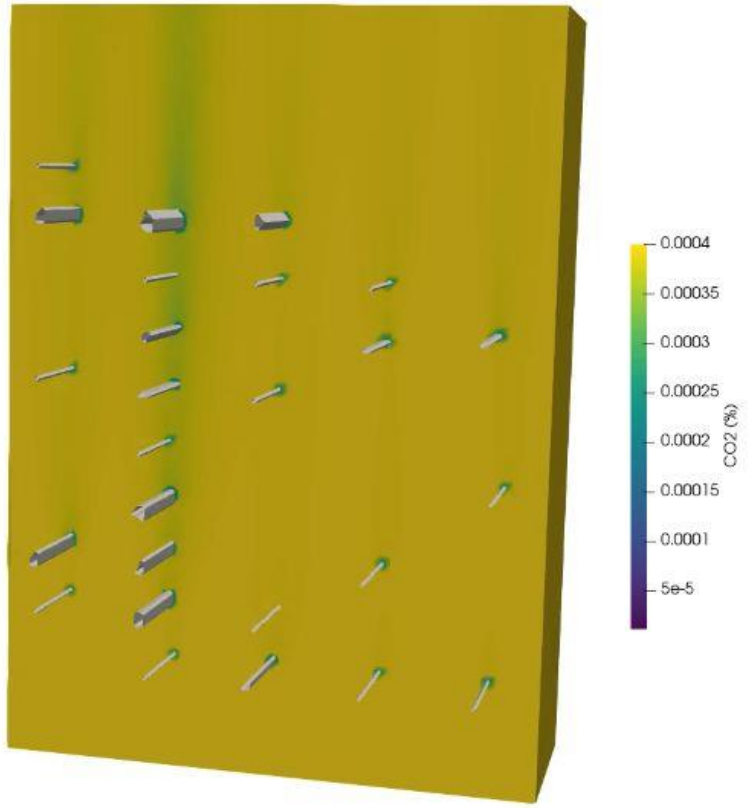
STL file

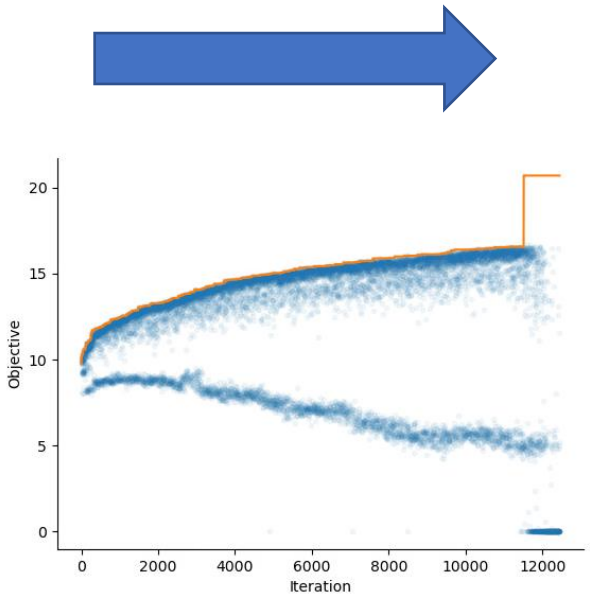
Mesh

Model

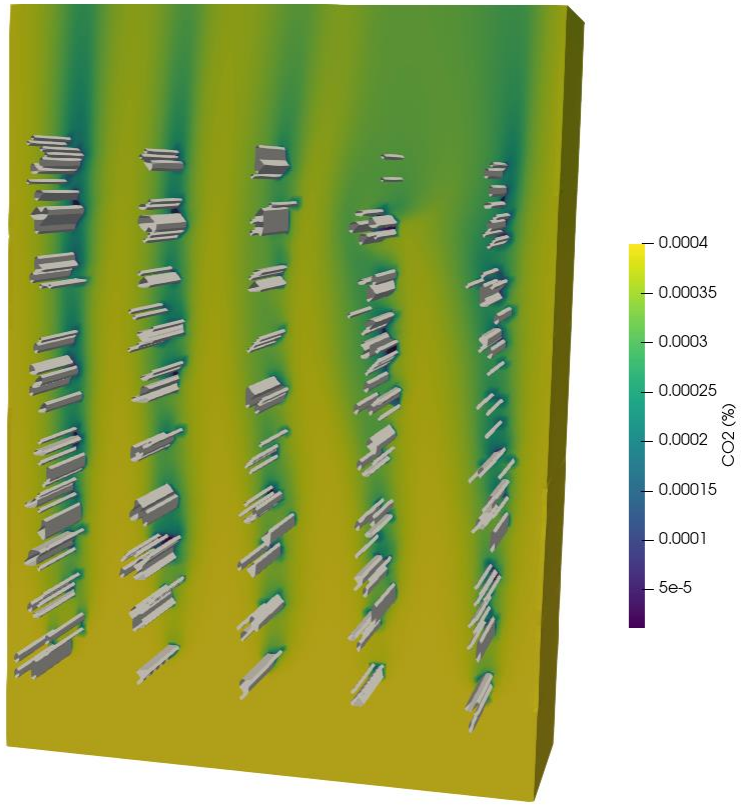
Binary Level set: Results

Score: 5.156



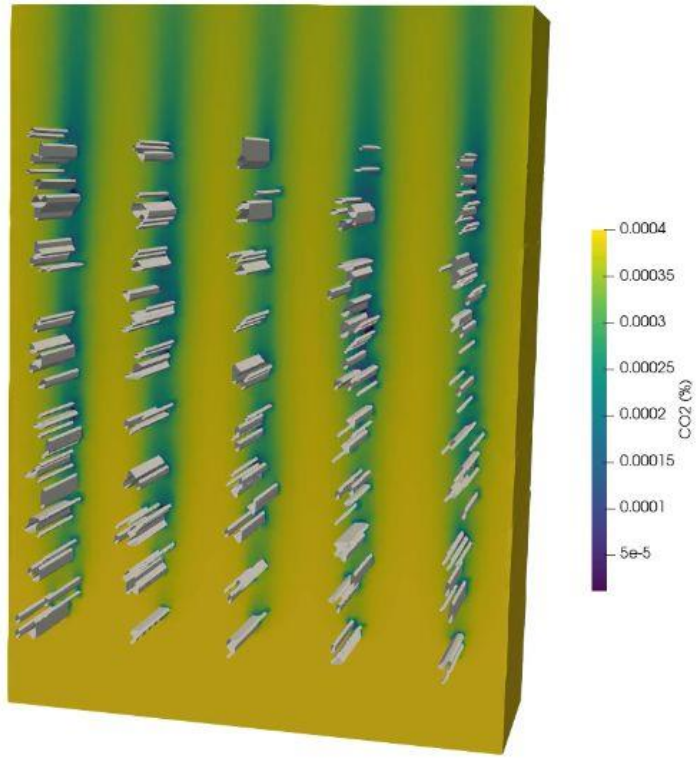


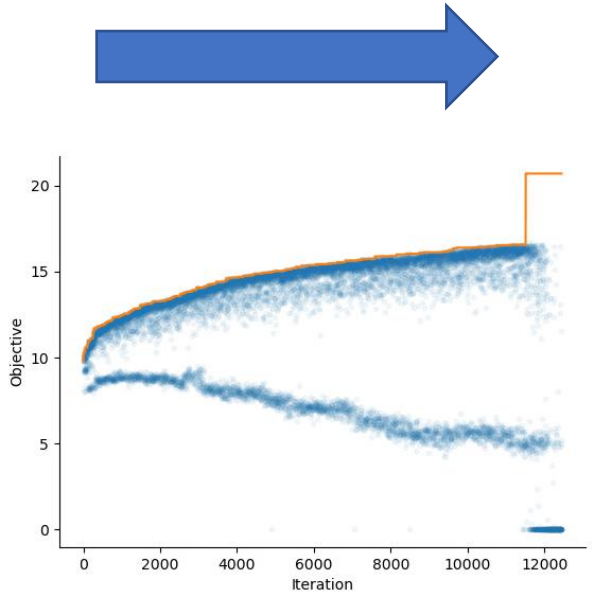
Score: 20.693



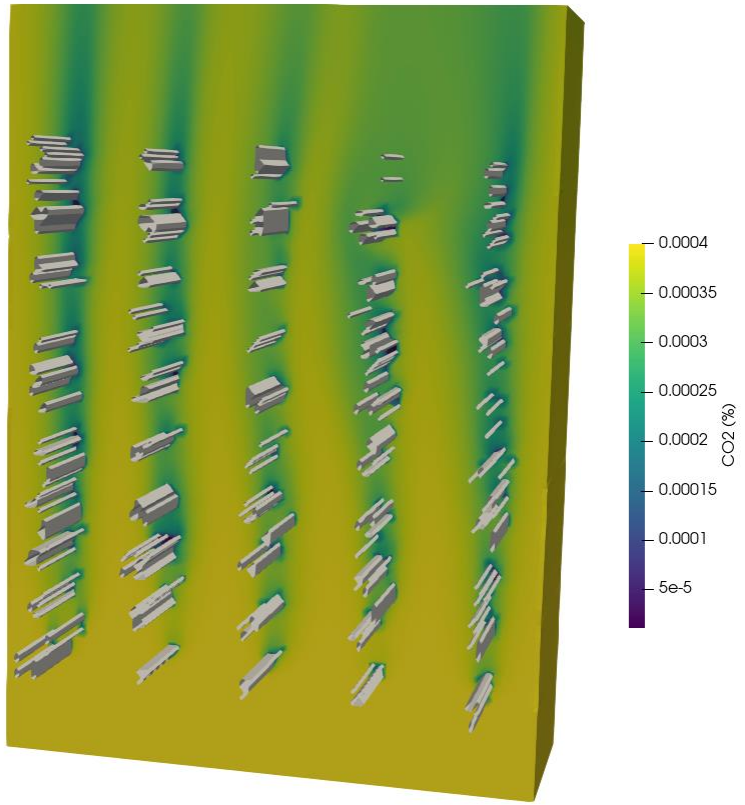
Binary Level set: Results

Score: 16.020





Score: 20.693



What's the best configuration?

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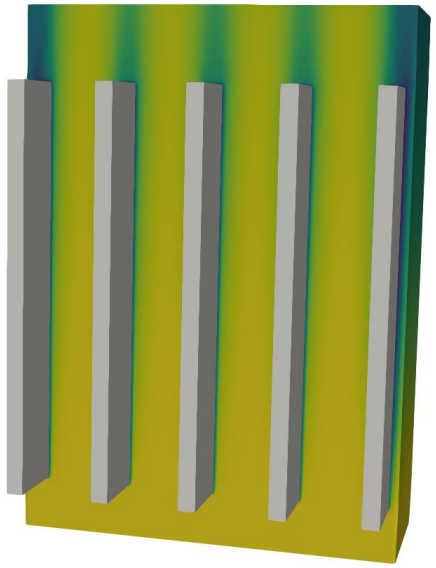
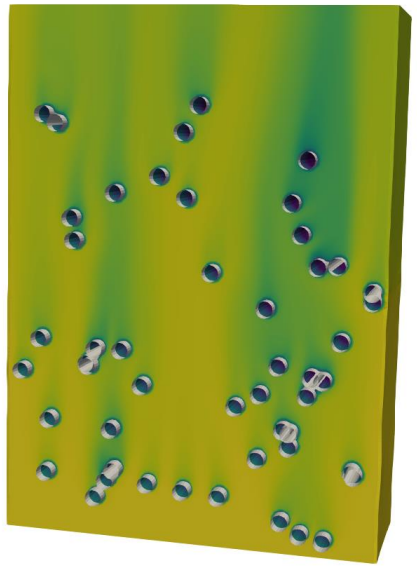
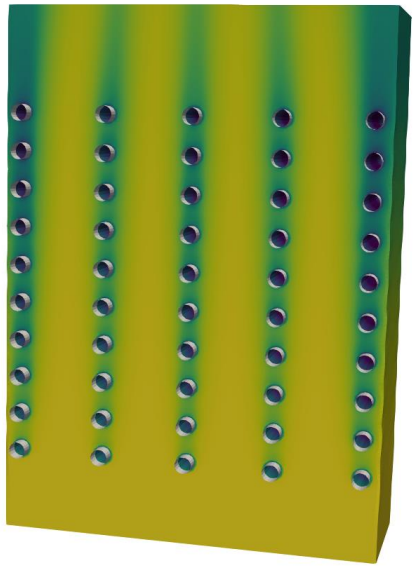
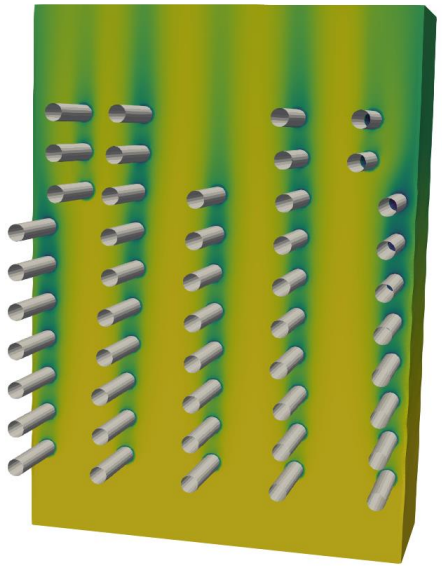
Algorithmic





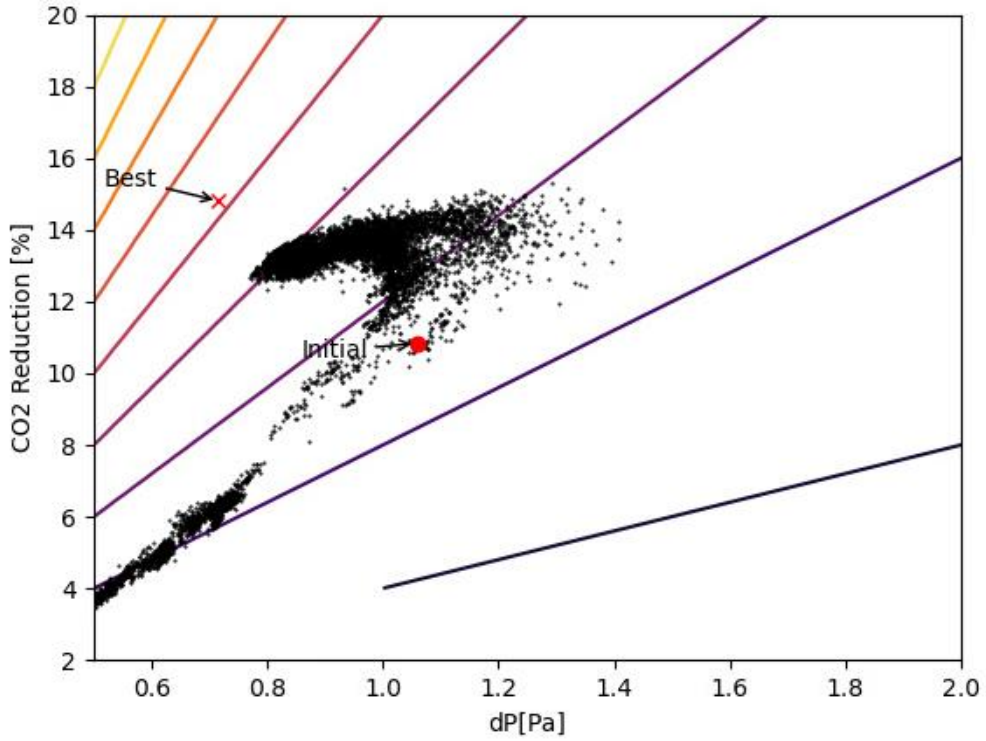




Score	18.1	4.0	10.2	11	20.7
	Plates	Random tubes	Structured tubes	Optimized tubes	Free form

Summary

- Need to reduce energy consumption → reduce pressure drop
  - Use generative algorithms to optimize the design
  - Successfully ran OpenFoam simulations of the lab scale test unit geometry
- Next steps
  - Refine reactions in OpenFoam model to calculate more realistic objective function
  - Build and test promising design candidates
  - Validate optimization process with experimental data
  - Extend to multi-objective



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