CCSI²
Carbon Capture Simulation for Industry Impact

Solvent Model Validation Hierarchy

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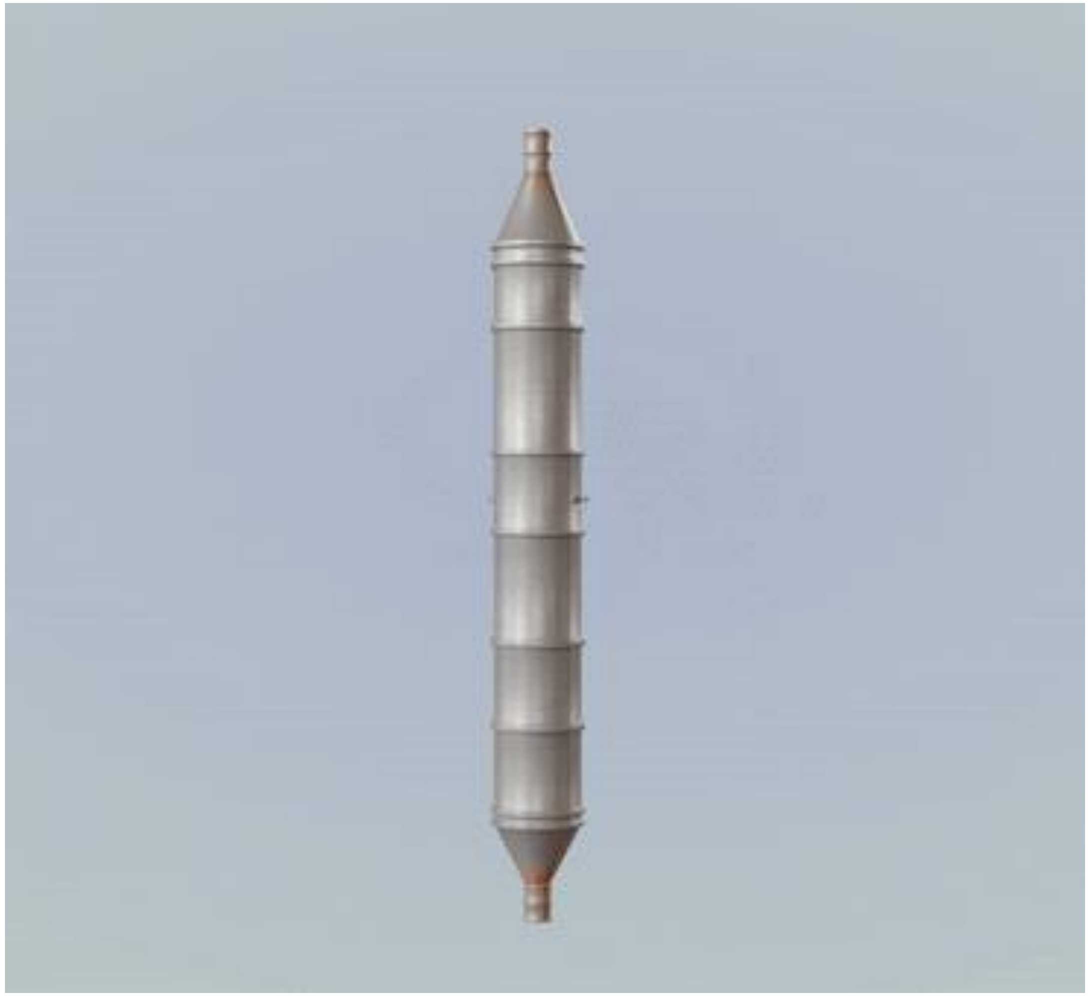
Solvent model validation framework to optimize CO_2 capture

Absorber column with commercial packing and intensified packing device for intrastage cooling ▶



Intensified device for intrastage cooling to control absorber column temperature profile

Absorber columns have complex multiscale, multiphysics dynamics.

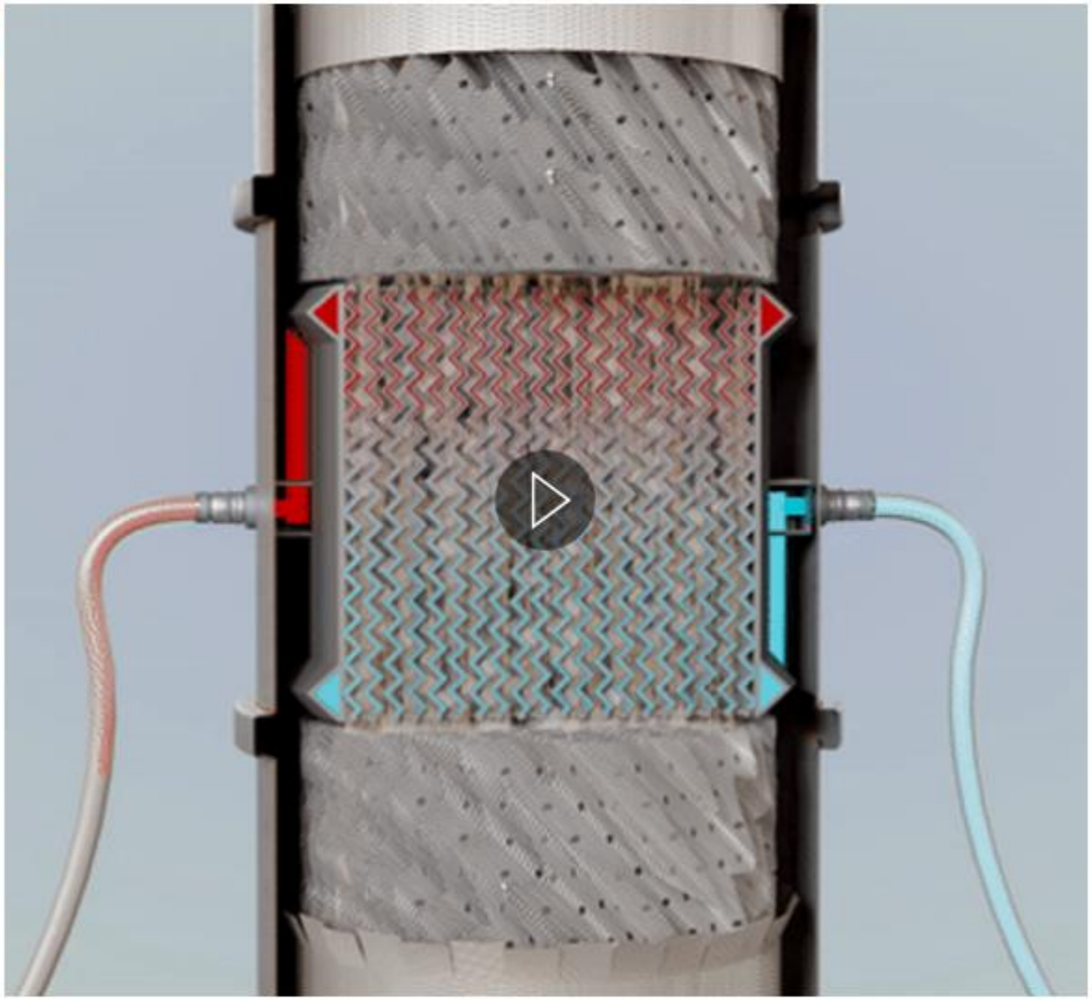
Intrastage cooling using a non-optimized intensified device can increase CO_2 capture efficiency by 5–25%, with almost 40% reduction in column size.

We have developed an integrated approach for process optimization.

Solvent model validation framework to optimize CO_2 capture

Absorber column with commercial packing and intensified packing device for intrastage cooling ▶

Intensified device for intrastage cooling to control absorber column temperature profile



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Intrastage cooling using a non-optimized intensified device can increase CO_2 capture efficiency by 5–25%, with almost 40% reduction in column size.

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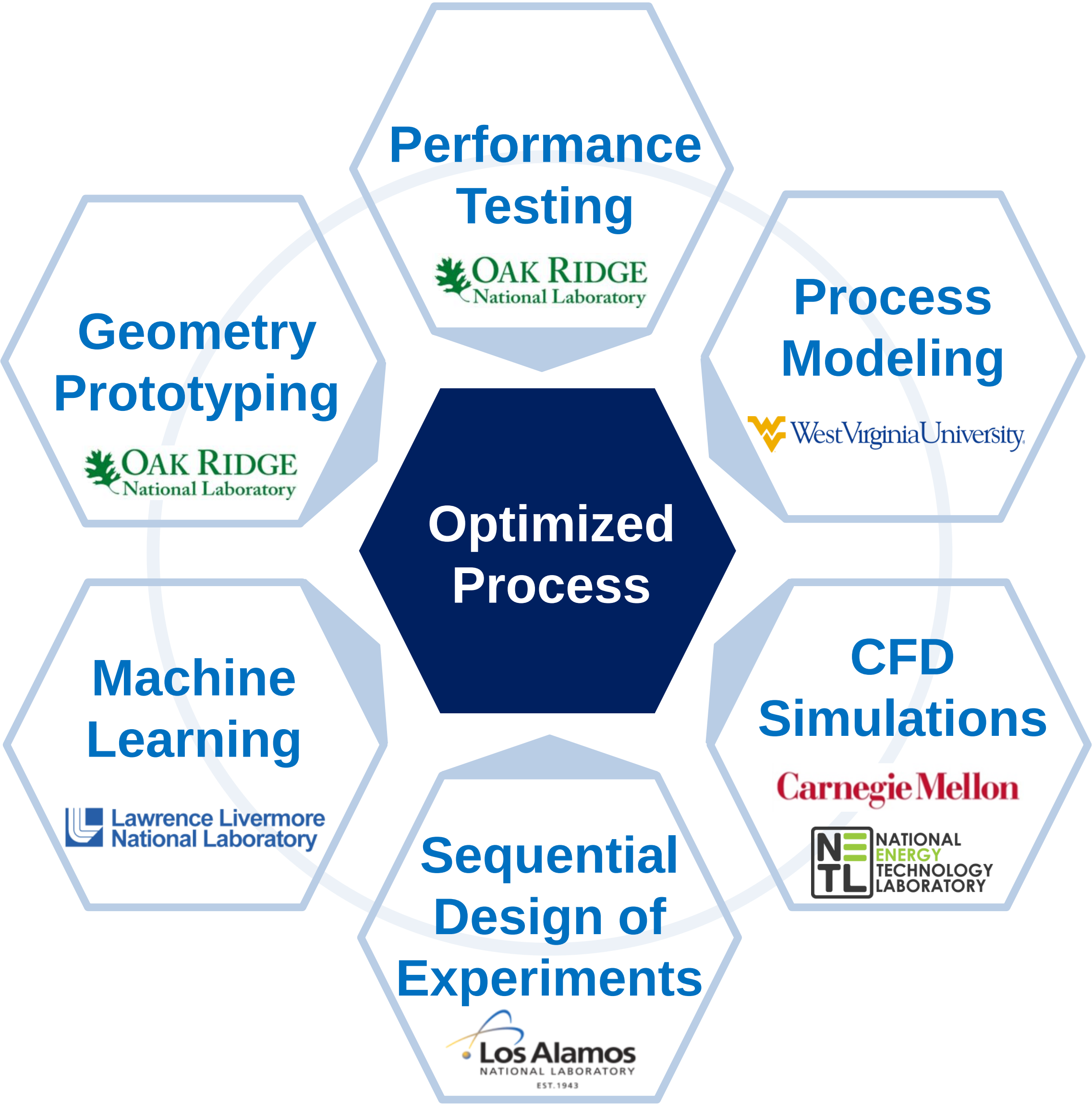
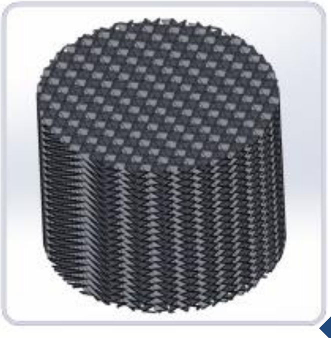
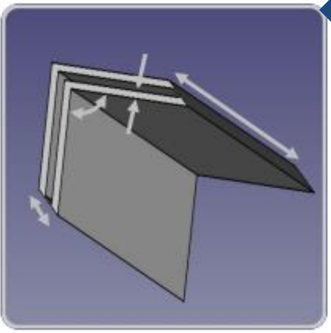
Multi-pronged approach to validate solvent models



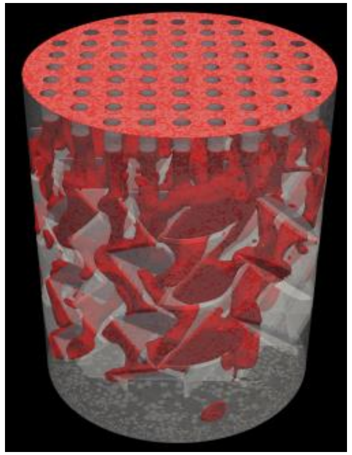
Overall optimization strategy

Candidate geometry & operating conditions

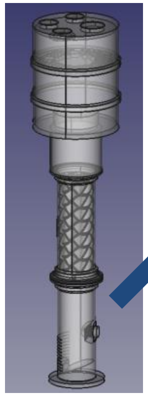


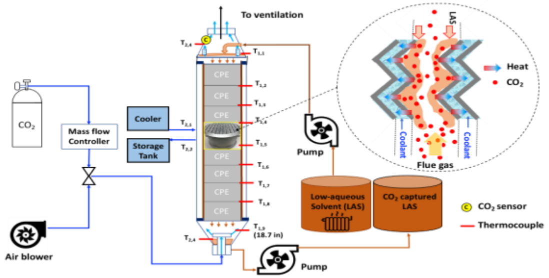


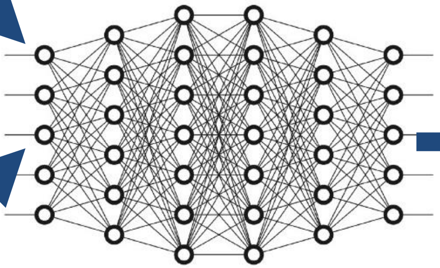
CFD model & simulations



Device manufacturing, column setup and experimentation

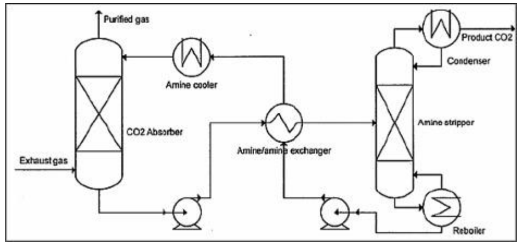




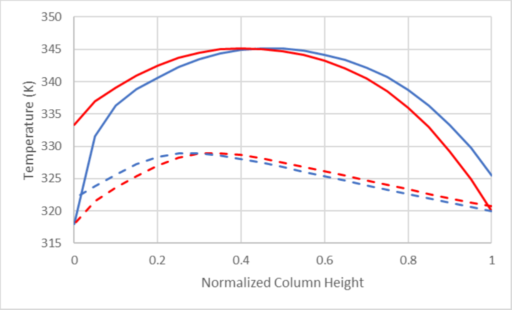


ML Training

Process modeling & optimization

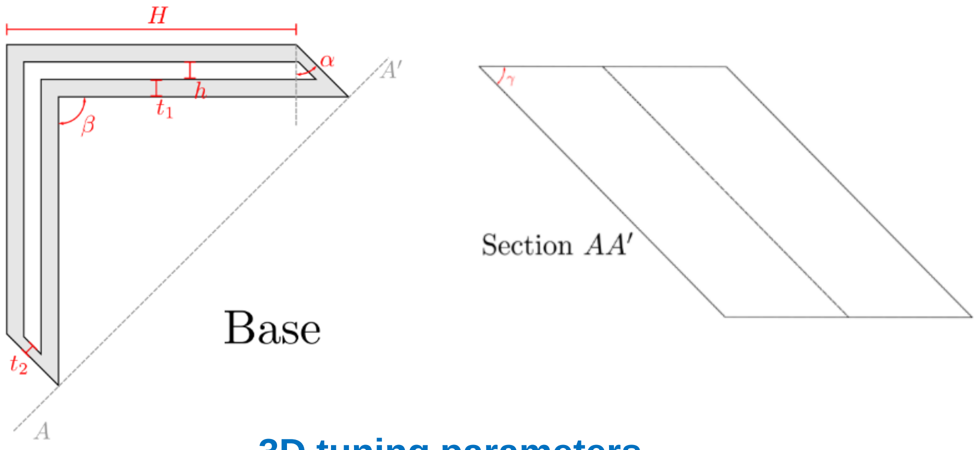


$$min f(x)$$
$$s.t. g(x) \geq b$$
$$h(x) = 0$$
$$x \geq 0$$



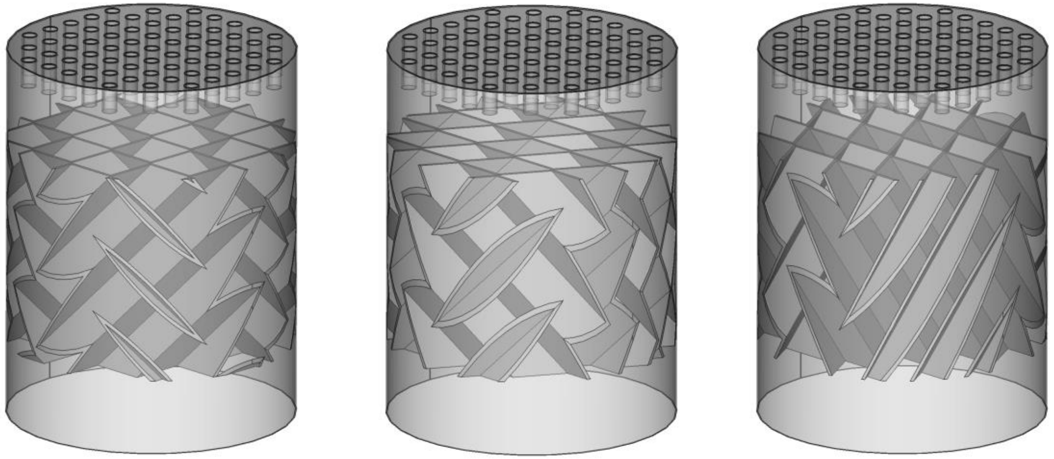
Update Geometry/UQ

Geometric parametrization in 2D and 3D



3D tuning parameters

3D candidate geometries



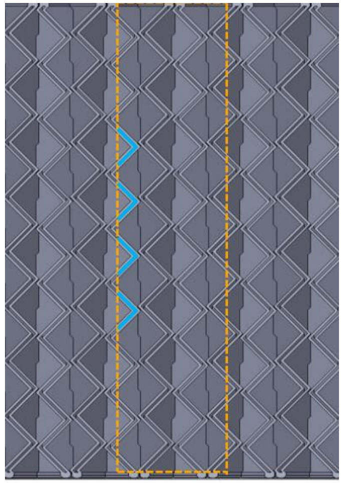
$\beta = 60°$
$\gamma = 45°$

$\beta = 90°$
$\gamma = 45°$

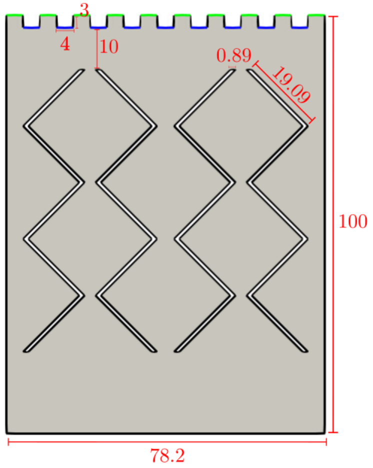
$\beta = 60°$
$\gamma = 60°$

```
#L_mat # 3 permutations
#pack_gap # 3 permutations
#t_mat # 2 permutations

# ========= User Parameters ===============
dName = "doc1"
column_radius = 38.1
column_height = 100
Ldrip = 3
Wdrip = 4
Ndrip = 9
Wgas = (2.*column_radius - Ndrip*Wdrip)/(Ndrip + 1)
tcol = 0.89
Lpack = 12 #13.5 #13.5*np.sqrt(2.)
dpack = 17
dpack_wall = Wgas*1.
pack_gap = 2.*tcol
#NpackY = 7
#theta1 = 30.
#theta2 = 2.*theta1
# ========================================

theta_mat = [30., 45., 60.]
L_mat = [11., 13., 15.]
pack_mat = [2.*tcol,3.*tcol,4.*tcol]

permutations = []
for k in range(len(pack_mat)):
    for j in range(len(L_mat)):
        for i in range(len(theta_mat)):
            permutations.append((i,j,k))
```

Scripts for automated packing generation 2D/3D

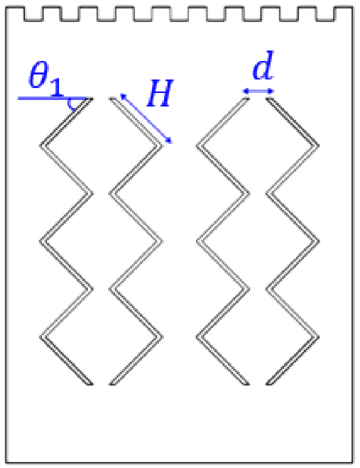


Cross-section of intensified packing design



2D packing

(All dimensions in mm.)

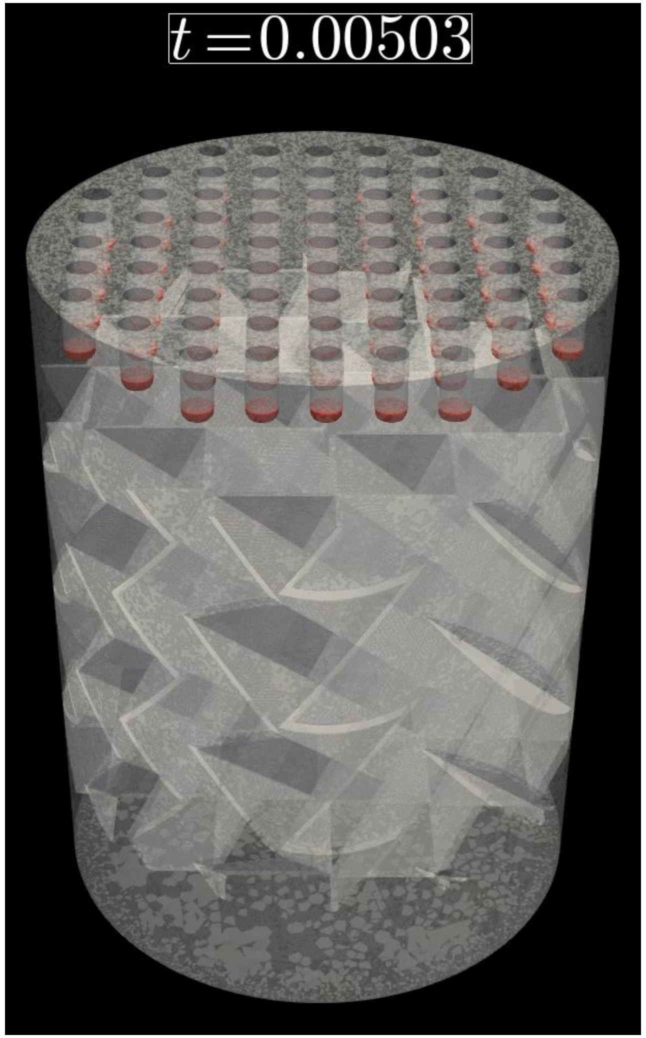


2D tuning parameters

Packing #	θ_1	H (mm)	d (mm)
1	30	10	1.78
2	45	10	1.78
3	60	10	1.78
4	30	13	1.78
5	45	13	1.78
6	60	13	1.78
7	30	14.8	1.78
8	45	14.8	1.78
9	60	14.8	1.78
10	30	10	2.67
11	45	10	2.67
12	60	10	2.67
13	30	13	2.67
14	45	13	2.67
15	60	13	2.67
16	30	14.8	2.67
17	45	14.8	2.67
18	60	14.8	2.67
19	30	10	3.56
20	45	10	3.56
21	60	10	3.56
22	30	13	3.56
23	45	13	3.56
24	60	13	3.56
25	30	14.8	3.56
26	45	14.8	3.56
27	60	14.8	3.56

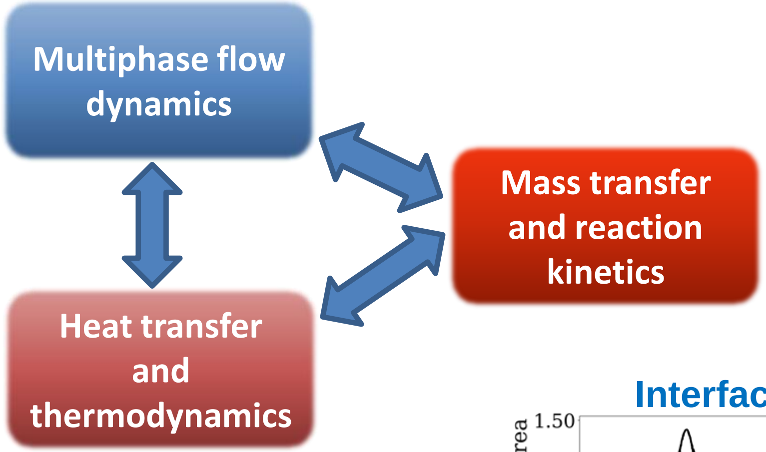
27 packing design permutations

3D simulation framework



Solvent: 30% MEA, 70% H_2O (by mass)
Flue gas: 10% CO_2, 1.5% H_2O, 88.5% N_2 (by mass)

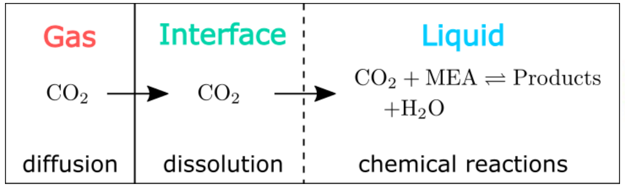
Coupled multiscale, multiphysics



IDAES framework in Fluent & OpenFOAM

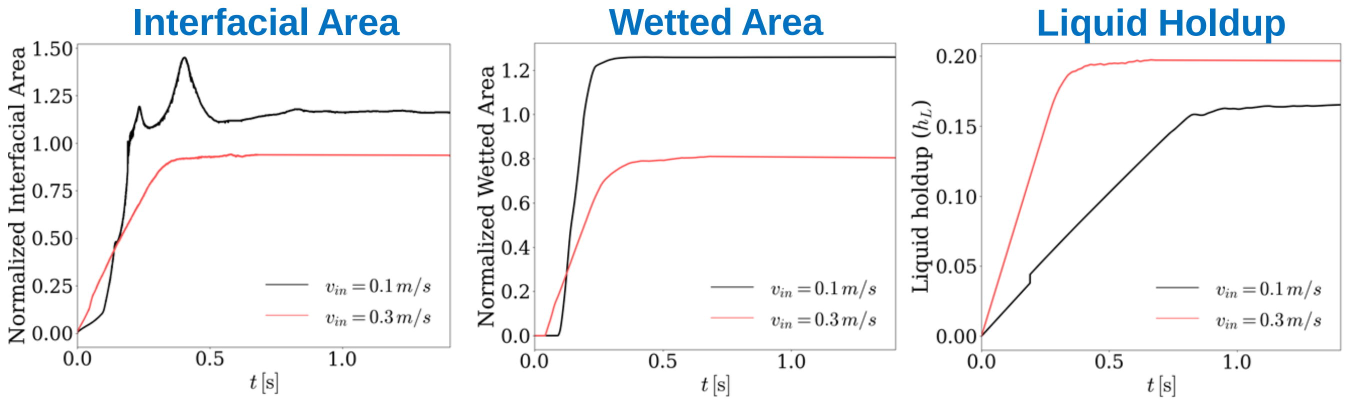
$$2MEA + CO_2 \rightleftharpoons MEACOO^- + MEA^+$$

$$MEA + H_2O + CO_2 \rightleftharpoons MEA^+ + HCO_3^-$$



IDAES Institute for the Design of Advanced Energy Systems

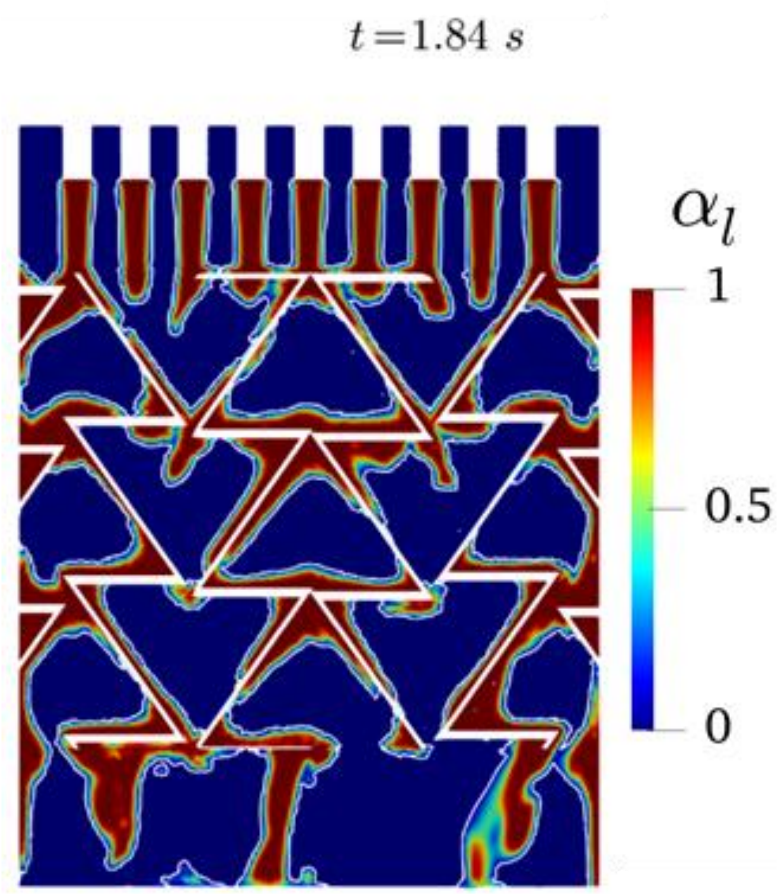
Flow predictions



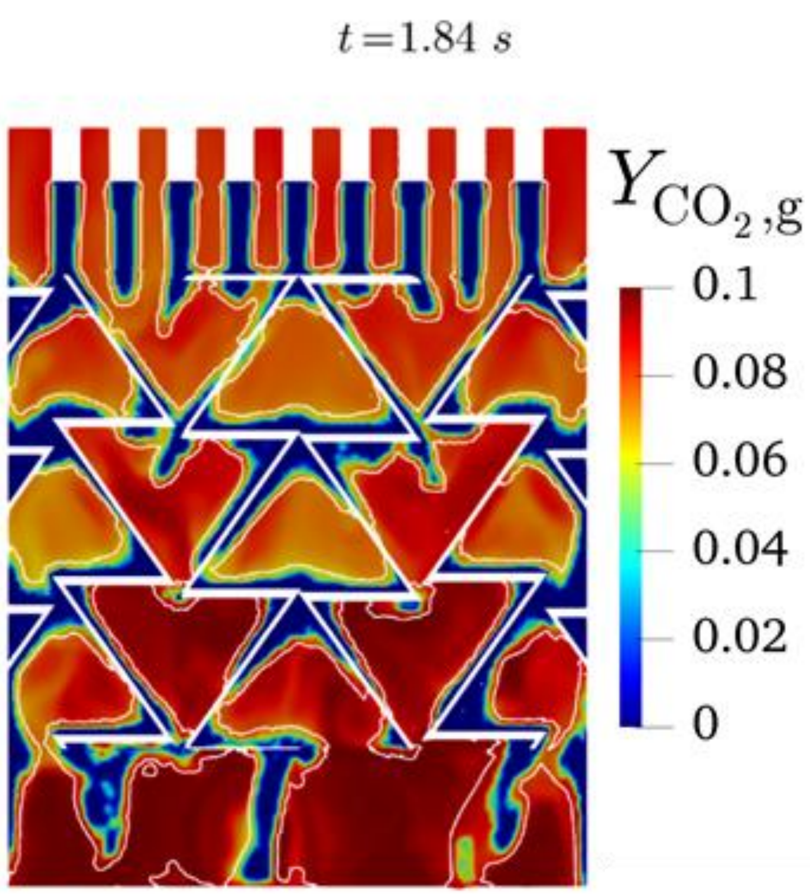
INNOVATIONS ►

- **First-ever implementation of the IDAES detailed reaction dynamics and thermodynamics in absorption CFD**
- **Unique, coupled multiphysics approach covering mass, momentum and heat transfer**
- **Locally dependent material properties**

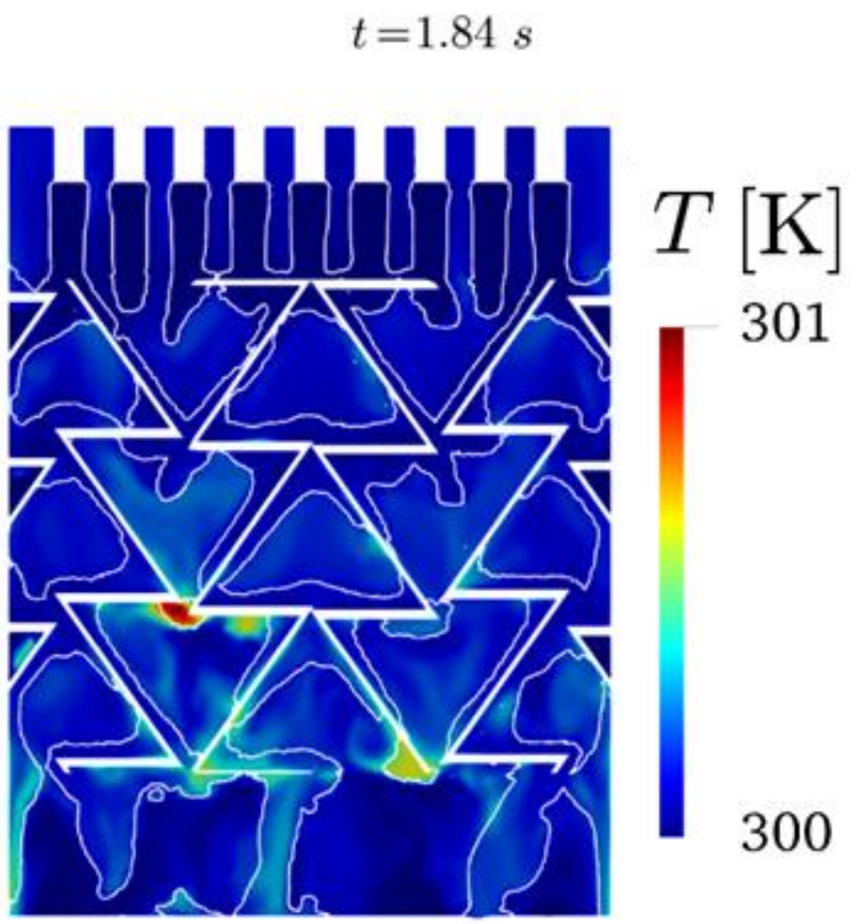
Preliminary indicative 3D simulation results



Liquid fraction (α_l)



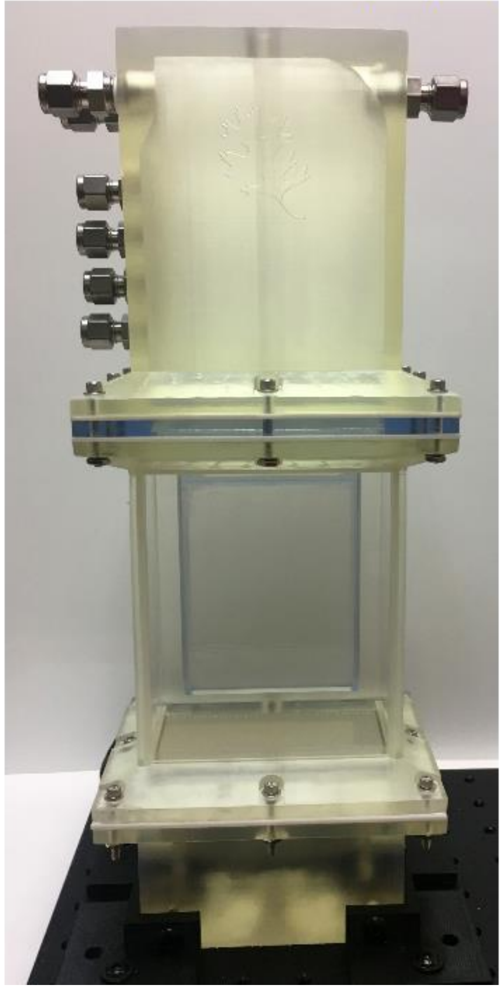
Mass fraction of CO_2 (Y_{CO2})



Temperature (T)

2-inch columns for higher-fidelity validation data

Fluid–Structure Interface (FSI) setup

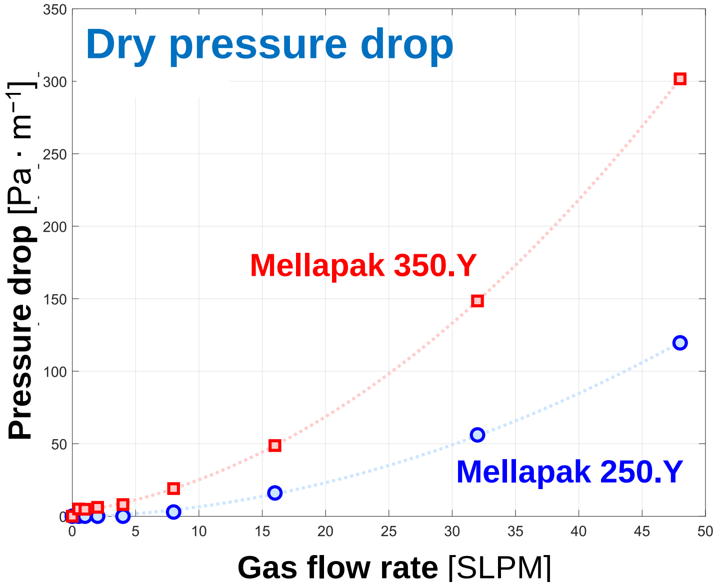


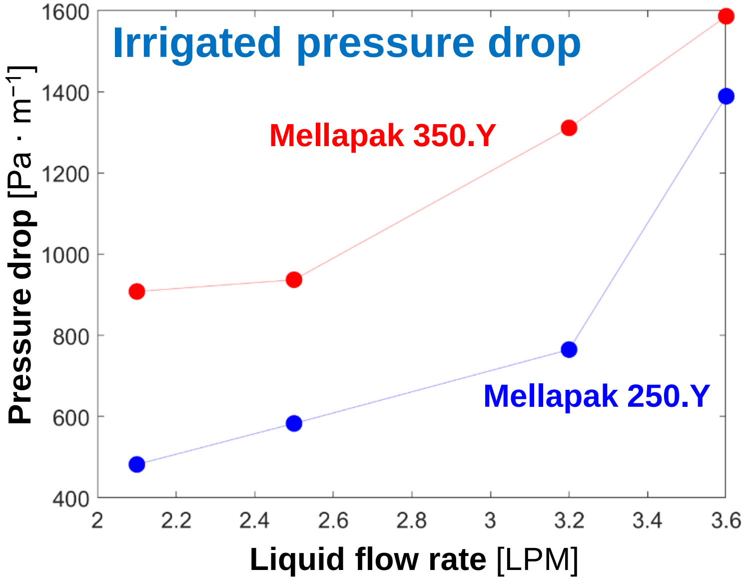
To measure solvent flow behavior on column material of construction

Packing Prototype Performance (PPP) setup

To characterize specific geometry performance for validation data

◀ **3D printed column, with full-size packing structures, for rapid prototyping & testing**





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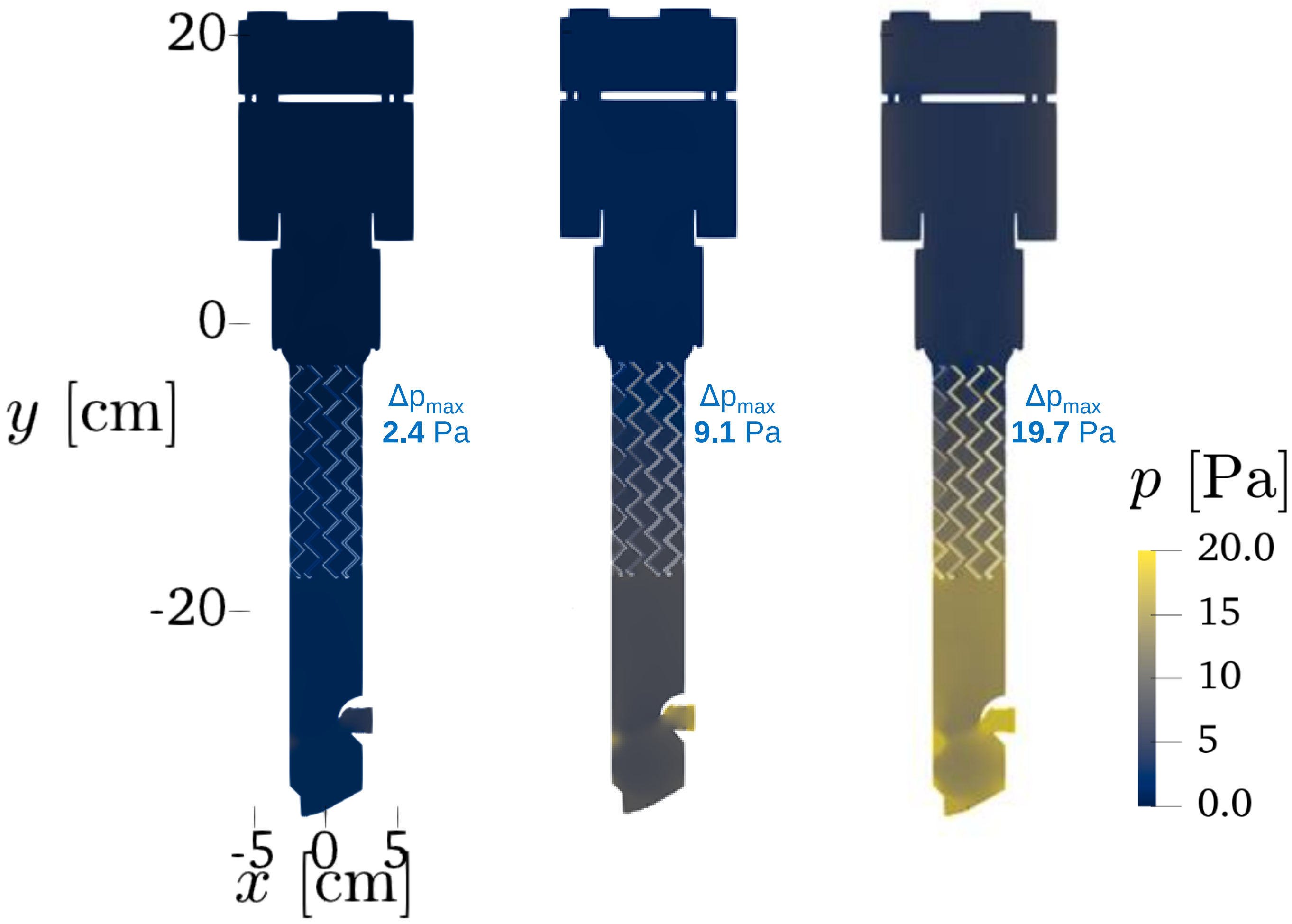
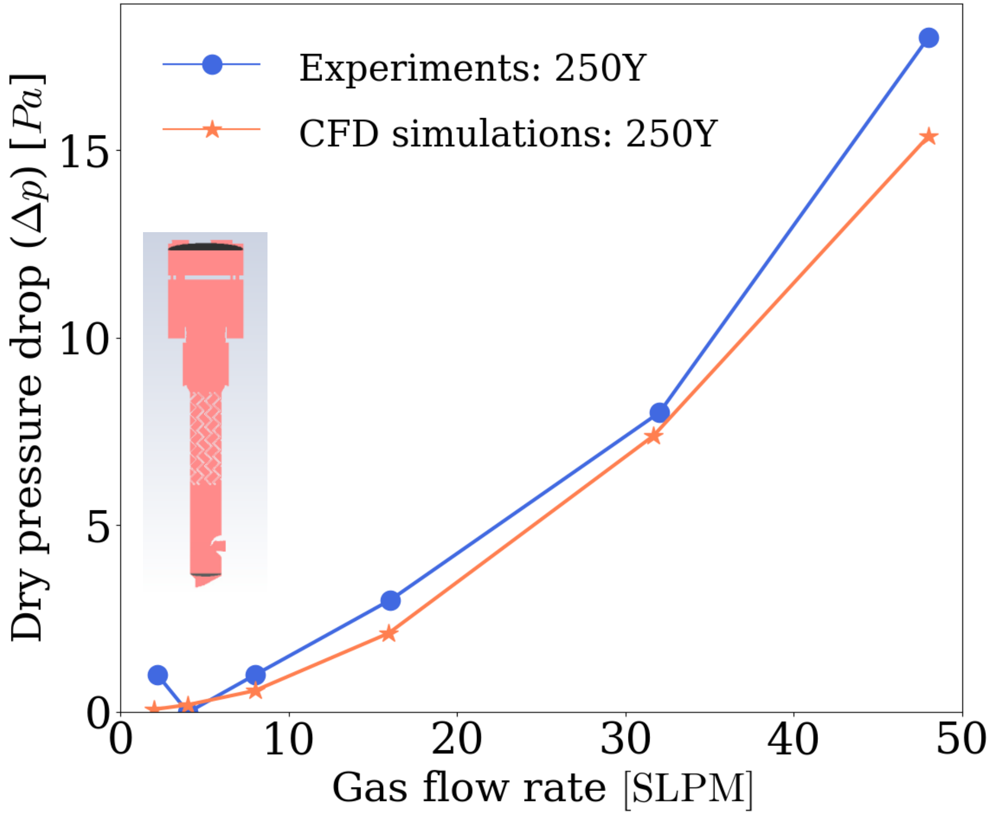
Dry pressure distribution for the 2-inch column



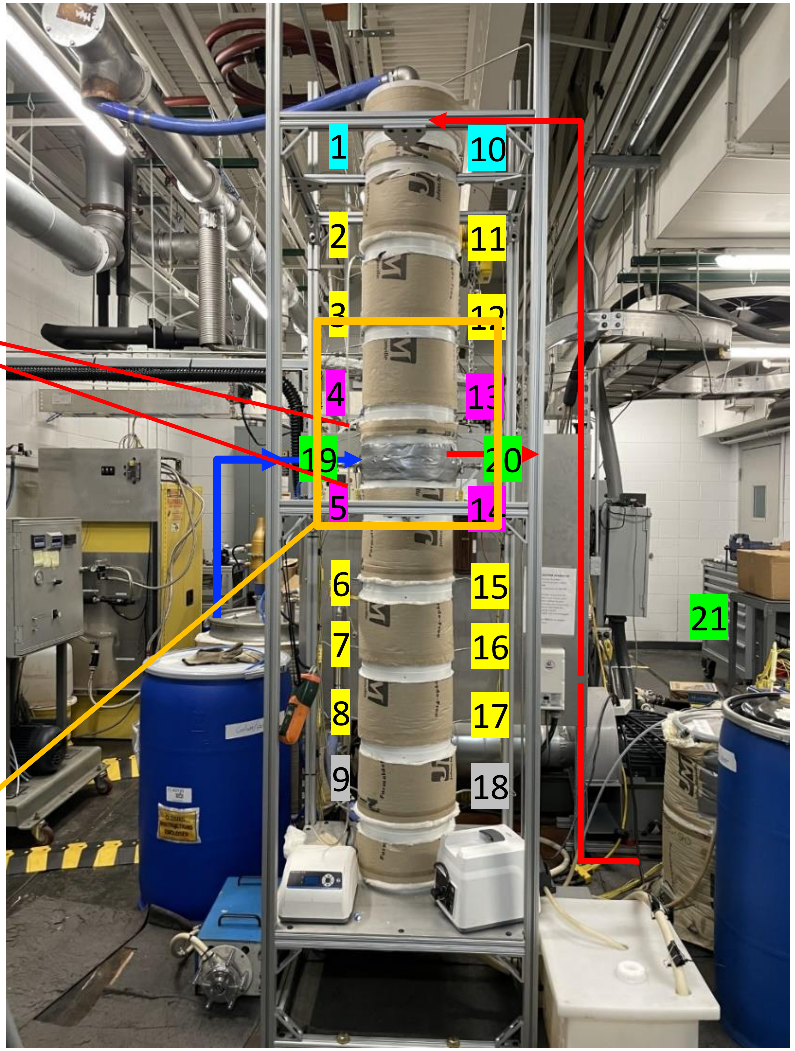
16 LPM **32 LPM** **48 LPM**



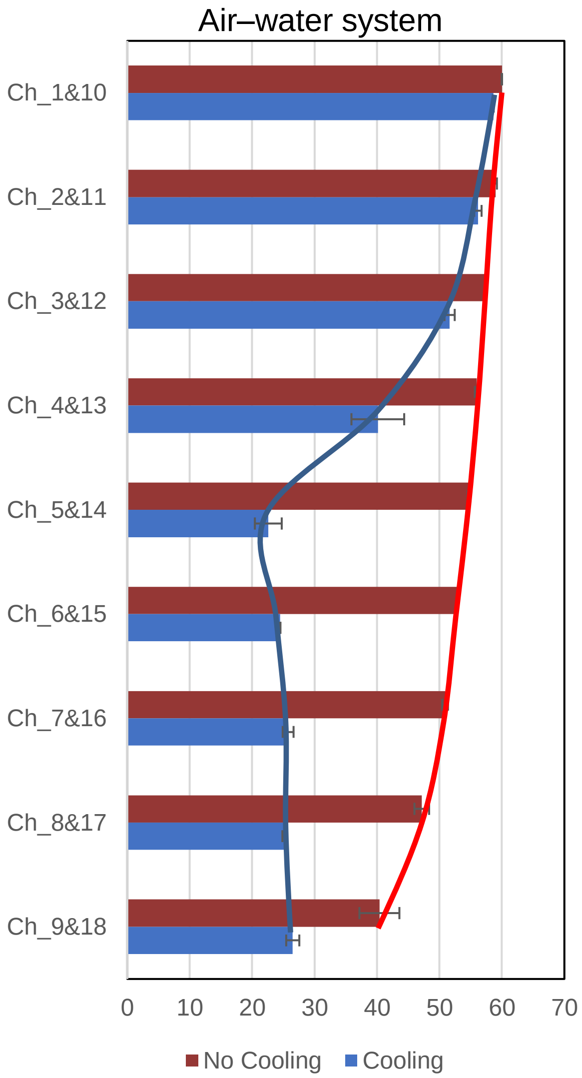
"Measure what you model; model what you measure."

8-inch column for model scaling testing

Two 3D-printed intensified device sections



Current focus is on enhanced instrumentation to provide high-fidelity boundary conditions and performance data for simulations



Temperature profiles

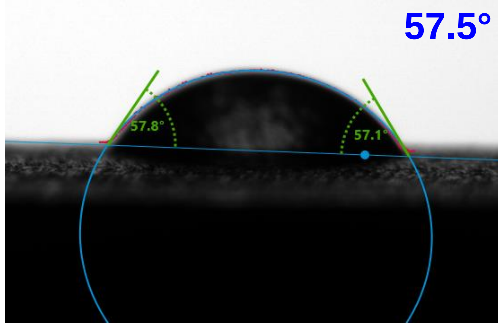
[AMO-funded]

Solvent properties measurements improve simulation accuracy

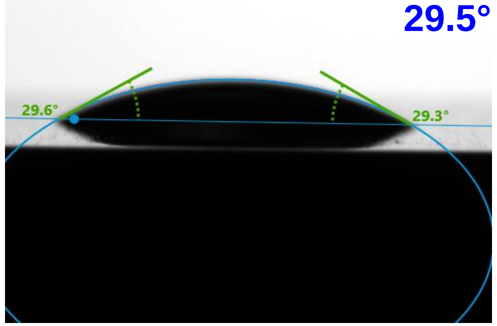
We have a wide range of capabilities to measure specific **solvent interaction** with our specific packing **materials of construction** to improve simulation accuracy.

Static Contact Angles

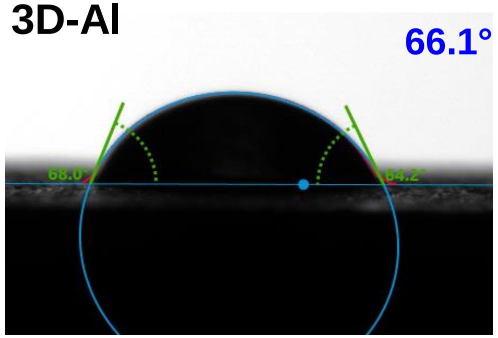
MEA30 on 3D-Al



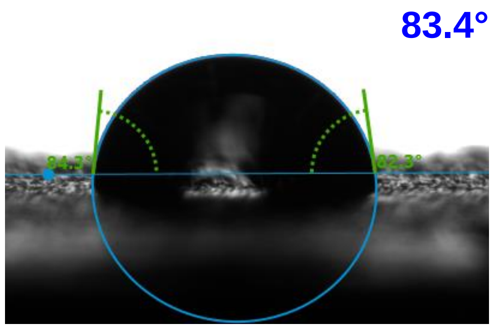
MEA30 on 410 SS



CO_2–aged MEA30 on 3D-Al

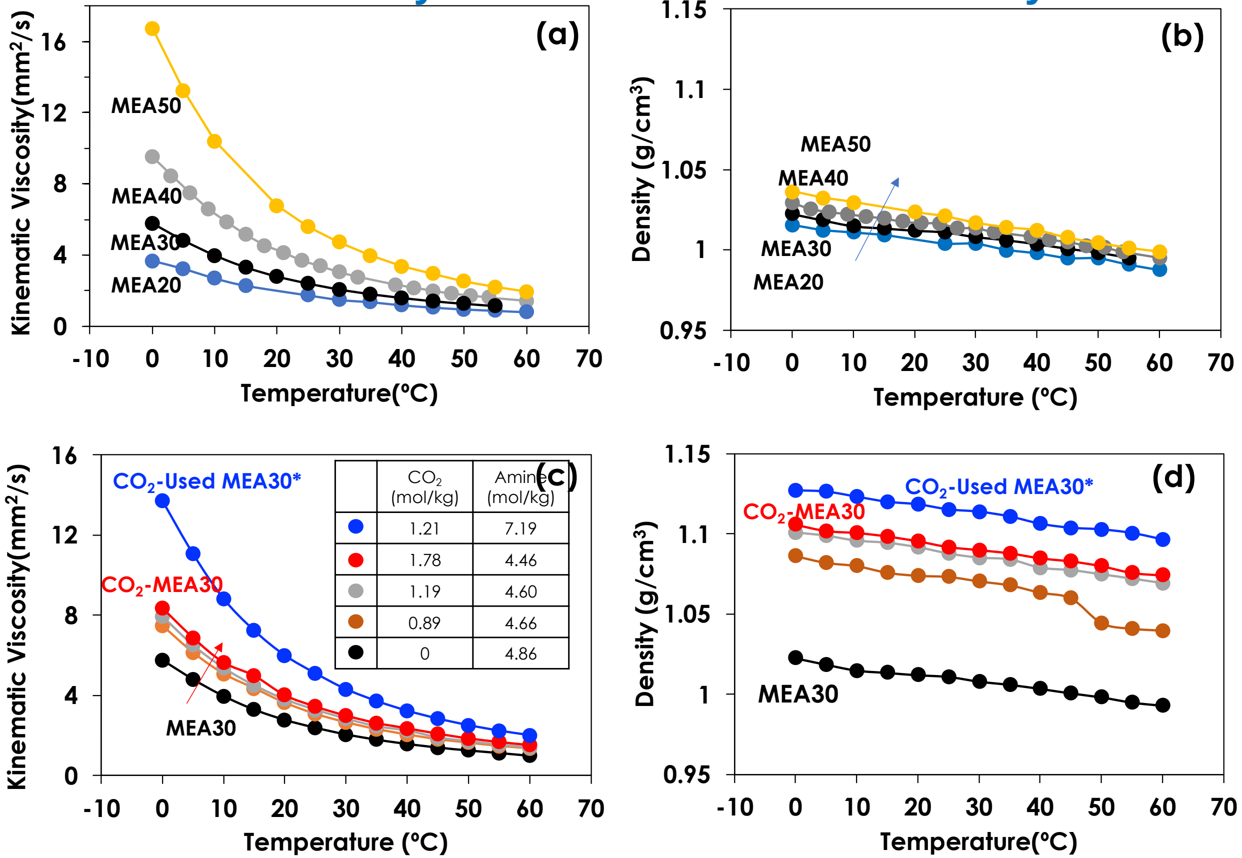


Water on 3D-Al



Viscosity

Density



Scaling sequence and capabilities

12-inch column, 1 T_{CO2}/day

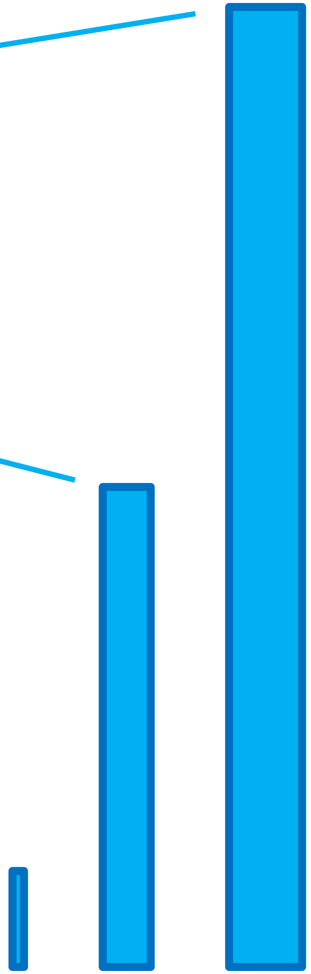
Candidate geometry validation & CFD/process/ML model support

8-inch column, 0.1 T_{CO2}/day

Candidate geometry validation & CFD/ML model support

2-inch column

CFD film-modeling validation and candidate geometry testing



APPROXIMATELY TO SCALE

Commercial packing

Intensified devices

Packing Prototype Performance Column
2-in (5 cm) diameter
0.7 m tall

Column A
8-in (20 cm) diameter
2 m tall

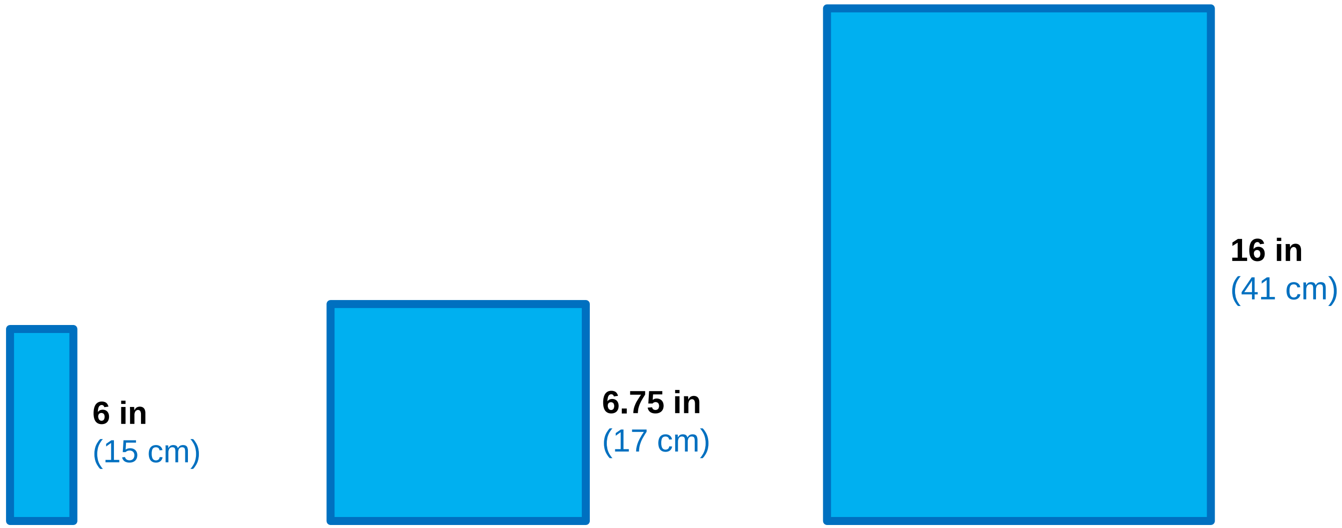
Column B
12-in (30 cm) diameter
4 m tall

PHOTOS NOT TO SCALE

Scale-up sequence – intensified-device sections

- Objective: provide high-fidelity performance data sufficient to support process models, CFD, ML–ROM surrogates

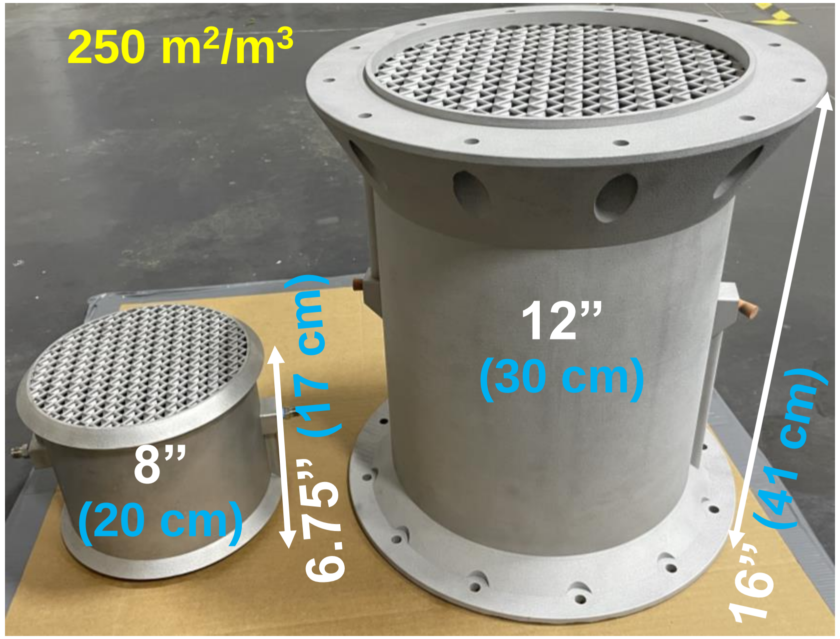
0.3 L → 19 × → 5.6 L → 5.3 × → 29.7 L



2-inch (5 cm) section | **8-inch (20 cm) section** | **12-inch (30 cm) section**

▲ APPROXIMATELY TO SCALE

3D-printed intensified devices



Highlights

Unique capabilities

- Special treatment of solvent layer incorporating IDAES framework for MEA chemistry, heat transfer, and transport properties for direct CFD simulation of solvent wetting, thermodynamics, and CO_2 absorption

- Additive manufacturing for prototype packing fabrication and testing for process intensification

- Experimentation at multiple scales for scale-up validation

Because of the complexities of the solvent–packing interaction, scaling up of an optimized process is facilitated by the application of machine learning.

MACHINE LEARNING FOR ACCELERATING CFD AND DESIGN OPTIMIZATION

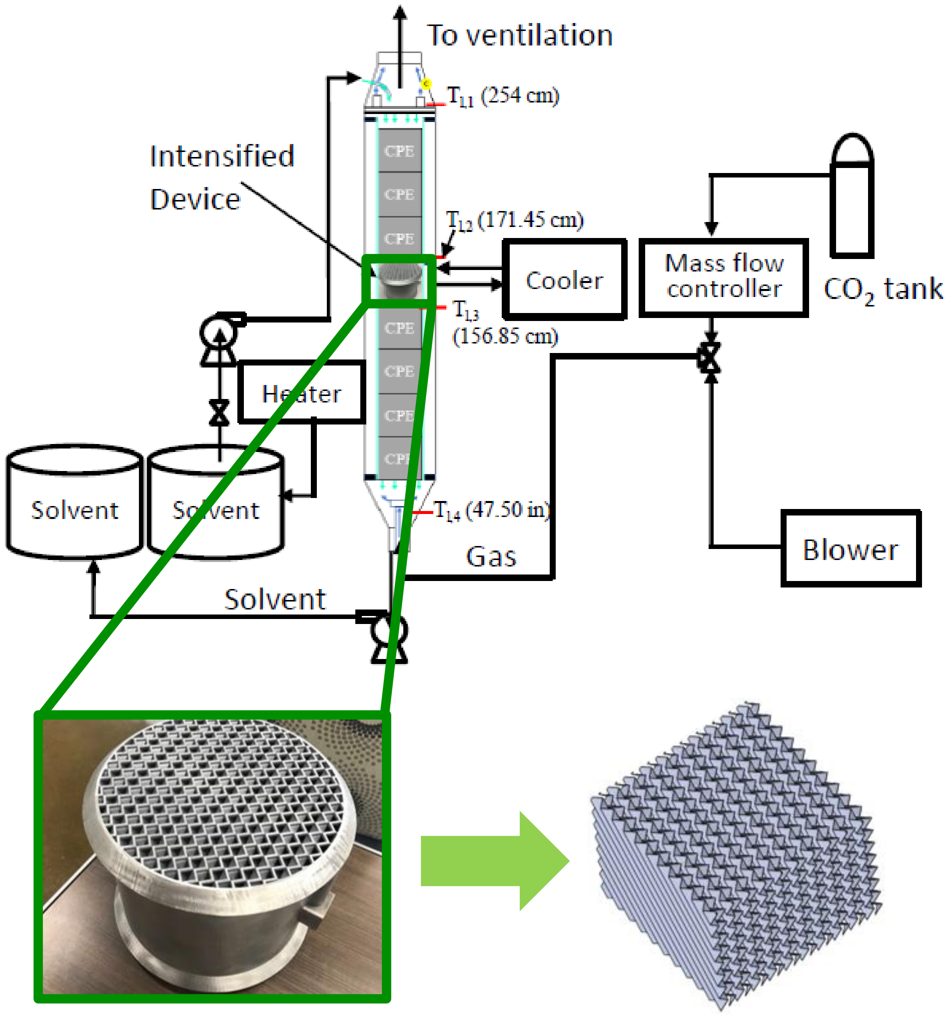
Machine learning for CFD

CFD is critical for the fundamental understanding, to inform process and system level modeling.

- **Need local information on transport phenomena to understand driving forces**
- **Can be incorporated into design optimization to optimize the device**

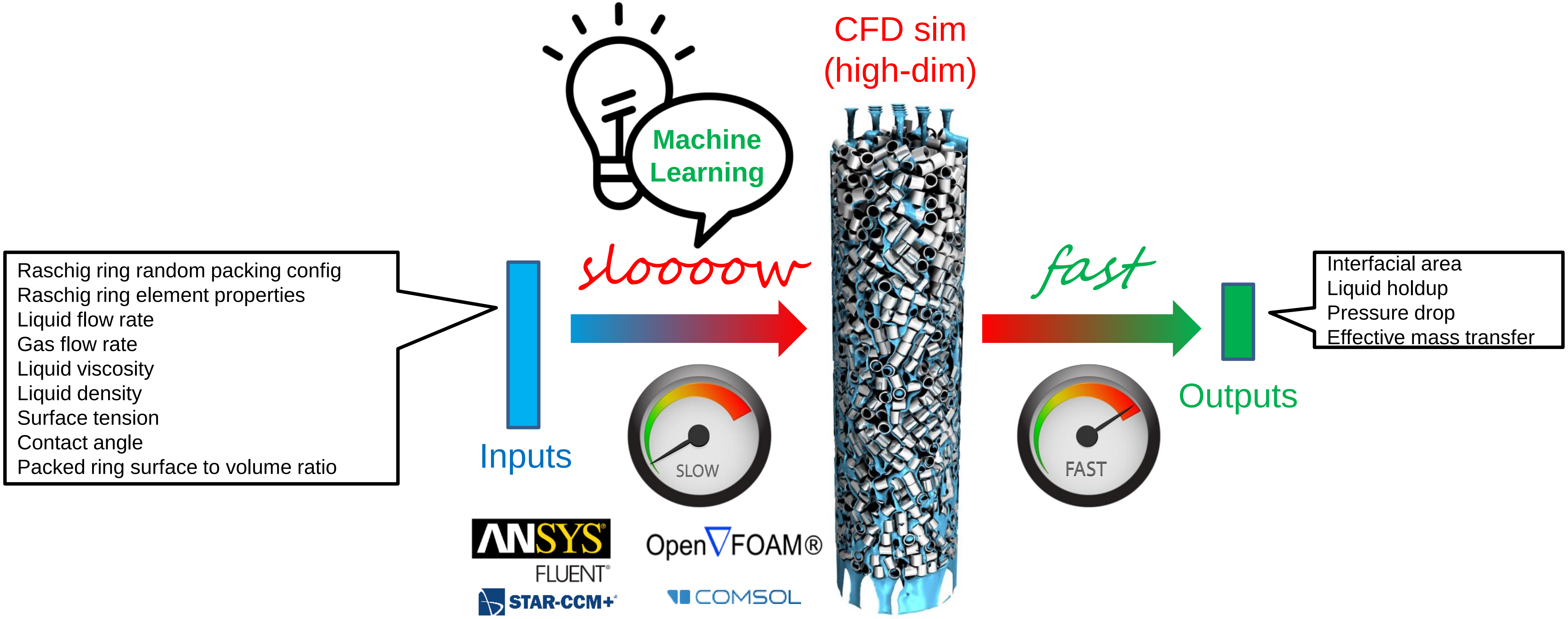
Simulation time is a bottleneck that impedes high-level modeling.

Machine learning surrogates, such as Deep Fluids (DF) and MeshGraphNets (MGN), can reduce the computational burden of time-consuming simulations.

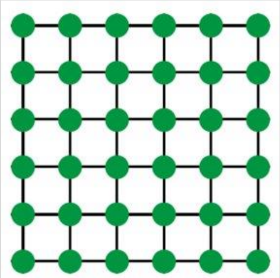
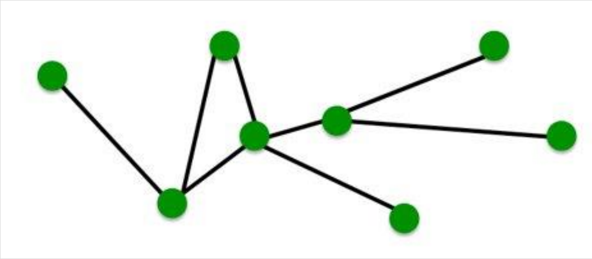
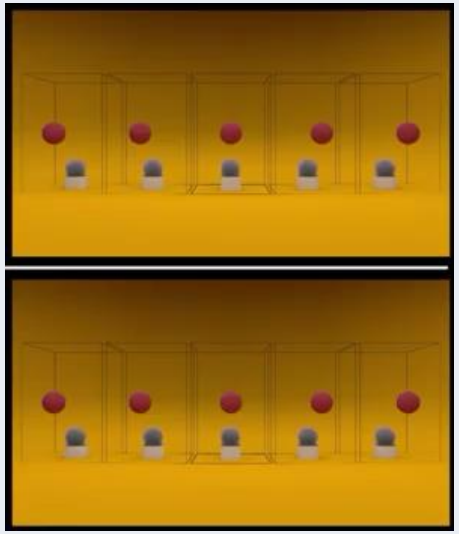
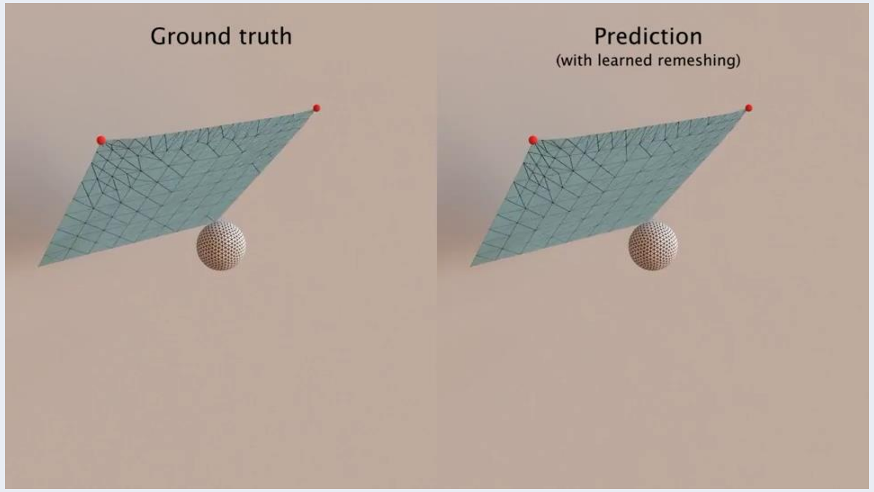


Fast Surrogates for CFD Simulation Model

- **Machine learning** surrogates to speed up computational fluid dynamics (CFD) simulations

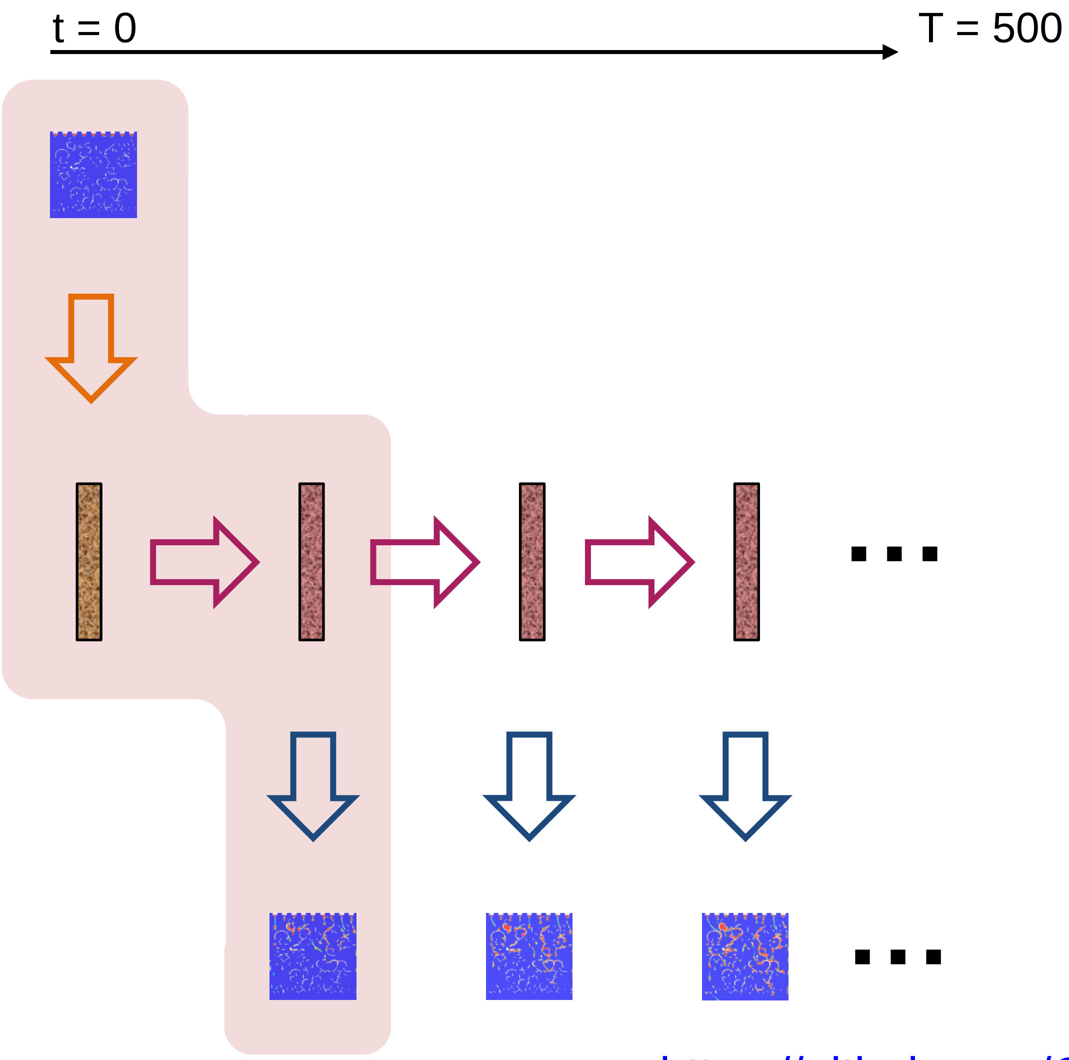


CCSI^2 ML for CFD

	DeeperFluids (DF)	MeshGraphNets+ (MGN)
Representation	 Treats data as an **image** For structured grids	 Treats data as a **graph** For unstructured meshes
Prior work	**Deep Fluids** **[Kim et al., Eurographics 2019]** 	**MeshGraphNets** **[Pfaff et al., ICLR 2021]** 

DeepFluids / DeeperFluids (DF)

During prediction, the ML model uses the first frame to predict subsequent frames.



Input
A single frame

Encoding
The frame is mapped to a feature vector (embedding) in latent space.

Forward Pass
Predict the next embedding.

Decoding
Embeddings are mapped back to the physical space.

https://github.com/CCSI-Toolset/DeeperFluids

arXiv:2112.11656

MeshGraphNets (MGN)

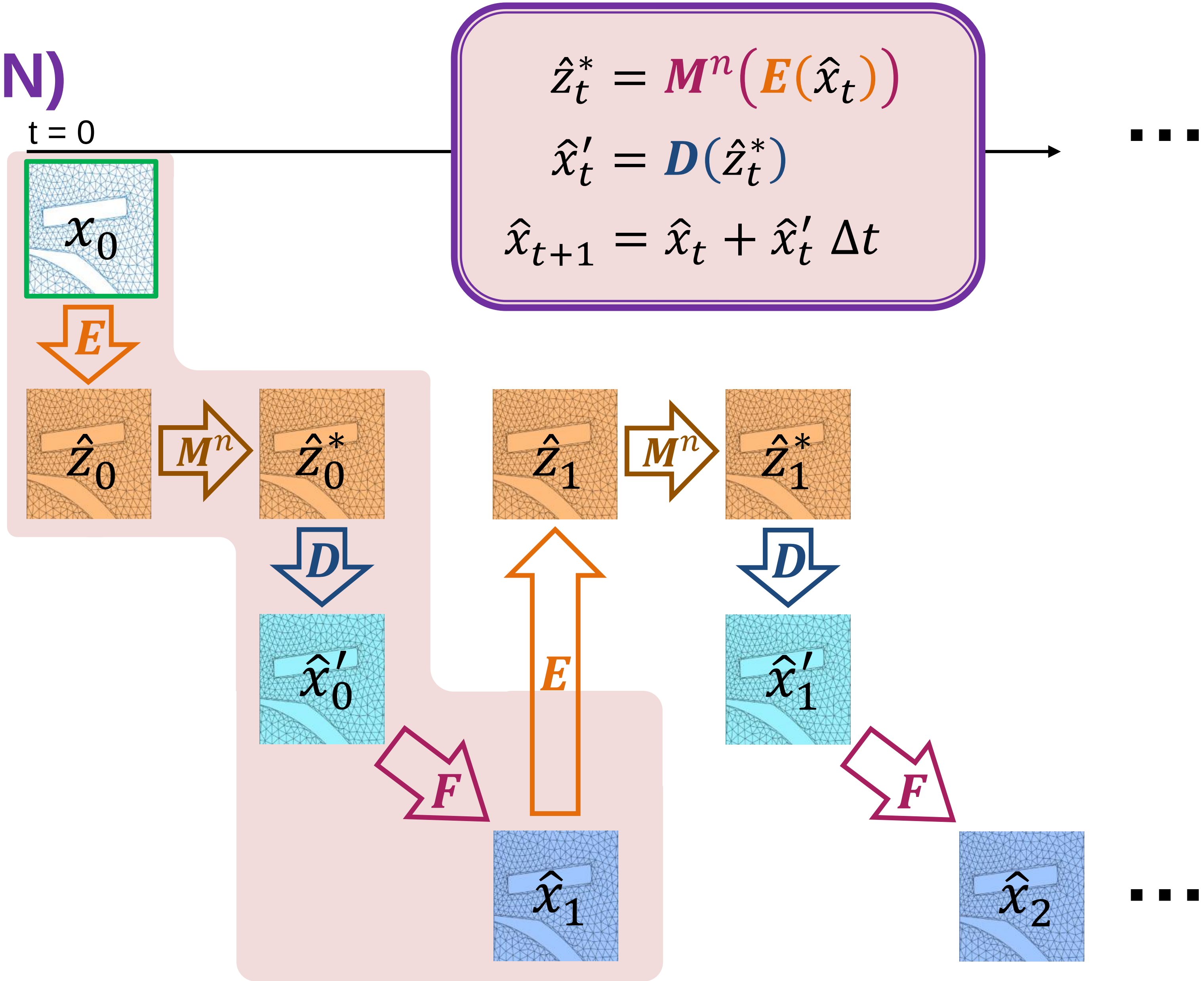
Input
A ***mesh*** within the original frame

Encoding *E*
Each node and edge has its own embedding.

Message Passing *M*
Neighboring edges and nodes exchange info to update embeddings.

Decoding *D*
Updated embeddings are decoded, which represent the gradient in physical space.

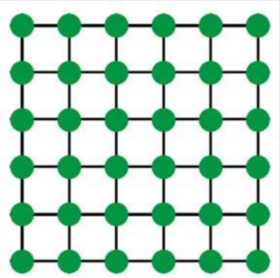
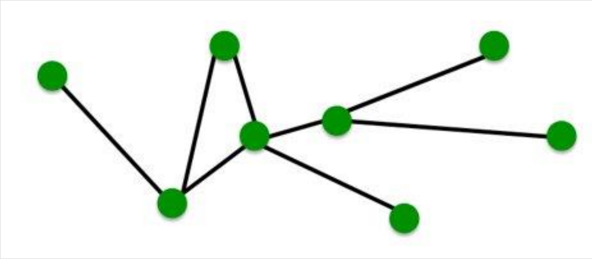
Forward pass *F*
Via forward Euler



https://github.com/CCSI-Toolset/MGN

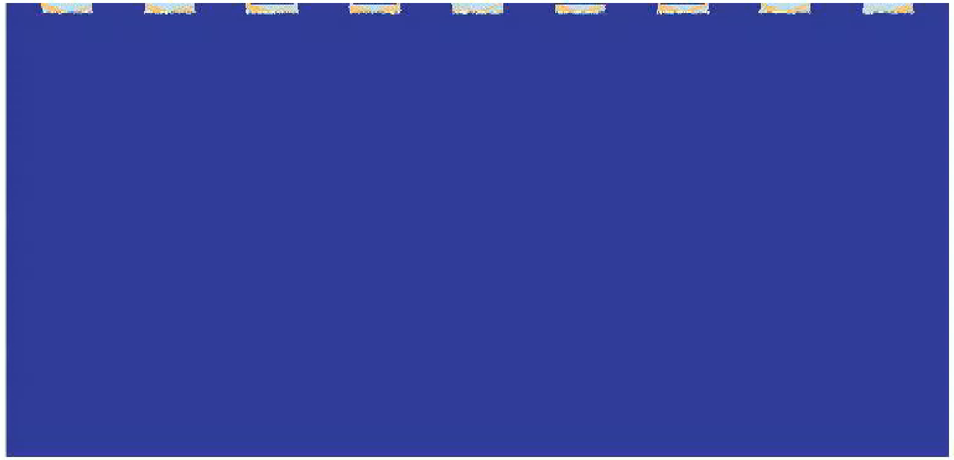
arXiv:2304.00338

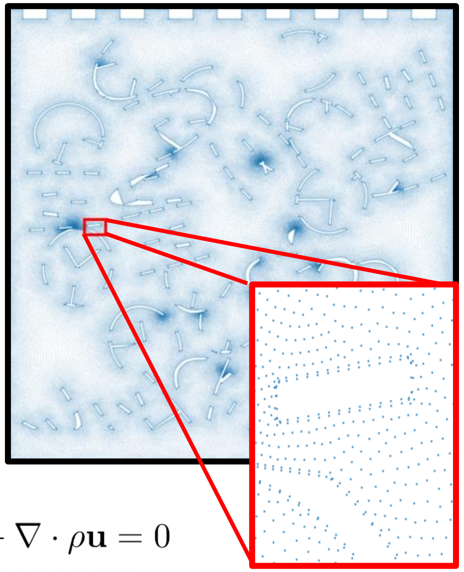
CCSI² ML for CFD

	DeeperFluids (DF)	MeshGraphNets+ (MGN)
Representation	 Treats data as an **image** For structured grids	 Treats data as a **graph** For unstructured meshes
Physics	Physics constraints are **difficult to incorporate** after compression into images and latent spaces. Dynamics is learned within **latent space**.	Node dynamics is learned through interactions with other nodes via **message passing**, making it easier to impose physics constraints. Dynamics is learned within the **physical space**.
Accuracy	DF will be **less accurate** than MGN, but should still be **visually acceptable**.	MGN should yield much higher accuracy, but at the expense of higher computational resources.
Transferability	DF **needs to be retrained** to predict for new meshes/packings.	MGN learns the physics independent of mesh shape and **can transfer well** to new meshes/packings.
Speed-up	DF **favors speed** over accuracy and transferability; up to **5000x faster** than CFD.	MGN **favors accuracy and transferability** over speed; currently up to **200x* faster** than CFD.

2D RCM data

– 2 packing configurations (vertical slice of 3D packing)
  - 50 simulations (different inlet velocities)
  - 500 timesteps
    – Velocity, pressure, volume fraction measurements
  - 150K irregularly spaced points (nodes)

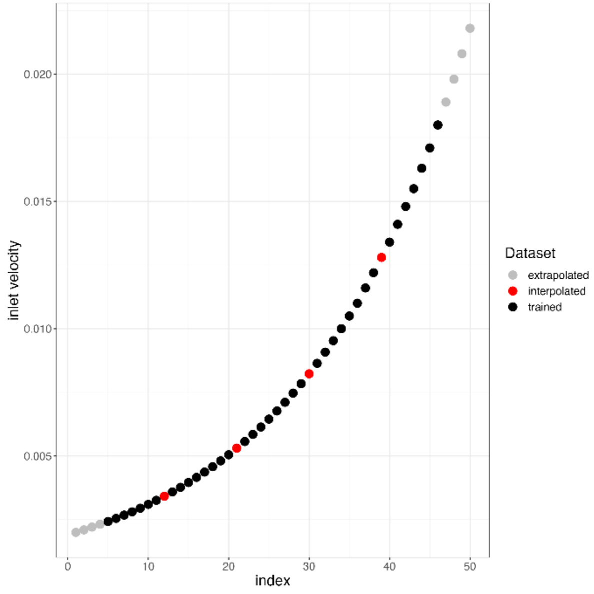




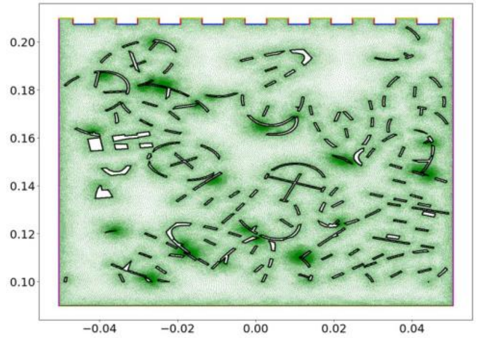
$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = -\nabla p + \mu \nabla^2 \mathbf{u} + \rho \mathbf{g} + \mathbf{F}_\sigma$$

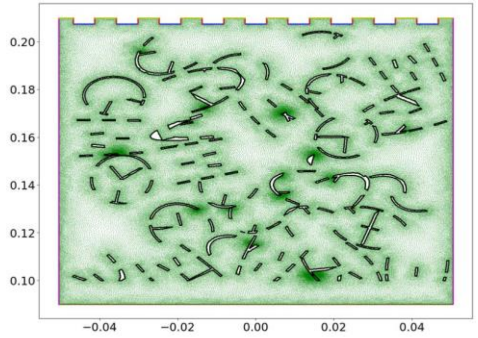
$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\mathbf{u}\alpha) = 0$$



Trained on:



Tested on (MGN only):



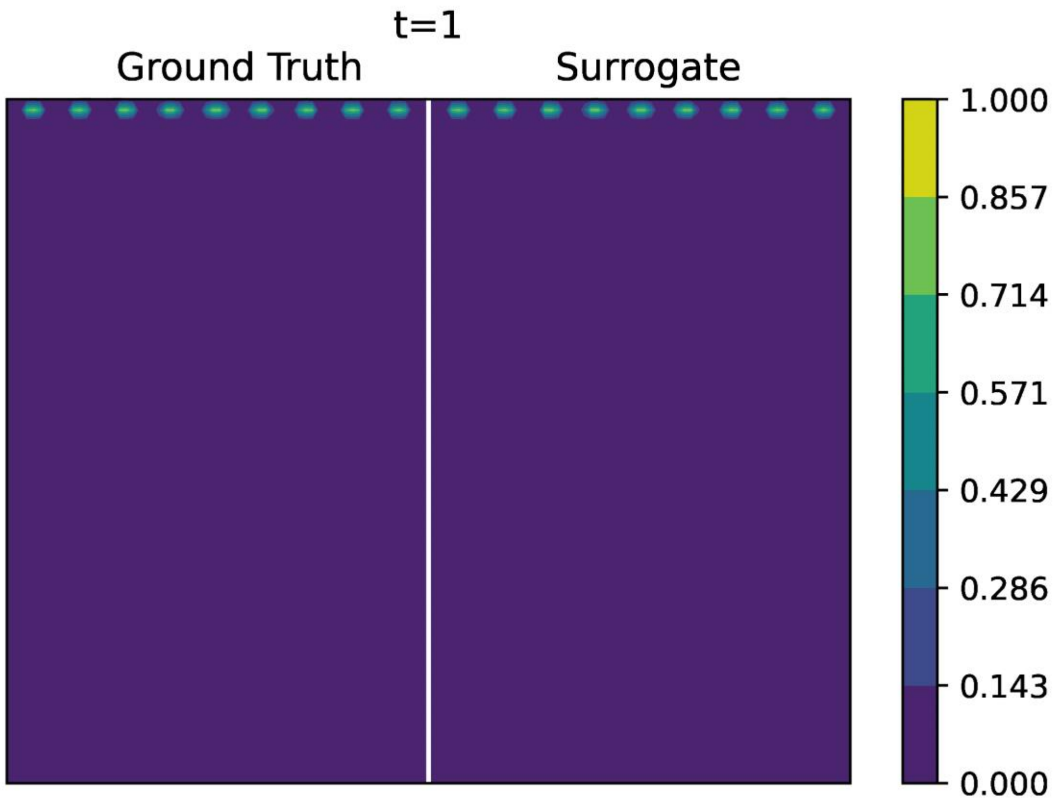
DeeperFluids surrogates

Building on the original surrogates…

H	Error_{IA}					
	w=20	50	150	200	300	499
1024, 512	0.33 (0.14)	0.08 (0.00)	0.09 (0.00)	0.10 (0.00)	0.11 (0.00)	2.53 (0.26)
128, 128, 128	0.64 (0.11)	0.08 (0.01)	0.08 (0.00)	0.07 (0.00)	**0.06** (0.00)	2.25 (0.18)

We find better performance

LIN	s	Error_{IA}		Error_{VF}	
		L_{RE}	RMSE	L_{RE}	RMSE
ARC	1	0.12	0.09	0.53	0.55
	6	0.15	0.14	0.51	0.53
LSTM	1	0.12	0.06	0.56	0.54
	6	0.09	0.09	0.52	0.54
MLP	1	0.07	0.07	0.53	0.55
	6	0.08	0.12	**0.49**	0.52
Transformer	1	0.08	**0.04**	0.53	0.55
	6	0.06	0.22	0.53	0.80

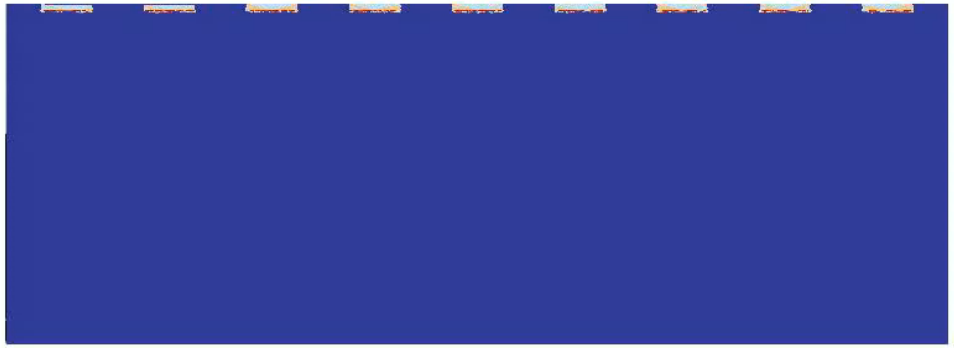


And big speedups!

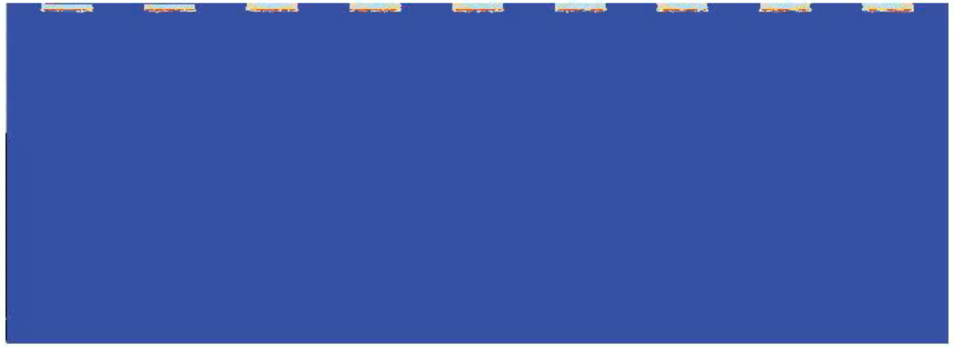
LIN	Error_{IA}	Error_{VF}	S_W
ARC	0.07 (0.00)	0.49 (0.00)	4800
LSTM	0.08 (0.01)	0.49 (0.01)	2700
MLP	**0.06** (0.00)	**0.47** (0.00)	5400
Transformer	0.08 (0.04)	0.51 (0.00)	4300

MeshGraphNets surrogates

Extrapolated velocities + unseen packings



Ground truth, sim 11 (extrapolated velocity, unseen packing)



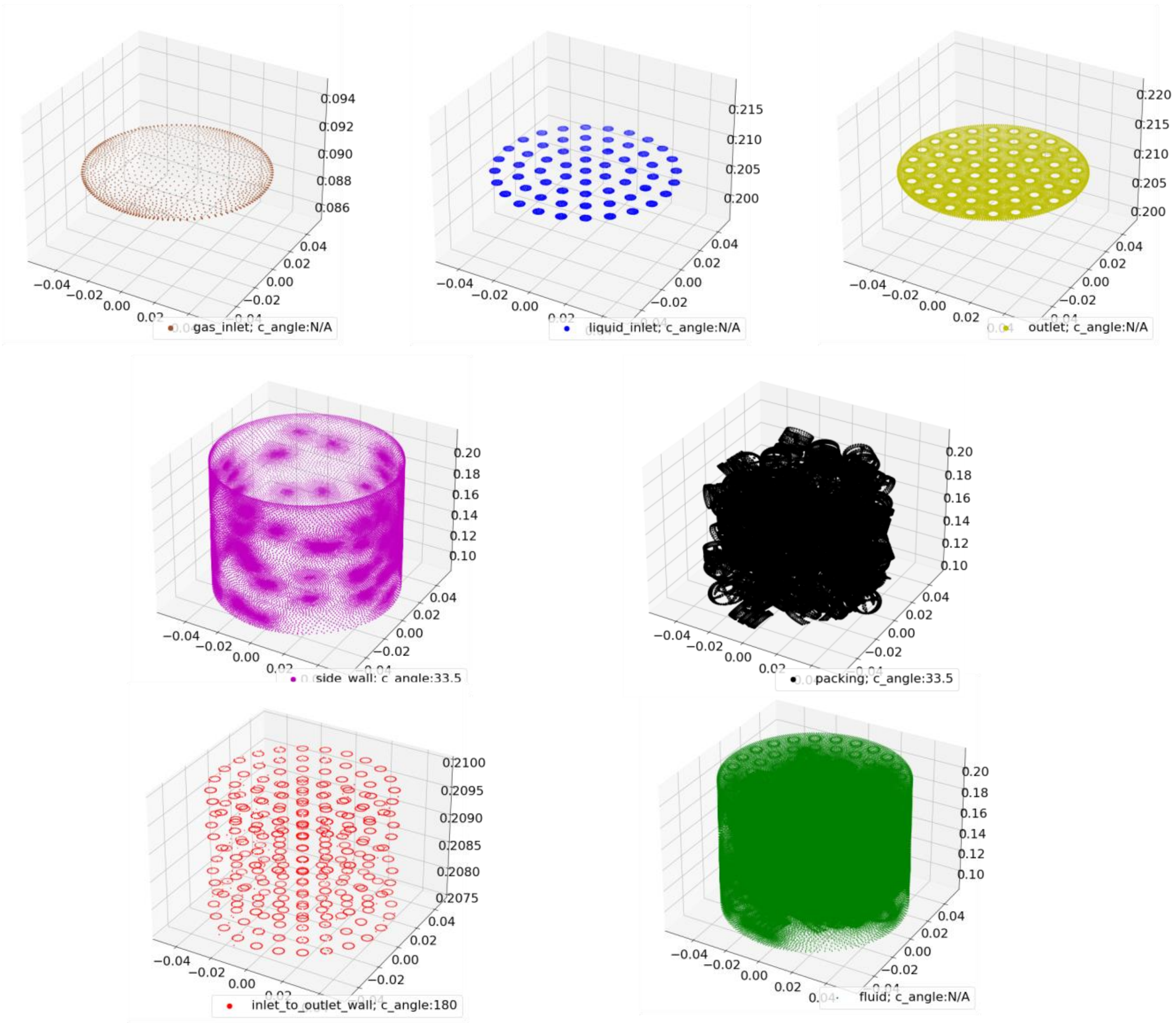
Predicted, sim 11 (extrapolated velocity, unseen packing)

Packing	Velocities	Avg. %-error in IA
Trained	Extrapolated	9.05
Unseen	Trained	5.42
Unseen	Interpolated	2.24
Unseen	Extrapolated	7.79

3D RCM data

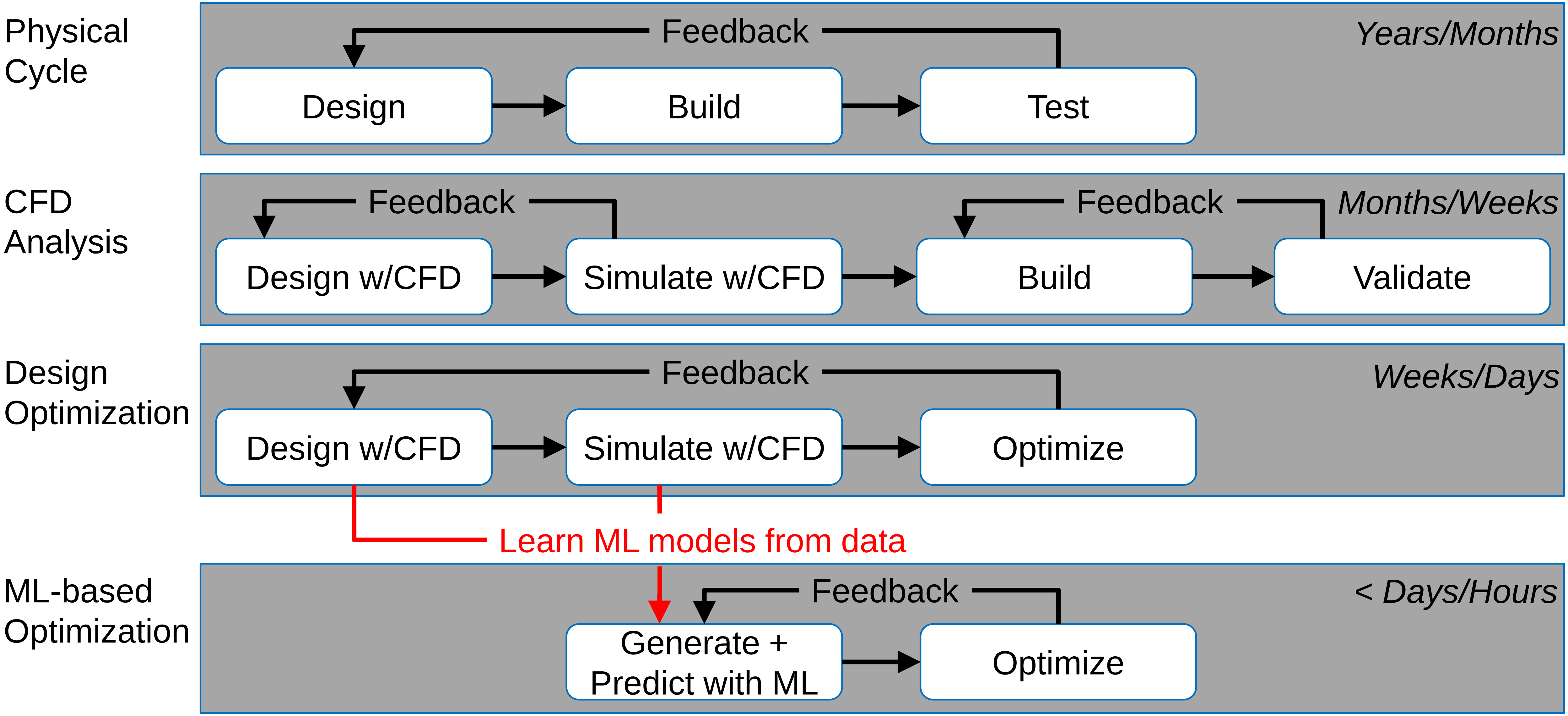
Data:
- 50 simulations
- 500 timesteps
  - Velocity, volume fraction, pressure measurements
- **3.1 million nodes** (vs. 150K in 2D)

- With patch training, higher-order integration and other enhancements, **MGN training is now feasible**
- Current speed-up over CFD: **~150-185x faster** with one V100 GPU
  - Targeting 1000x next



https://data.pnnl.gov/group/nodes/dataset/33472

ML + design optimization



ML for design optimization, TRL progression

- ML can accelerate CCS modeling and validation
  - Use some CFD data to train sufficiently accurate + faster ML surrogates
  - Once trained, replace CFD dependence with ML surrogates
- Multiphysics
  - ML transferability: able to update/fine-tune already-trained models to account for additional physics
- Novel packing configurations
  - MGN able to predict well on unseen packings/meshes
- Scaling up
  - MGN able to work on arbitrary domain/mesh sizes
  - Can update/fine-tune already-trained models to account for scale-up effects

Summary

Process-level optimization is facilitated by machine-learning models trained on detailed CFD simulations — experimentally validated at different scales — capturing the effects of design and operating conditions on the absorption performance for a given solvent.

Components

- Sequential Design of Experiments – see next talk by Abby Nachtsheim
- Experimental prototype performance fabrication and testing
- Process modeling and optimization
- Computational Fluid Dynamics modeling
- Machine Learning

CCSI²

Carbon Capture Simulation for Industry Impact

For more information

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BACKUP SLIDES