Computational Design and Process Intensification of CO_2 Absorbers

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Oak Ridge National Laboratory

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Project Team
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Yash Girish Shah (NETL/Leidos)
Debangsu Bhattacharyya (WVU)

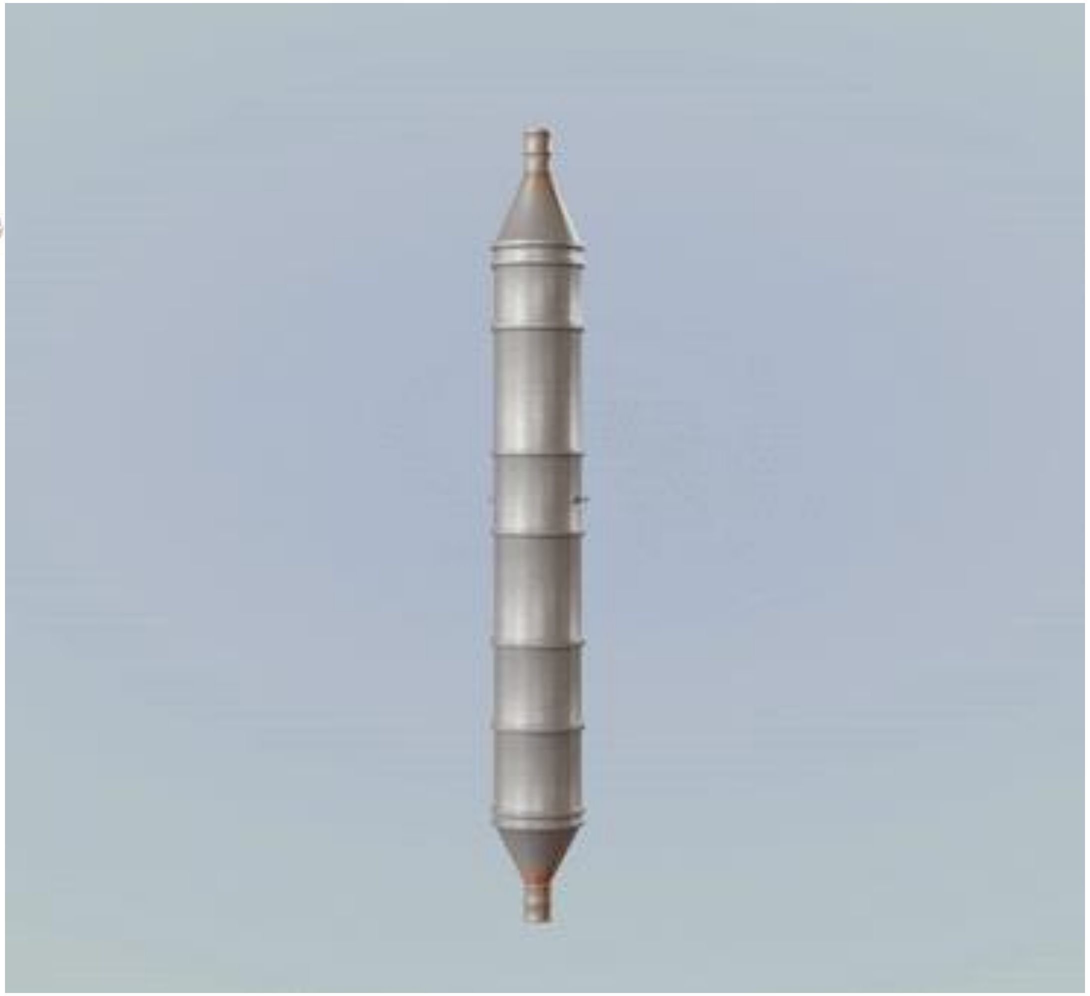
Acknowledgements: Many collaborators across CCSI^2

Project overview

Objective: Design and optimize performance of novel, process-intensifying structured packing specific to solvent characteristics.

Approach: Interface with other CCSI² teams to leverage CCSI² expertise, utilizing **ORNL capabilities** in **additive manufacturing** and existing **experimental infrastructure**.

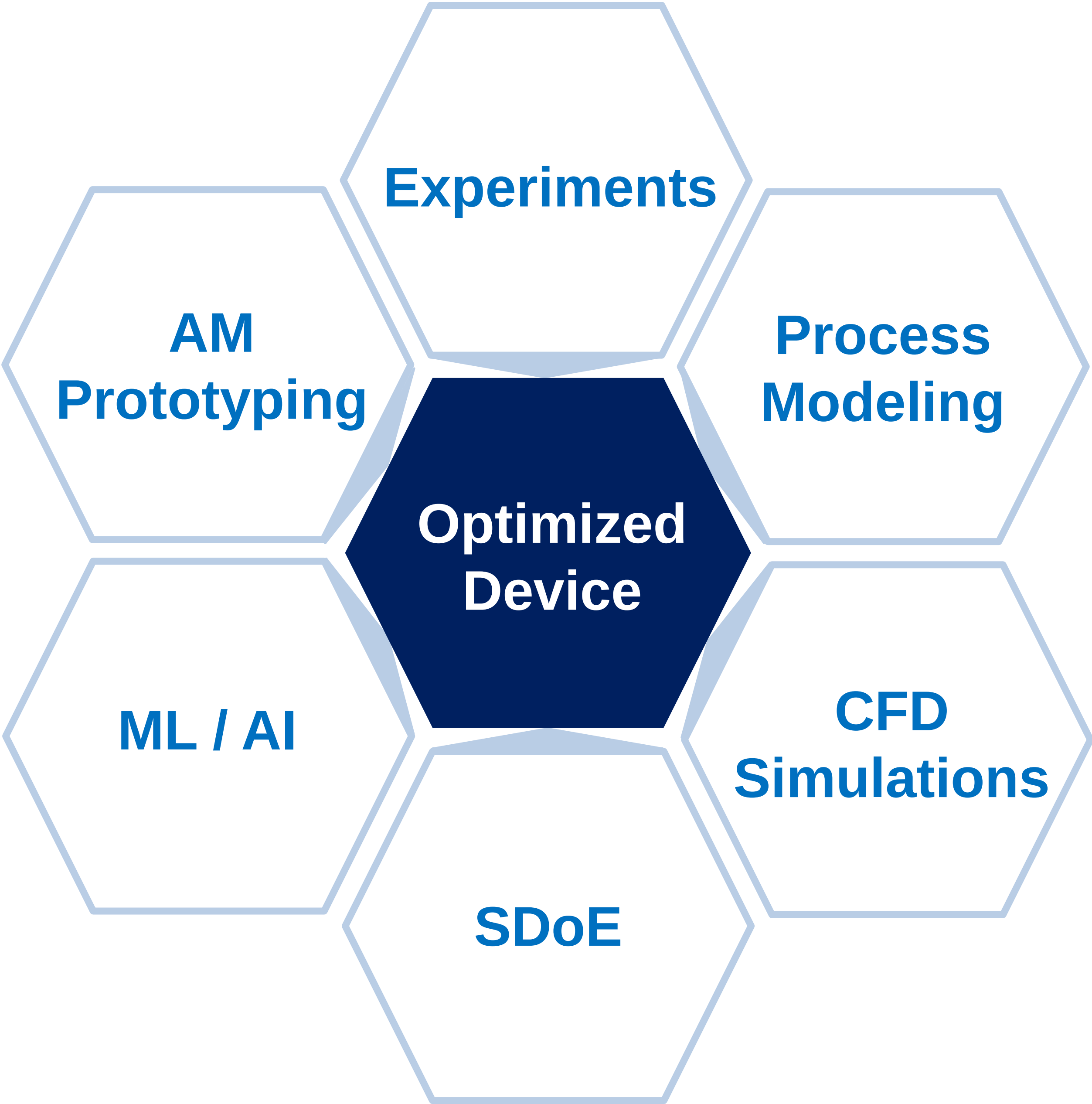
Absorber with intensified device



Commercial packing

The intensified device provides intrastage cooling to maximize capture efficiency ► process intensification

Device optimization relies on many components



EXPERIMENTS

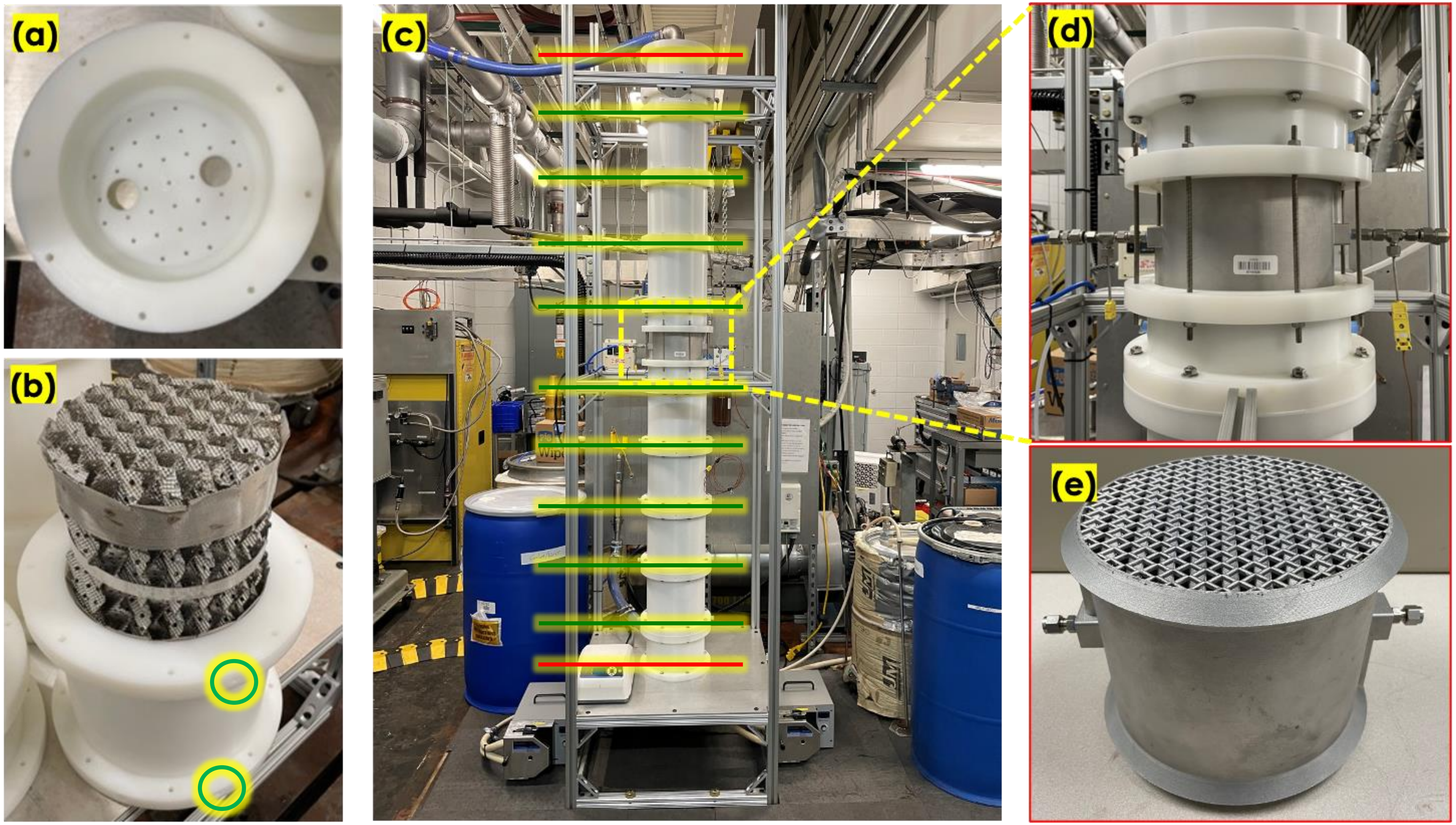
Costas Tsouris, Gyoung Yang,
Josh Thompson, Aimee Jackson

Experimental activities are prepared to maximize utility of performance data for CFD model validation and candidate geometry evaluation

- **Enhancement of existing 8-inch column for finer-grained measurements**
  - Each flange has 4 ports for column performance measurements
  - Improved characterization of *operando* solvent properties (e.g., CO_2 concentration, amine concentration, water content, etc.)

- **Designed reduced-size test section for more rapid simulations and experimental testing and prototyping**

The 8-inch column has fine-grained measurement points



8-inch column at ORNL
(Column A)

Existing measurement points

Added measurement points

a) HDPE solvent distributor
b) Commercial stainless-steel packing element with HDPE outer wall module
c) CO_2 absorption column setup
d) Installed intensified device
e) 3D printed intensified packing device

CCSI²
Carbon Capture Simulation for Industry Impact

Performance data tools for model validation and candidate packing geometry evaluation are in place

Current measurement variables

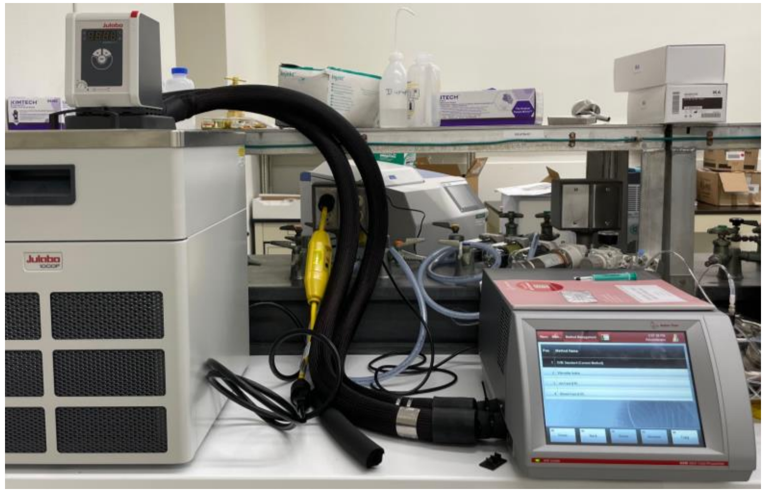
On the column

- Pressure
- Temperature
- Gas flow rate & CO_2 concentration
- Solvent flow rate [column top & bottom]

In the lab

- Solvent CO_2 concentration
- Solvent density
- Solvent viscosity
- Solvent water content
- Solvent amine concentration
- Solvent–solid surface contact angle

Instruments for solvent contact-angle and density/viscosity measurements



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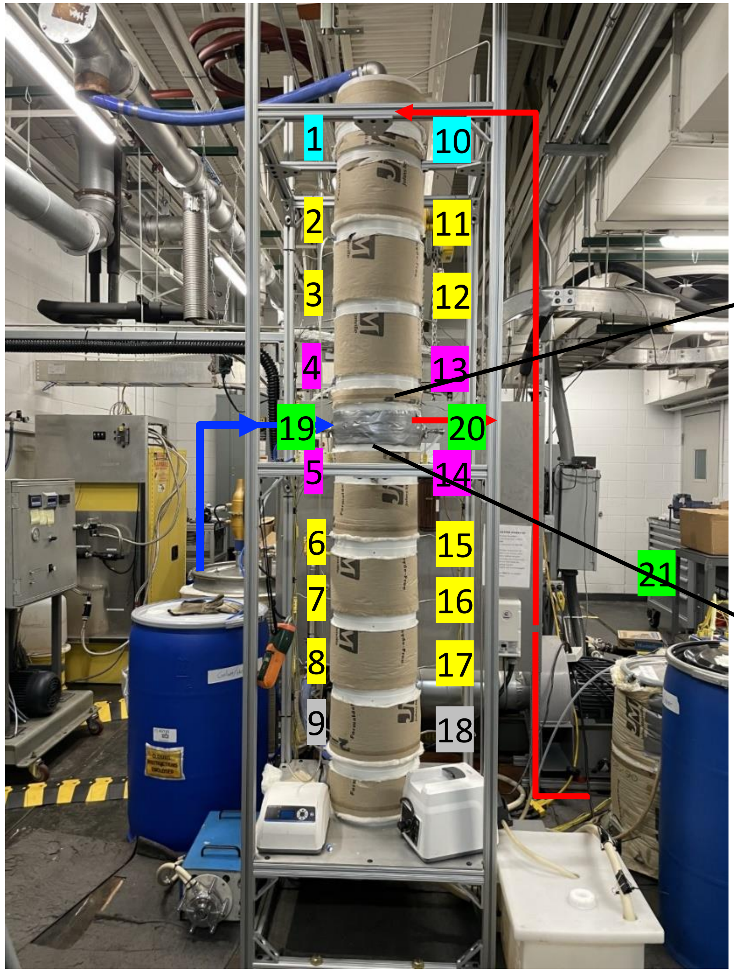
Heat-transfer experiments were conducted to evaluate two intensified device geometries



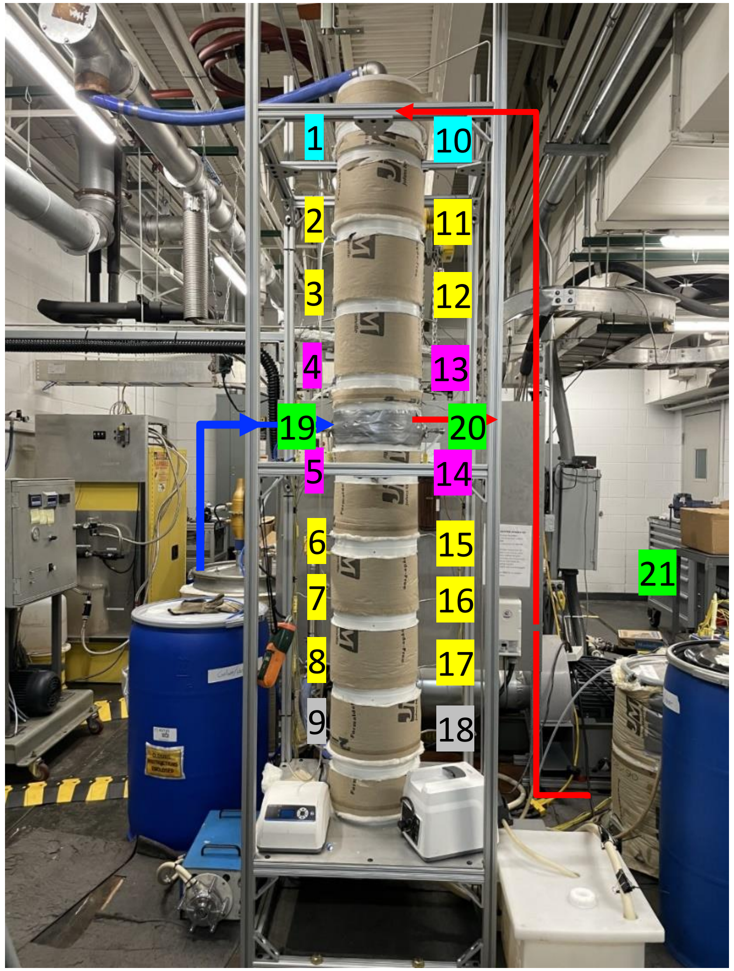
Experiments with the 8-inch diameter Column A

►Measured pressure drop, holdup, and residence time distribution of the solvent using intensified devices

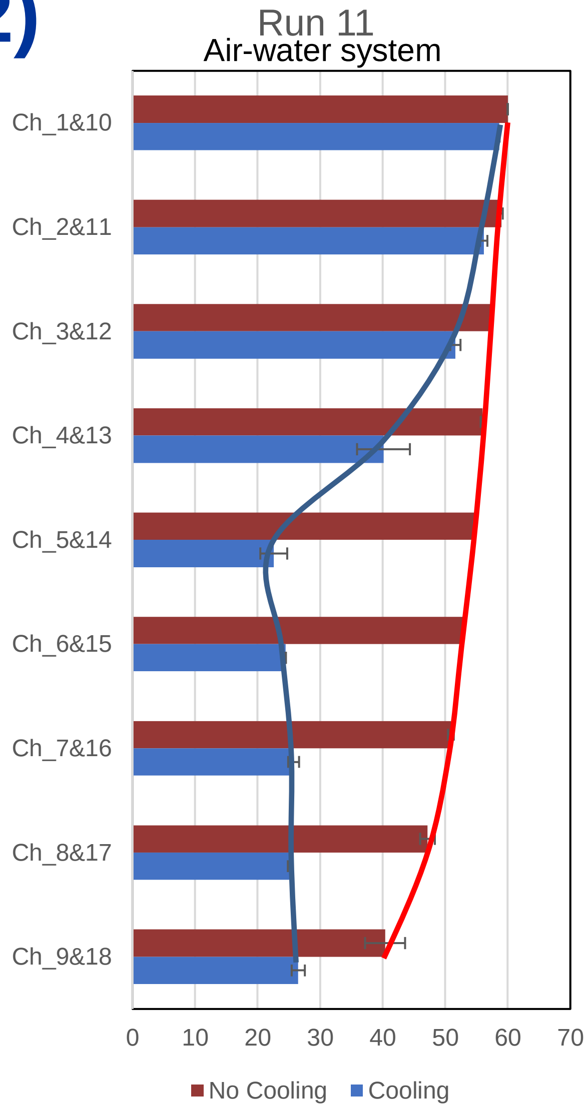
Absorber column performance (1/2)

D=8” H=6.75” device for Column A (left) and D=12” H=16” device for Column B (right)

[FEAA384]



Heat-transfer experiments using Column A



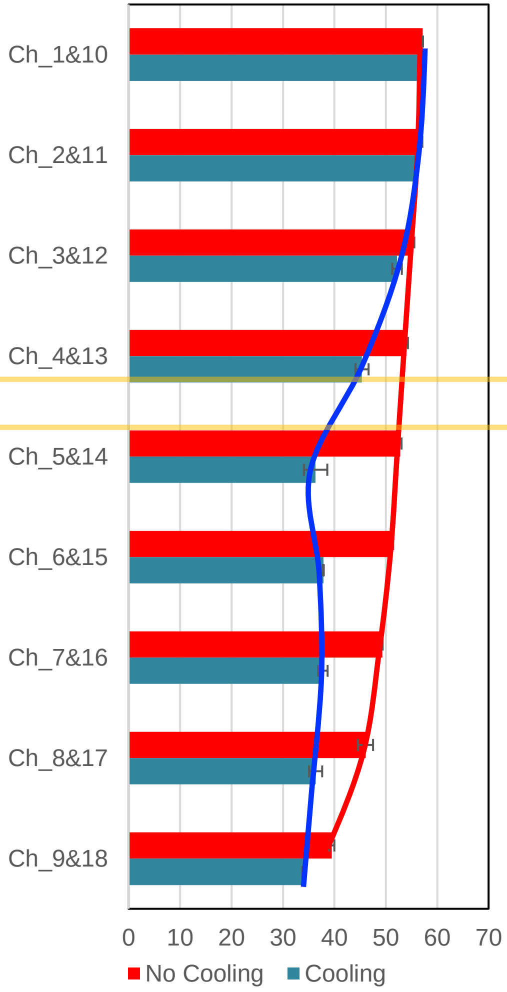
Temperature profiles

[AMO-funded]

Absorber column performance (2/2)

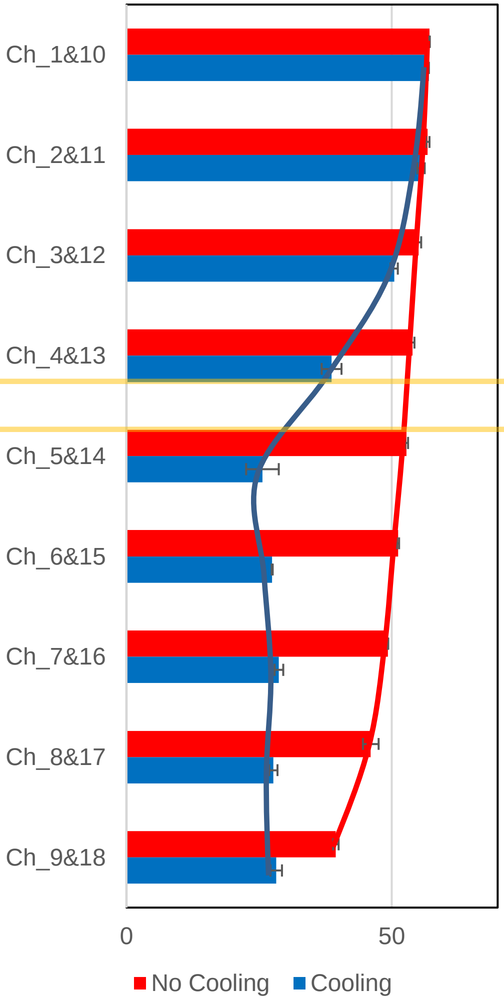
Coolant: 0.96 LPM, 15.6 °C

Run 14



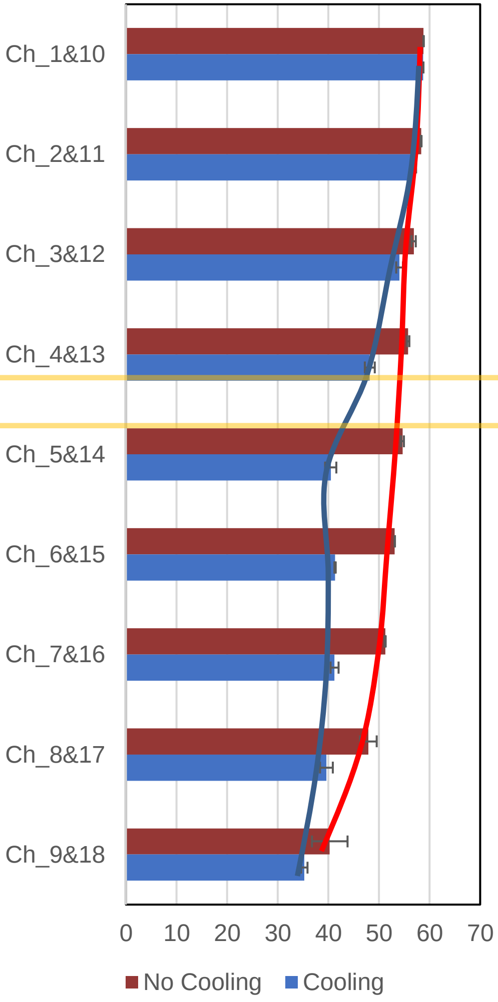
Coolant: 2.25 LPM, 15.8 °C

Run 15



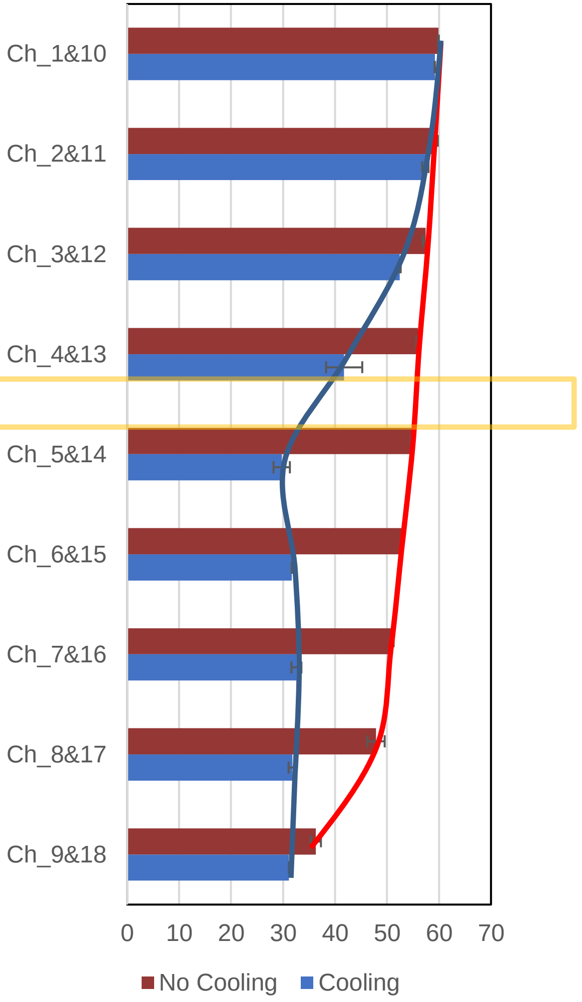
Coolant: 0.96 LPM, 21.1 ° C

Run 12



Coolant: 2.25 LPM, 21.5 °C

Run 13

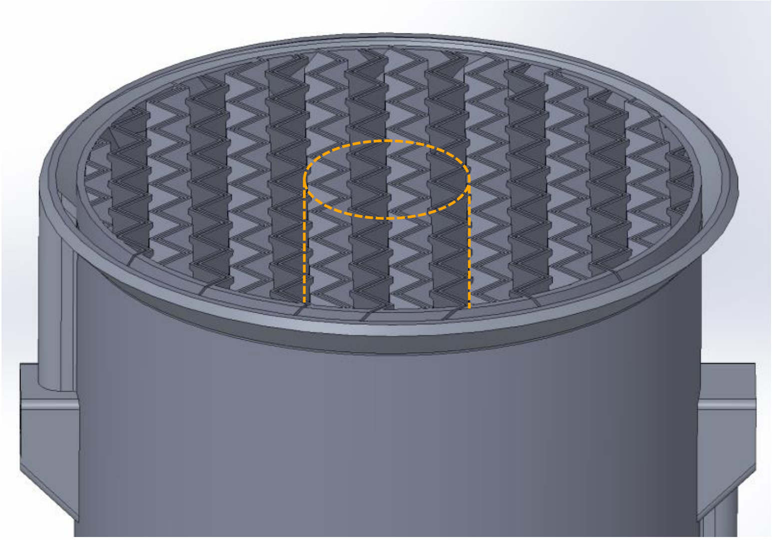


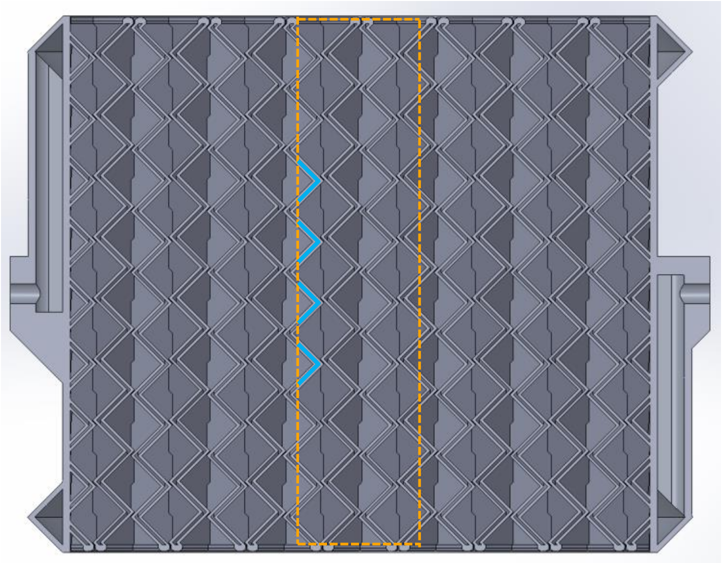
CCSI[2] Carbon Capture Simulation for Industry Impact

Future R&D Plan and Challenges

- Provide ground proof for iterative, progressive route to scale up absorber columns using commercially relevant and model-improved packing geometries
- Provide platform for computationally tractable validation data and rapid printed prototype testing

Perspective (L) and center-plane cut (R) views of 8” diameter section, with virtual CFD domain cut out [orange cylinder]





<u>Virtual</u>, reduced-size test section problems

- **Boundary flows** — handling boundary fluxes can cause numerical problems (solution stability)
- **Boundary conditions** — unknown spatial variations will be difficult to account for

<u>Physical</u>, reduced-size test section benefits

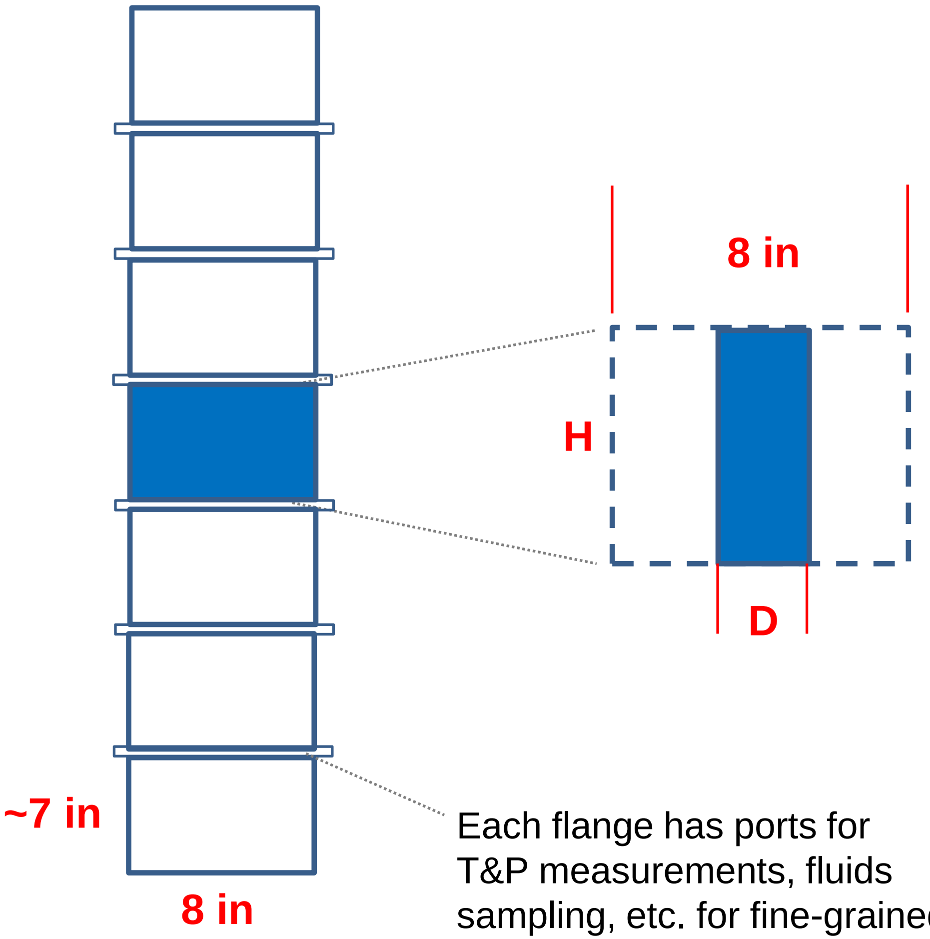
- **Exact validation target** — physical walls part of the simulation
- **Experimental operation ease** — less flow required
- **Tractable computational problem** — can run many tuning iterations using available resources in the limited time available

CCSI 2 Carbon Capture Simulation for Industry Impact

Later simulations will be run on larger sizes to discount wall effects

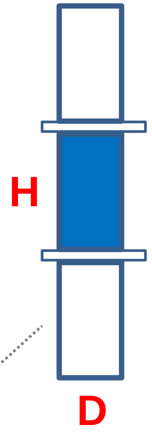
Options for reduced-size test sections (1/2)

Option 1: New section in Column A



Each flange has ports for T&P measurements, fluids sampling, etc. for fine-grained validation data.

Option 2: New benchtop column



Currently, **D = 2** inches is favored by the CFD team.

Sections can have nonequal heights etc.

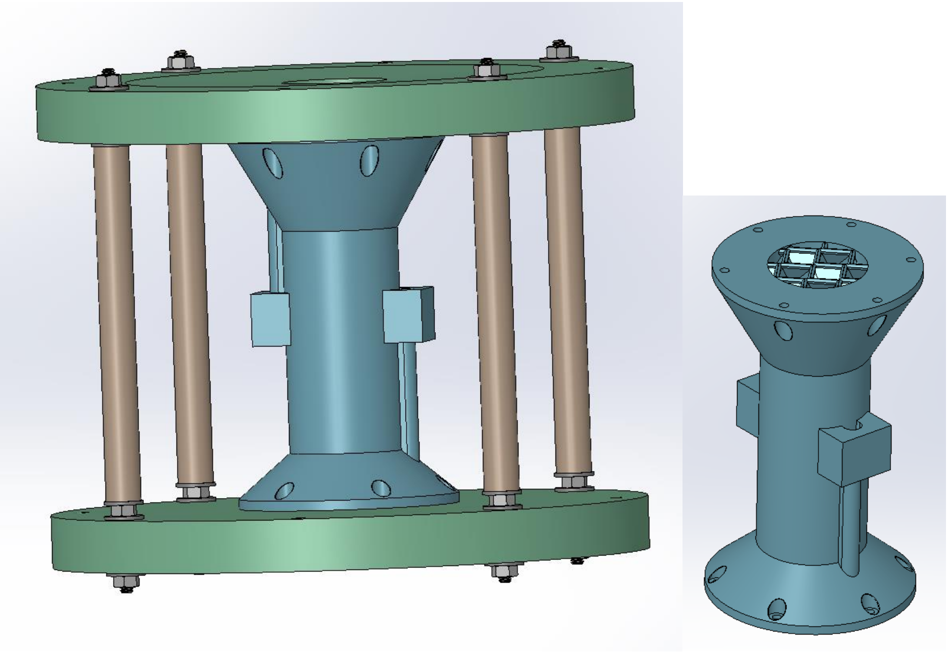
Printing can allow fine control of surface roughness for potential interfacial area improvement

Flows would be adjusted to compensate for different cross-sectional areas compared with the 8-inch column.

CCSI^2 Carbon Capture Simulation for Industry Impact

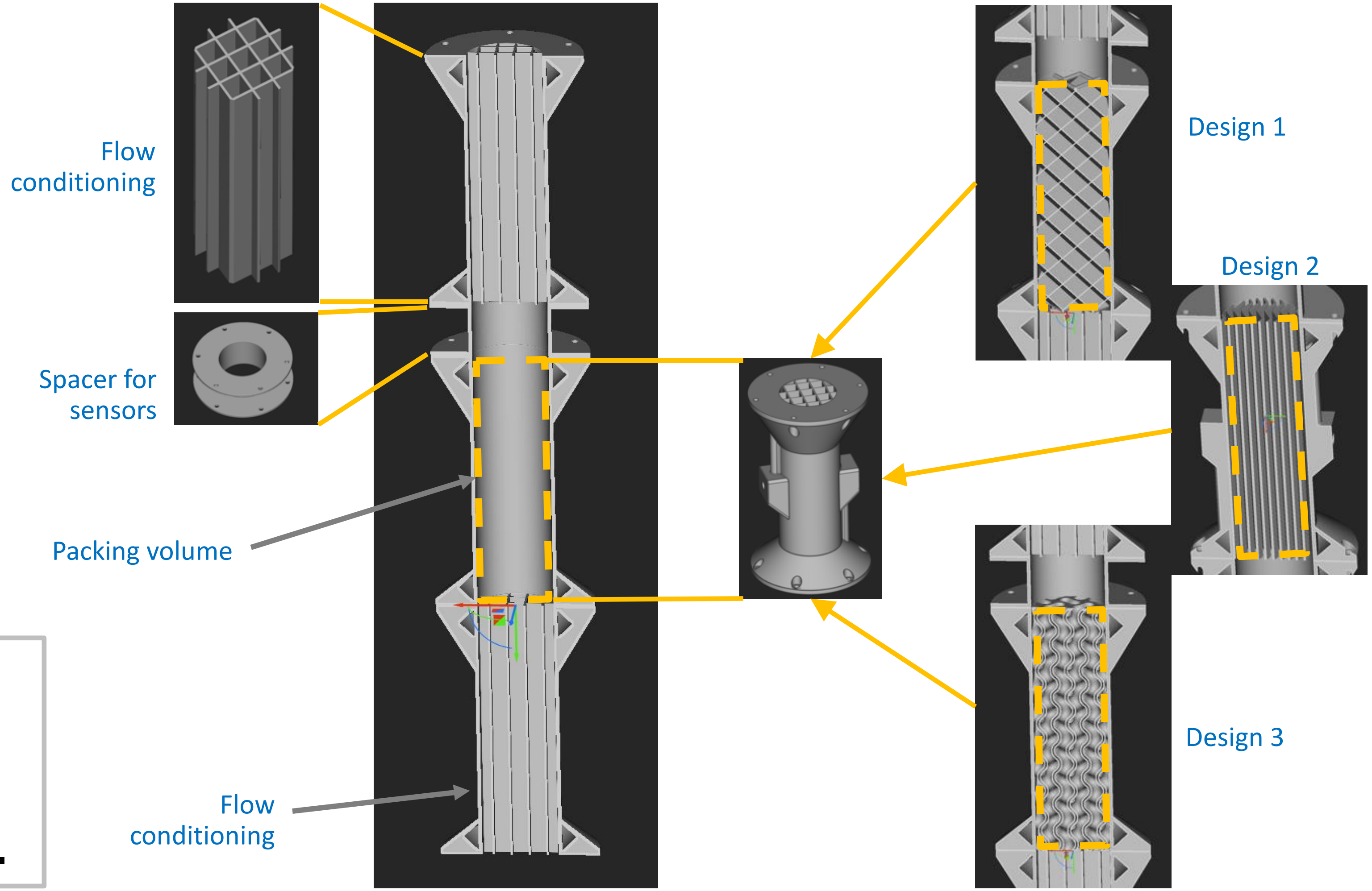
Options for reduced-size test sections (2/2)

Option 1



- ❖ A reduced-size test section will be printed this year.
- ❖ **Validation data will be measured and transferred to the CFD team.**

Option 2



CCSI²

Carbon Capture Simulation for Industry Impact

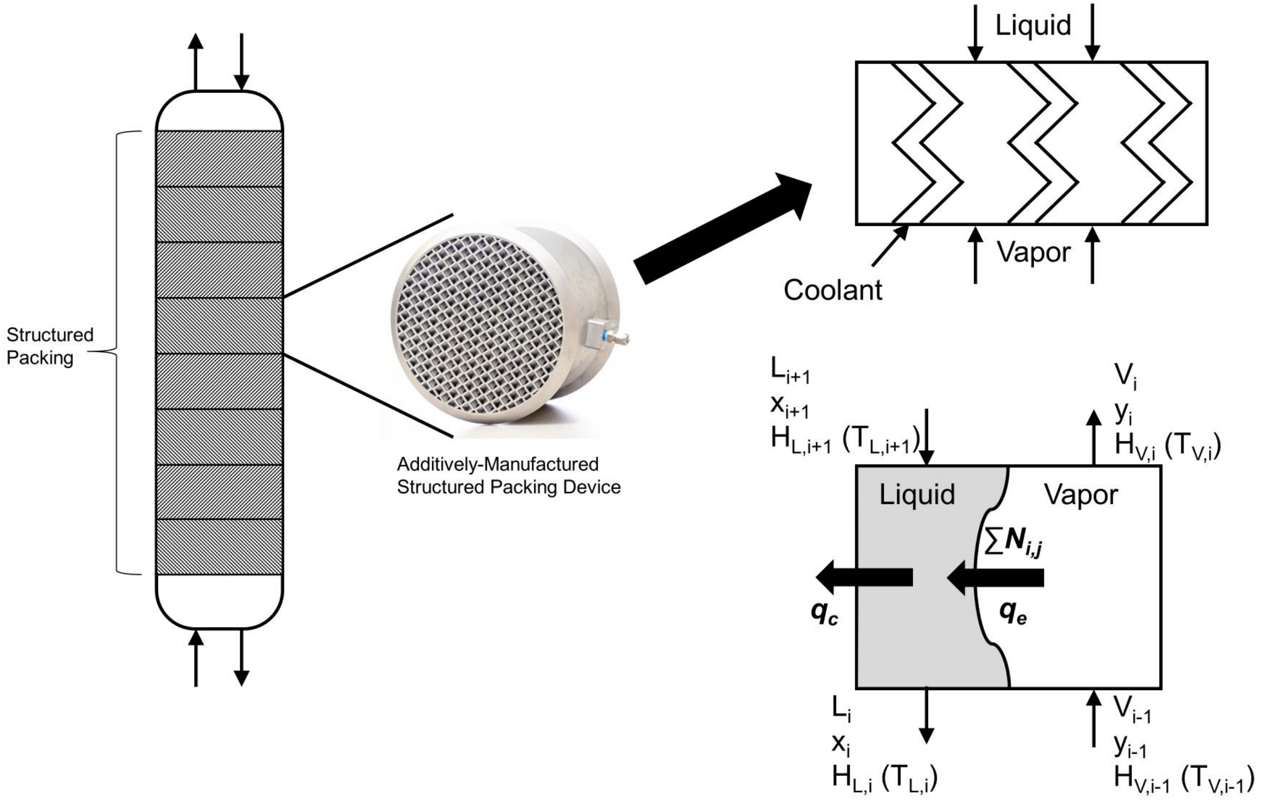
MODELING

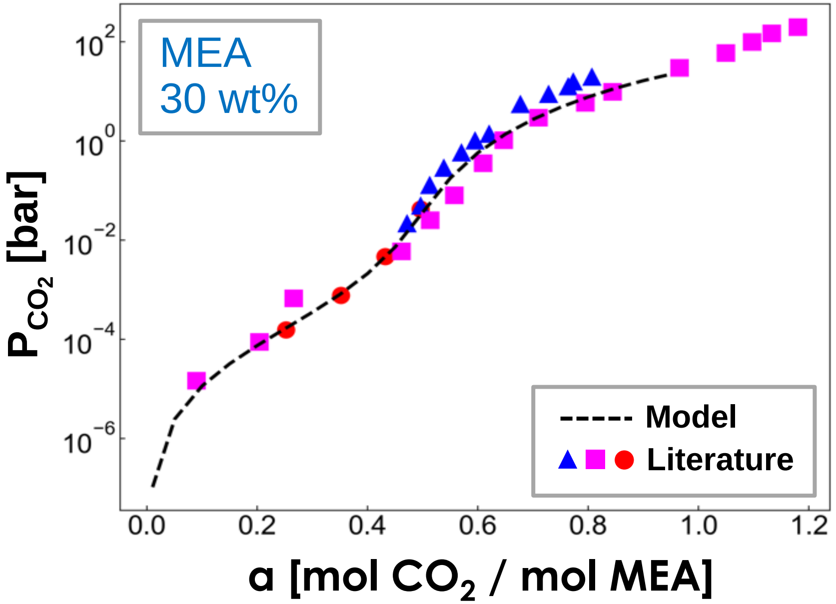
System-level modeling, with detailed intensified absorber dynamics, to plan & guide future validation experiments

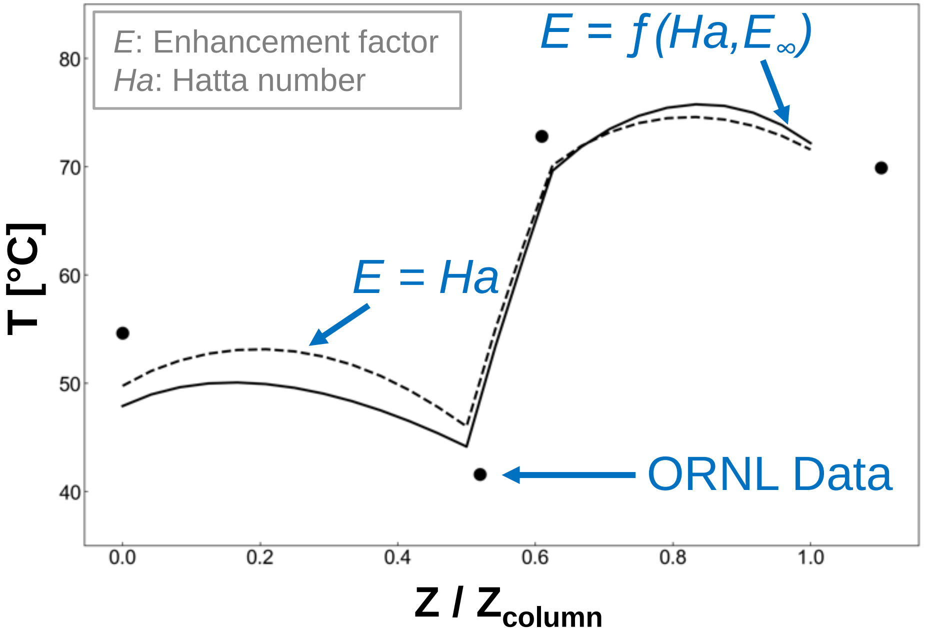
Josh Thompson (ORNL)

System-level modeling framework for design and planning

- Used to design ORNL 12” column [FEAA384] and plan experiments for ORNL 8” column [CCSI[2]].
- **Leveraging to prepare for CCSI² experiments to support CFD validation.**







CCSI² Carbon Capture Simulation for Industry Impact

Thompson, Tsouris (2021). Rate-based absorption modeling for post-combustion CO_2 capture with additively manufactured structured packing. *Industrial & Engineering Chemistry Research* **60**(41): 14845–14855. DOI:10.1021/acs.iecr.1c02756

Comparison of two intensified devices

		Device 1	Device 2
Wall thickness	mm	0.733	0.733
Surface area	m^2	**2.132** (100%)	**1.577** (74%)
Coolant volume	L	**0.784**	**0.539**
Channel area	mm^2	**4408**	**3030**

Device #1 **Device #2**

Experimental conditions

- Gas flowrate from 400–700 LPM
- Liquid flowrate from 2.34–4.49 LPM
- Coolant flowrate from 0.96–2.25 LPM
- Liquid Temp from 50–70 °C
- Coolant temp from 7–22 °C

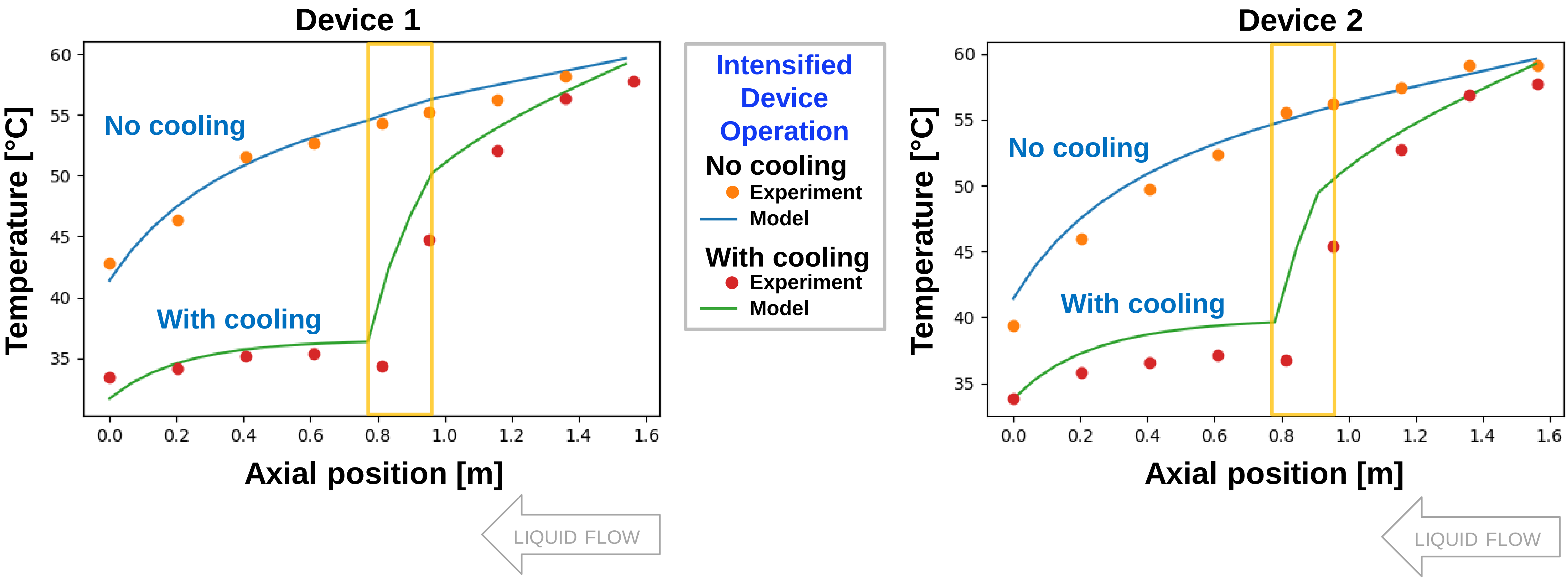
Modeling assumptions

- No reactions taking place – only air and water
- Temperature changes based entirely on enthalpy models of H_2O and air
- MEA modeling correlations and heat and mass transfer equations used

CCSI^2
Carbon Capture Simulation for Industry Impact

Devices and HT experiments: AMO
Model validation runs: CCSI^2

Model captures device heat-transfer performance



Experimental data from heat-transfer experiments shown above.
Column contains normal Mellapak™ 250.Y sections with different intensified devices (gold boxes).

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MODELING

Incorporation of MEA-property models from IDAES code into CFD simulation frameworks

Zachary Mills (ORNL) (OpenFOAM) and Yash Shah (NETL/Leidos) (ANSYS Fluent)
In consultation with WVU

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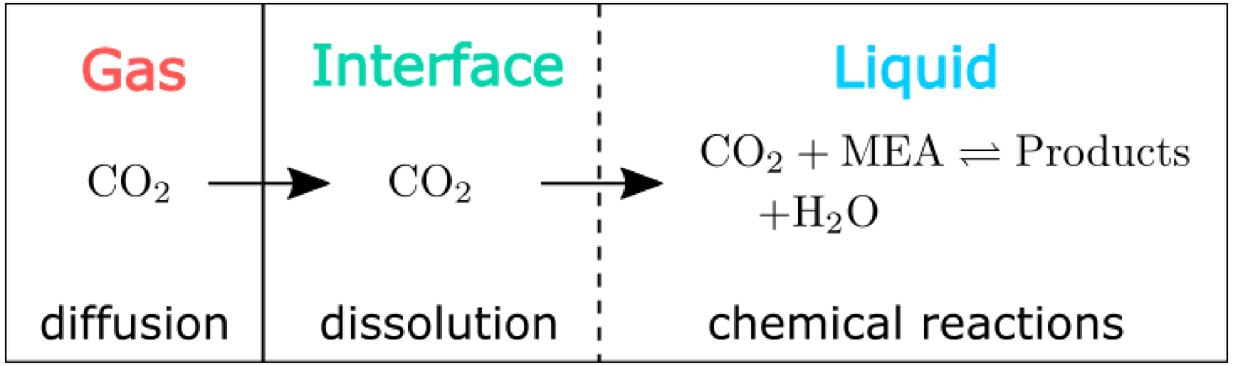
MEA mass transfer and thermochemical model

Mass Transfer model:

- Interface assumed at equilibrium
- Henry's law: $\frac{c_l}{c_g} = He$
- Reactions considered within the bulk liquid



Thermochemical properties:

- Ideal gas property models for the gas phase
- MEA solvent properties extracted from the IDAES package
- Solvent reaction kinetics modeled using a two-reaction mechanism*:

$$\mathbf{2MEA + CO_2 \rightleftharpoons MEAH^+ + MEACOO^-}$$

$$\mathbf{MEA + CO_2 + H_2O \rightleftharpoons HCO_3^- + MEAH^+}$$

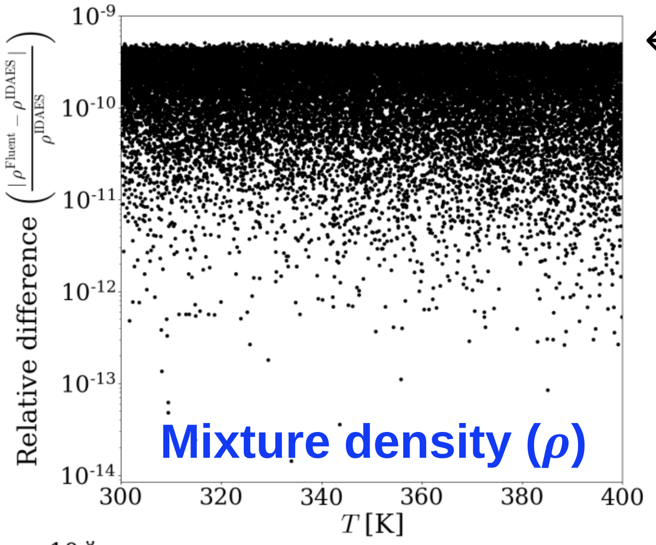
IDAES
Institute for the Design of Advanced Energy Systems

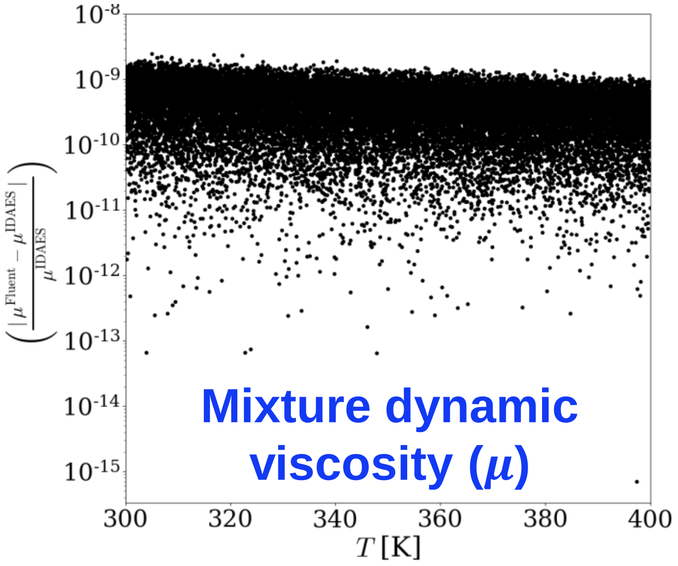
https://idaes.org/
https://github.com/IDAES/idaes-pse

CCSI2
Carbon Capture Simulation for Industry Impact

* Plaza, Van Wagener, Rochelle (2009). Modeling CO_2 capture with aqueous monoethanolamine. *Energy Procedia* **1**(1): 1171–1178. DOI: 10.1016/j.egypro.2009.01.154

IDAES property package for MEA imported into ANSYS Fluent





← Imported properties were verified to **correspond exactly** across the two frameworks (IDAES and Fluent; also, IDAES and OpenFOAM).

Properties and models incorporated include:

- **Instantaneous apparent/true species conversions**
- **Liquid-phase properties**:
  - Mixture density
  - Mixture viscosity
  - Mixture thermal conductivity
  - Mixture specific heat
  - Species diffusivities
- **Vapor-phase properties**:
  - Mixture density
  - Species & mixture viscosities
  - Species & mixture thermal conductivities
  - Species & mixture specific heats
  - Species diffusivities
- **Surface tension** (temperature & composition dependent)
- **Mass transfer** (liquid/gas) using Henry's law
- **Reaction kinetics** (MEA–H_2O–CO_2 two-reaction mechanism)

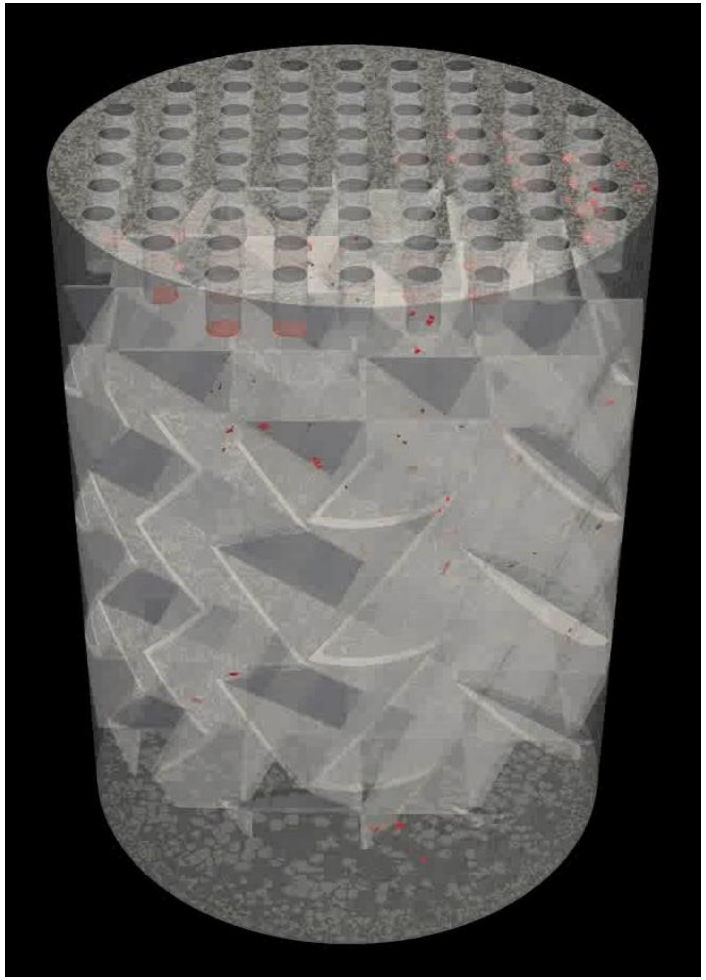
CCSI^2
Carbon Capture Simulation for Industry Impact

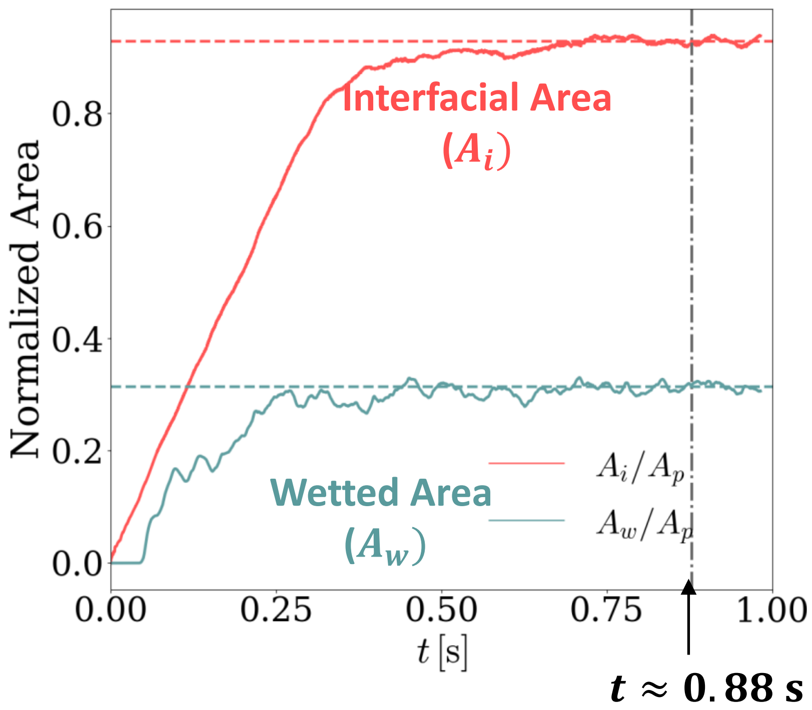
MODELING

CFD simulations with solvent thermochemical dynamics in new Volume of Fluids model of solvent layer in absorber device

Yash Shah (NETL/Leidos) (ANSYS Fluent) and Zachary Mills (ORNL) (OpenFOAM)
Simulations and visualizations shown here: Yash Shah

Simulation results: Interfacial and wetted areas



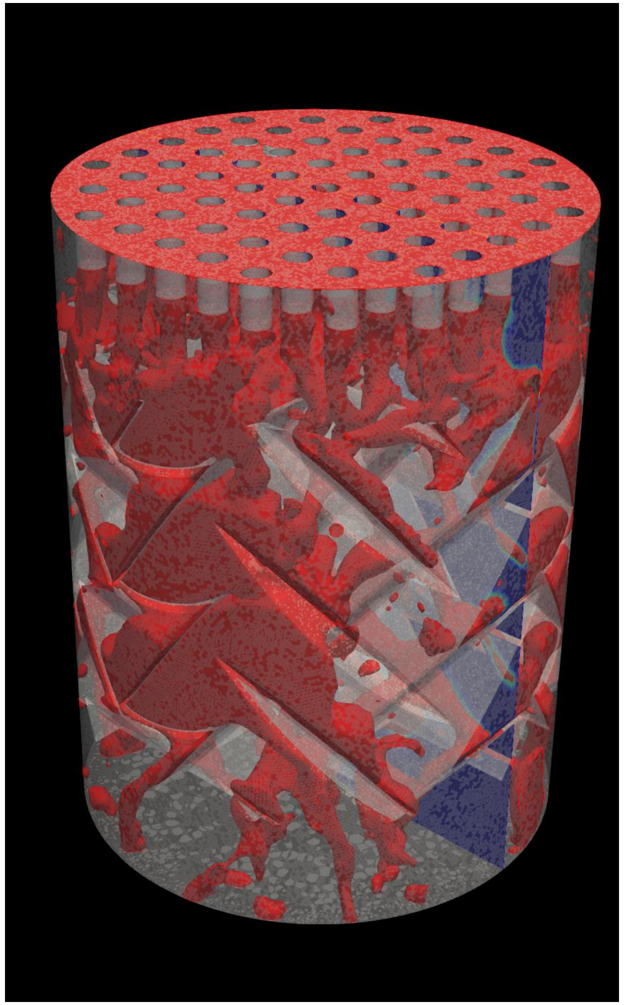


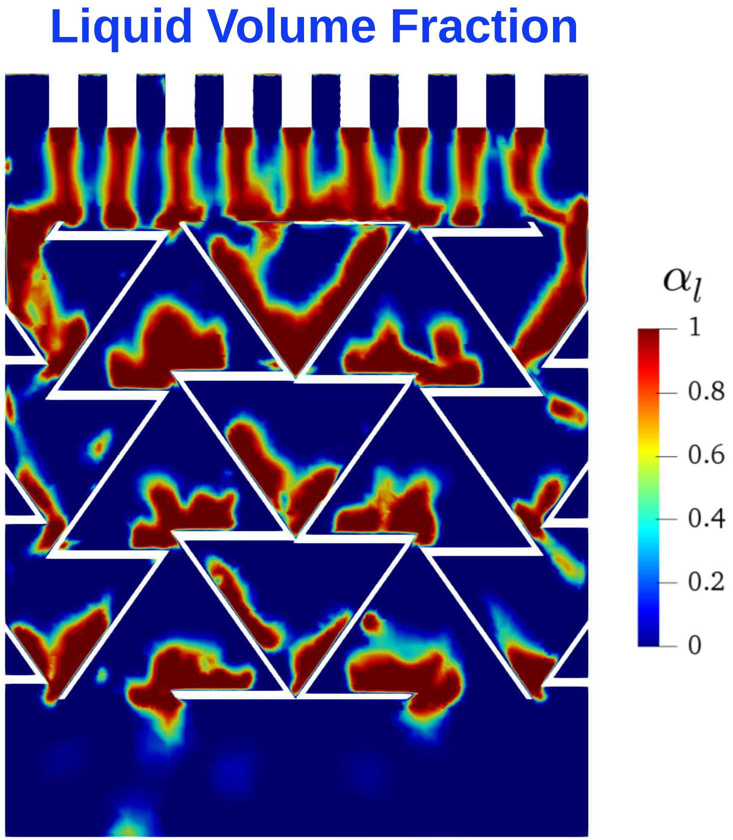
- Normalized interfacial area at pseudo-steady state: 0.928
- Normalized wetted area at pseudo-steady state: 0.314
- $(\Delta p)_{dry} = 4.754\ Pa$ calculated using a separate single-phase CFD simulation

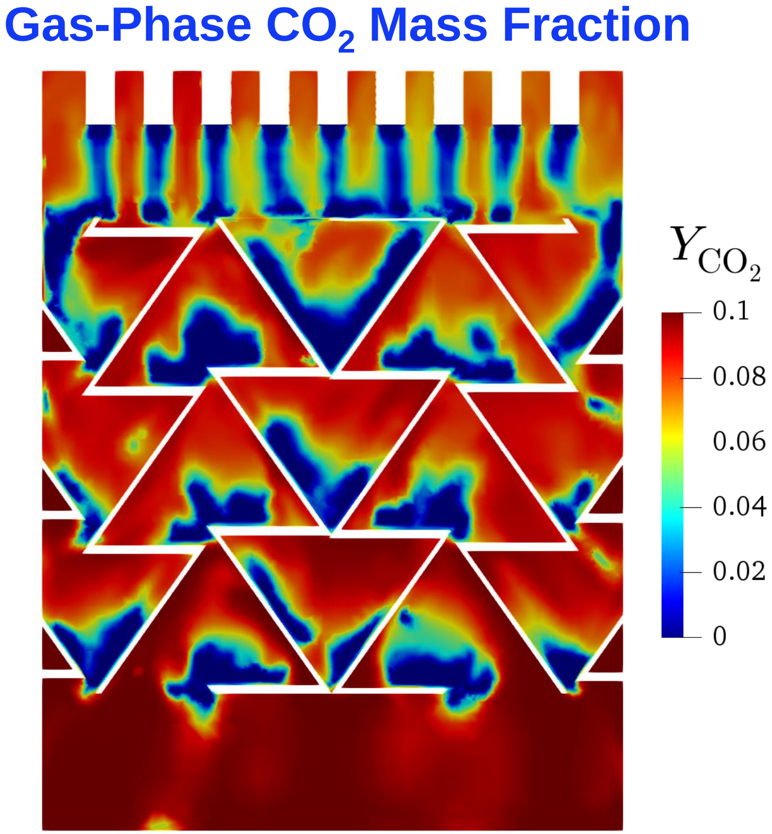
⇒Interfacial and wetted areas approach steady-state near $t = 0.88$ seconds

⇒Physical mass transfer and reaction rate kinetics were enabled after $t = 0.88$ seconds and continued for another 0.1 seconds

Simulation results: solvent and gas-phase distributions







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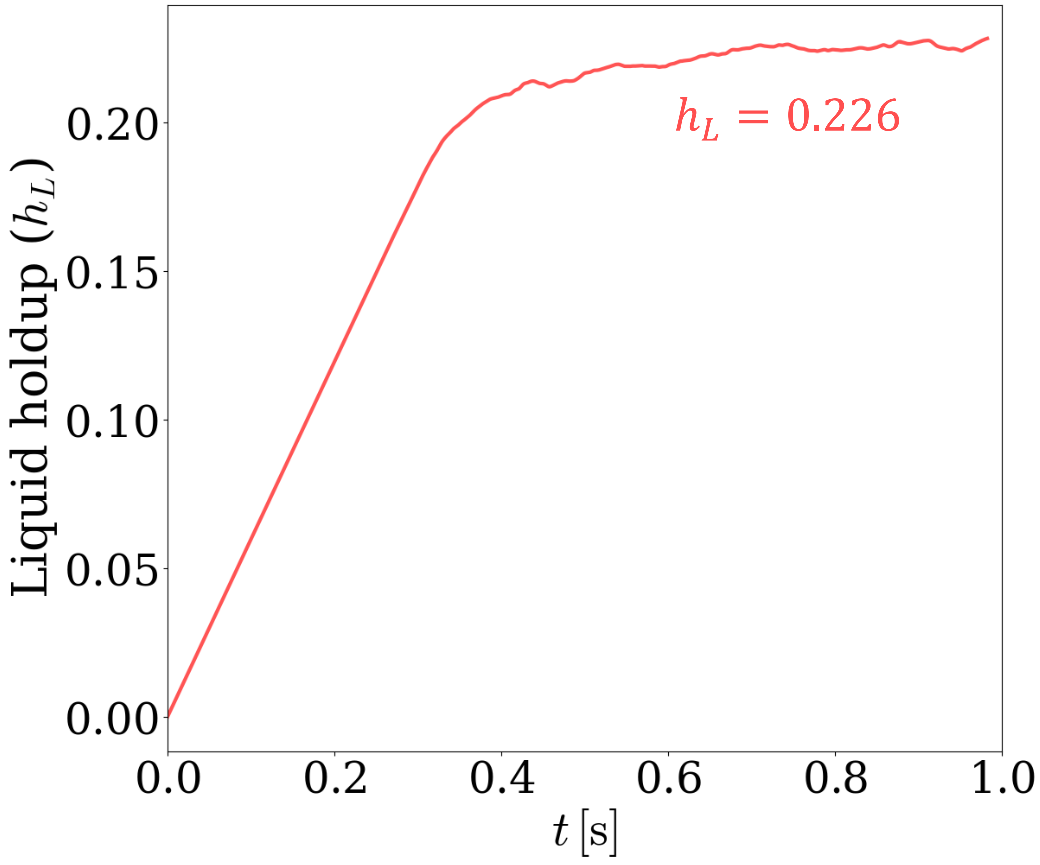
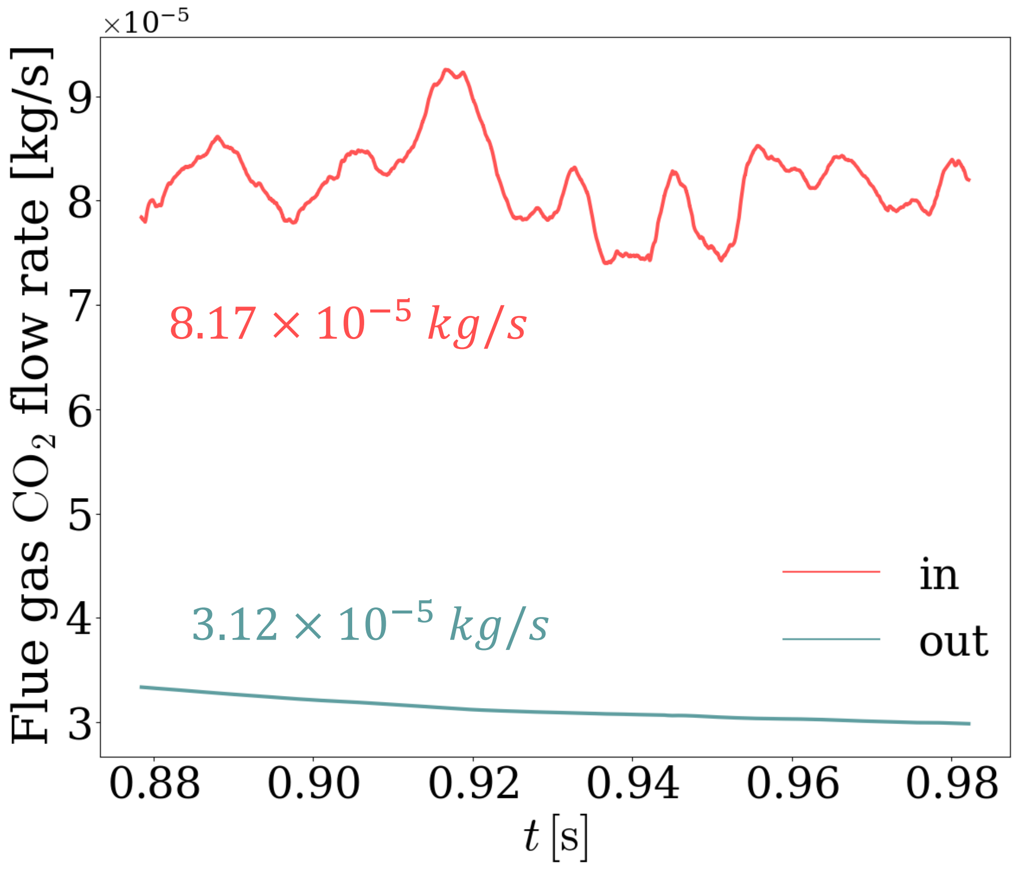
Simulation results: Liquid holdup & CO_2 absorption rate





Capture rate: 61.8%

CCSI^2 Carbon Capture Simulation for Industry Impact

Preliminary results from unvalidated model – work in progress

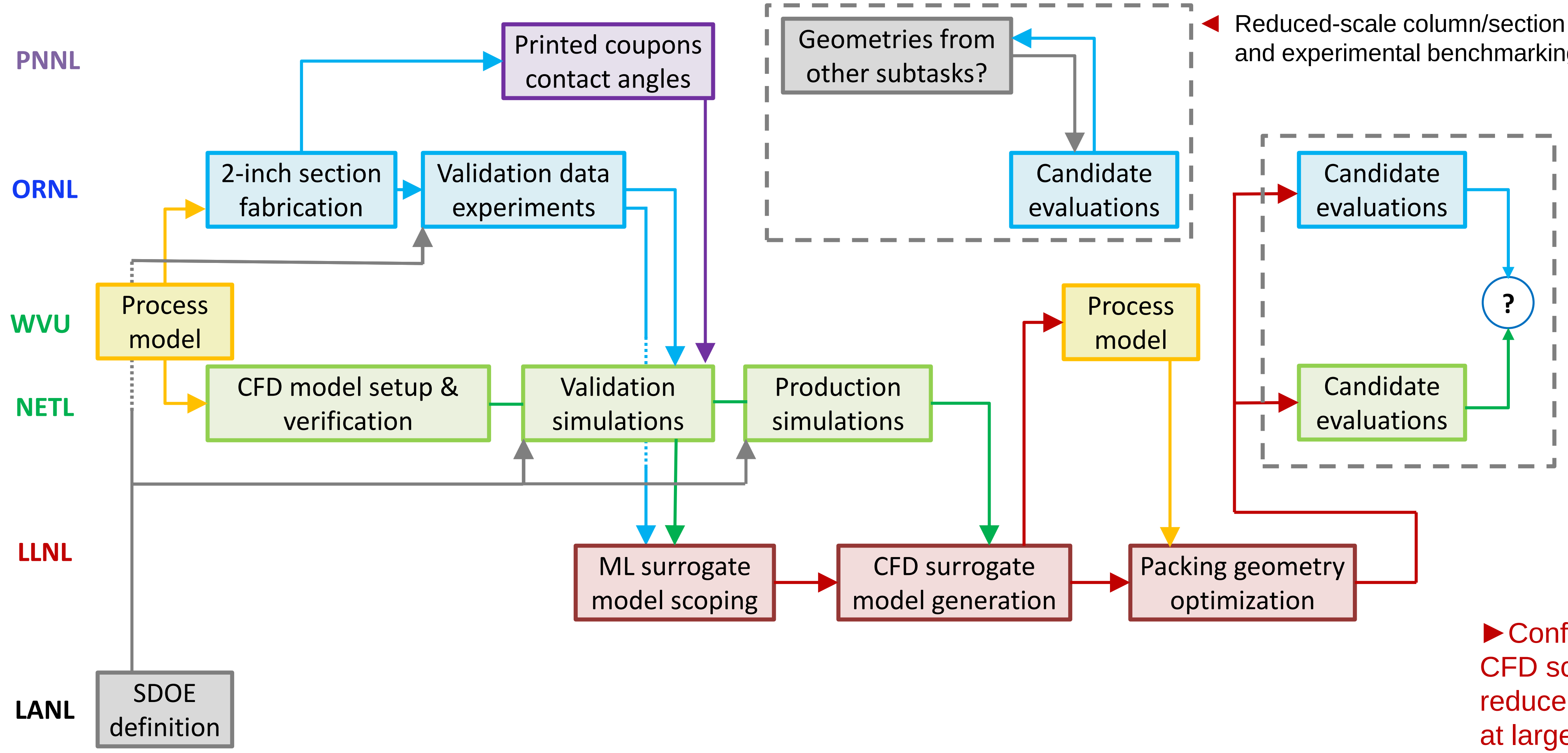
Future work

- Construct and operate rapid-prototyping, reduced-size test column section
  - CFD validation data
  - ML-identified candidate optimized geometries

- Scale up tests to 8- and 12-inch columns

- Consider effects of other solvents and/or materials of construction

Proposed pathway of dataflows & interfaces for application of modeling tools for optimized packing devices and columns



◄ Reduced-scale column/section allows rapid print prototyping and experimental benchmarking of other candidate designs

- Iterate progressively from 2- to 8- to 12-inch sections
- Fewer evaluation experiments are anticipated with each increase in size

►Confidence in the validated CFD scale-up process would reduce uncertainty in predictions at larger scales where experiments or CFD would be limited or not possible.

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For more information

https://www.acceleratecarboncapture.org/

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