Computational Fluid Dynamics (CFD) Simulations for Post-Combustion Carbon Capture

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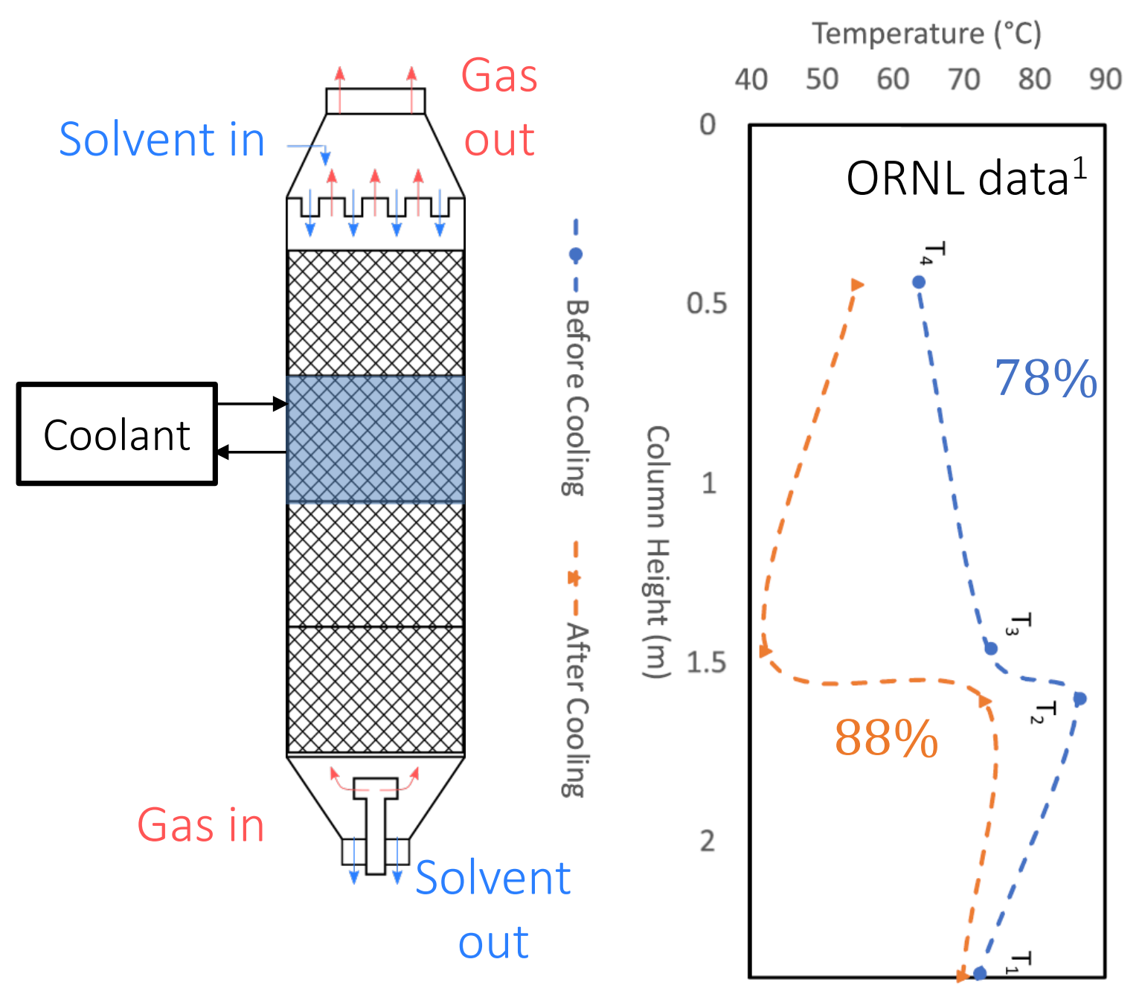
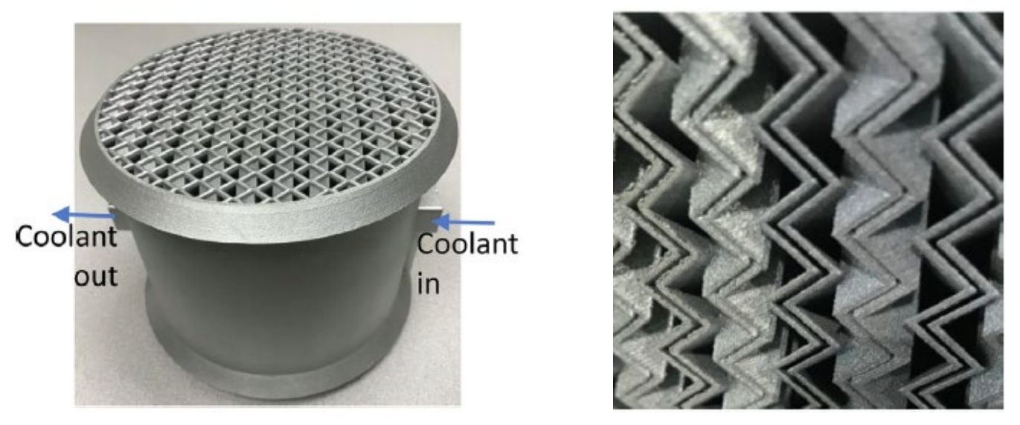
Motivation: Process Intensification of Packed Columns

- Temperature rise in the column leads to reduced reactivity and CO_2 absorption.
- Packing geometries with embedded cooling channels can enhance column performance and reduce operational and capital costs.
- **Computational Fluid Dynamics (CFD) is the only tool offering direct calculations of wetted area** (packing-solvent interface) **and interfacial area** (solvent-flue gas interface) **in the column, as a function of the design.**
- **CFD is the only tool that can inform process models for the effect of packing's design on the column's performance, within a process optimization framework.**



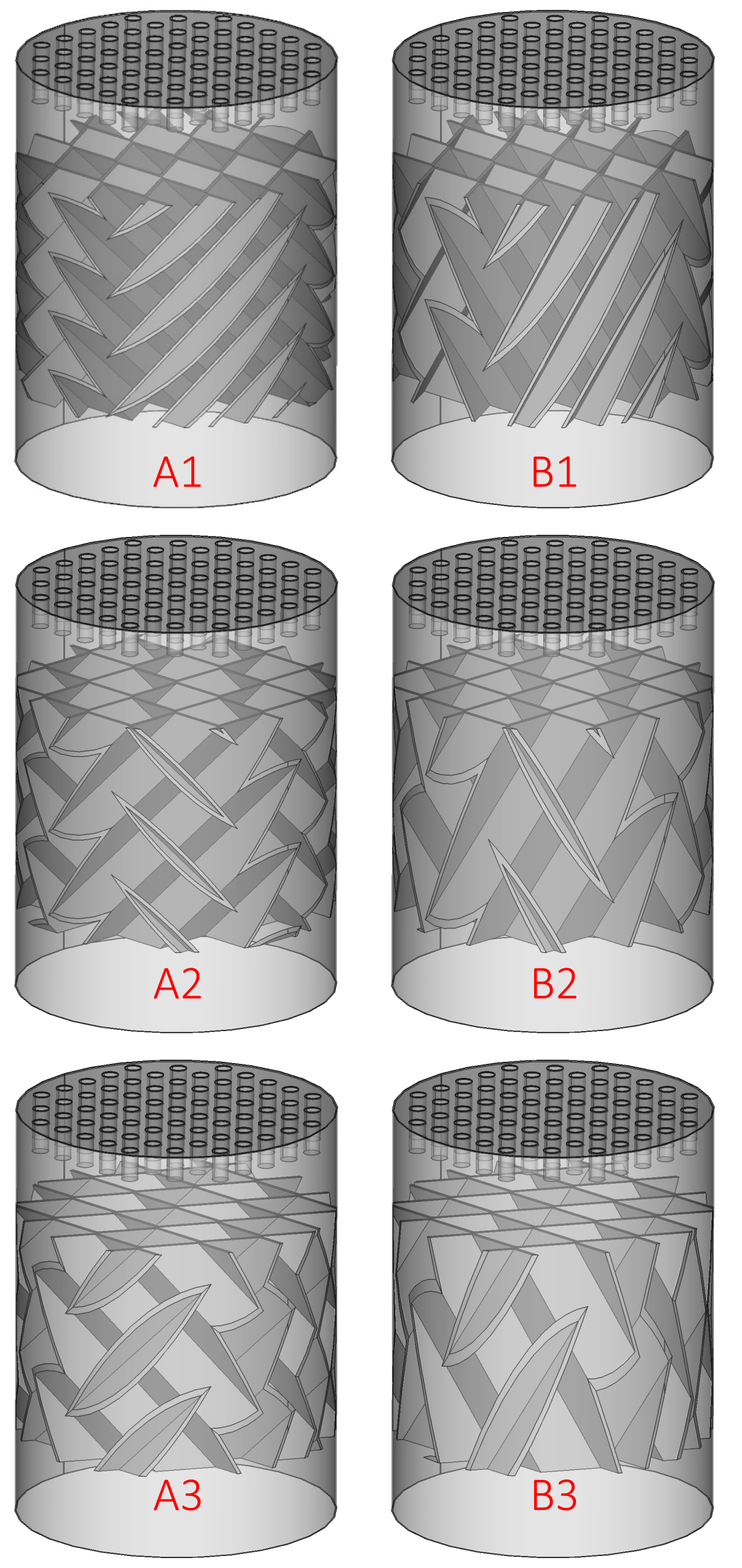
Longer-term Objective:

- Design structured packing to optimize carbon capture rate for given solvent and operating conditions.
- Develop a computational framework to map the geometrical features of the structured packing to column performance metrics.
- Create a computational tool for process optimization that can incorporate the effect of packing design and embedded cooling through reduced order models acquired from Machine Learning (ML) algorithms.

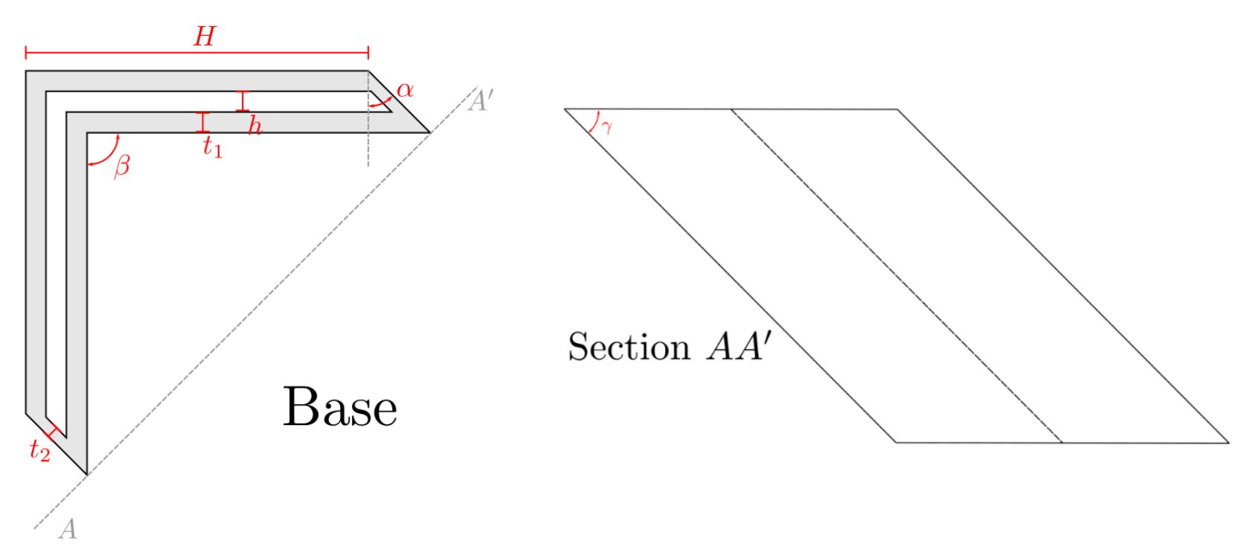


Intensified packing and coolant channels[2]

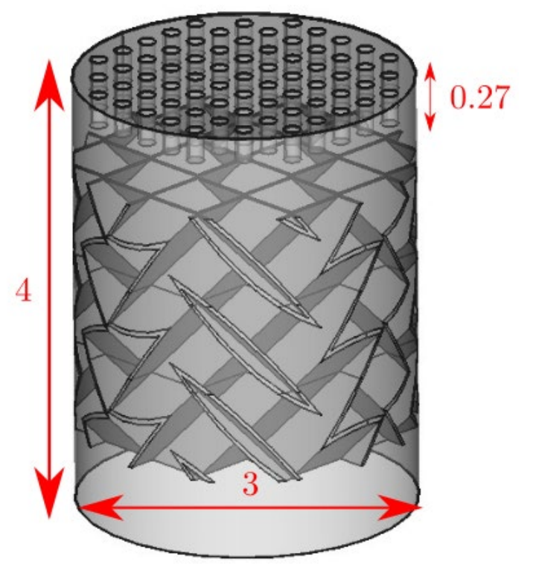
Parametric Construction of Alternate Packing Geometries for Optimal Column Performance



- FreeCAD based Python script automatically generates geometry for a user-defined set of parameters.



- Column performance metrics will be evaluated for each geometry using CFD simulations and mapped to the underlying geometrical parameters and operating conditions.



Design	β	γ
A1	60°	45°
A2	90°	45°
A3	120°	45°
B1	60°	60°
B2	90°	60°
B3	120°	60°

References

[1] *Miramontes, Jiang, Love, Lai, Sun, Tsouris "Process intensification of CO_2 absorption using a 3D printed intensified packing device." AIChE J.* 2020; 66:e16285.

[2] *Miramontes, Love, Lai, Sun, Tsouris "Additively Manufactured Packed Bed Device for Process Intensification of CO2 Absorption and Other Chemical Processes." Chemical Engineering Journal, 388, p. 124092.*

[3] Plaza, J.M., Van Wagener, D. and Rochelle, G.T., "*Modeling CO2 capture with aqueous monoethanolamine.*" *Energy Procedia*, 1(1), *pp.1171-1178.*

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Mass Transfer and Thermochemical Model

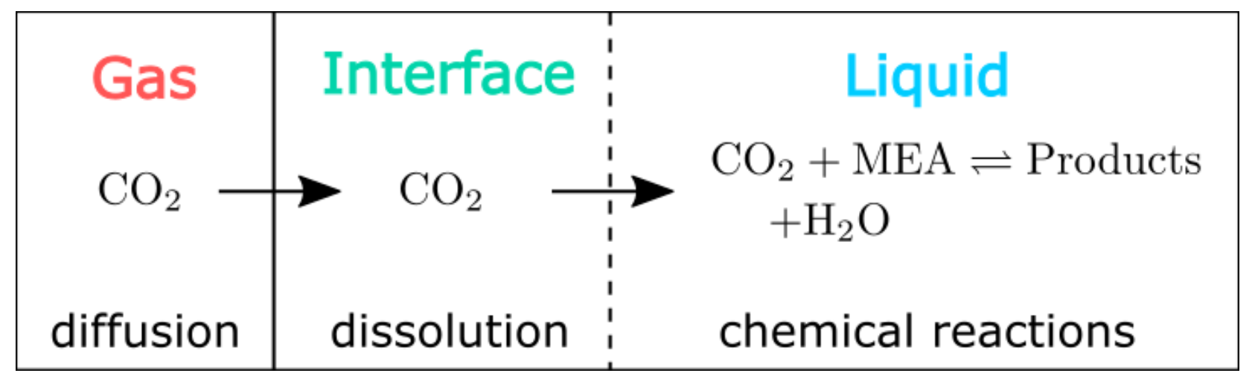
Mass Transfer model:

- 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[3]:

$$\mathbf{2MEA + CO_2 \rightleftharpoons MEACOO^- + MEA^+}$$
$$\mathbf{MEA + H_2O + CO_2 \rightleftharpoons MEA^+ + HCO_3^-}$$



Properties and models incorporated from IDAES:
Instantaneous apparent/true species conversions

- Liquid & vapor phase properties:
  - Mixture density
  - Mixture viscosity
  - Mixture thermal conductivity
  - Mixture specific heat
  - Species diffusivities
- Surface tension (temperature & composition dependent)
- Reaction kinetics

Numerical Setup

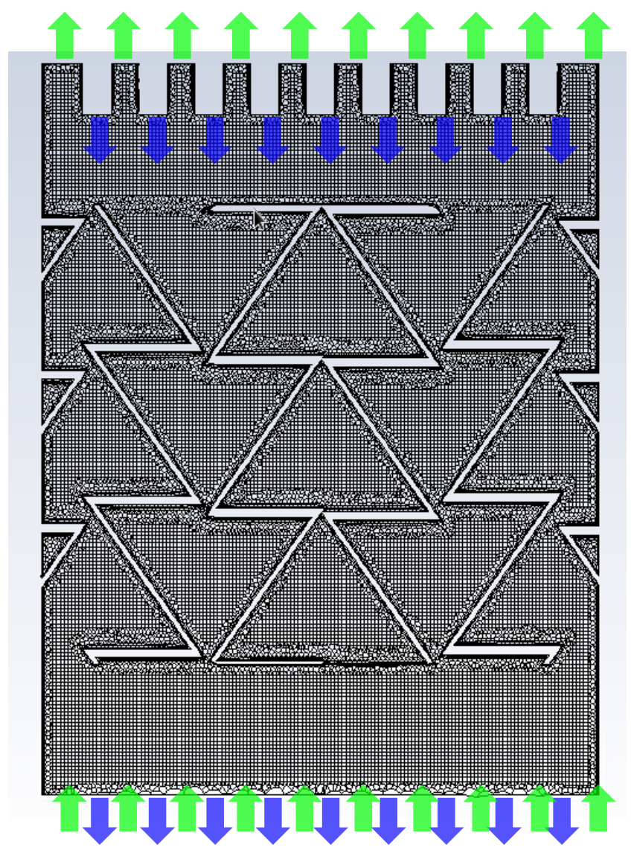
Numerical solver and algorithm:

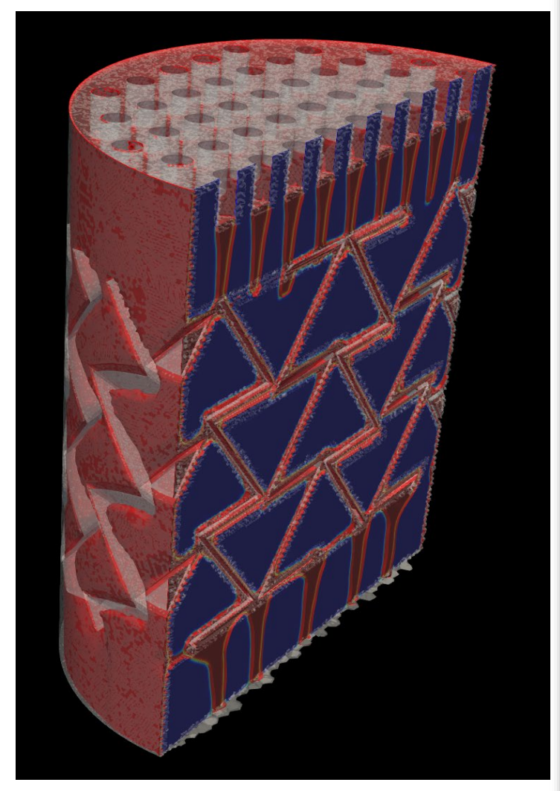
- Multiphase flow solver: ANSYS Fluent
- Interface tracking: Geometric Volume of Fluid (VOF) method
- Explicit reaction rate source terms

Simulation conditions:

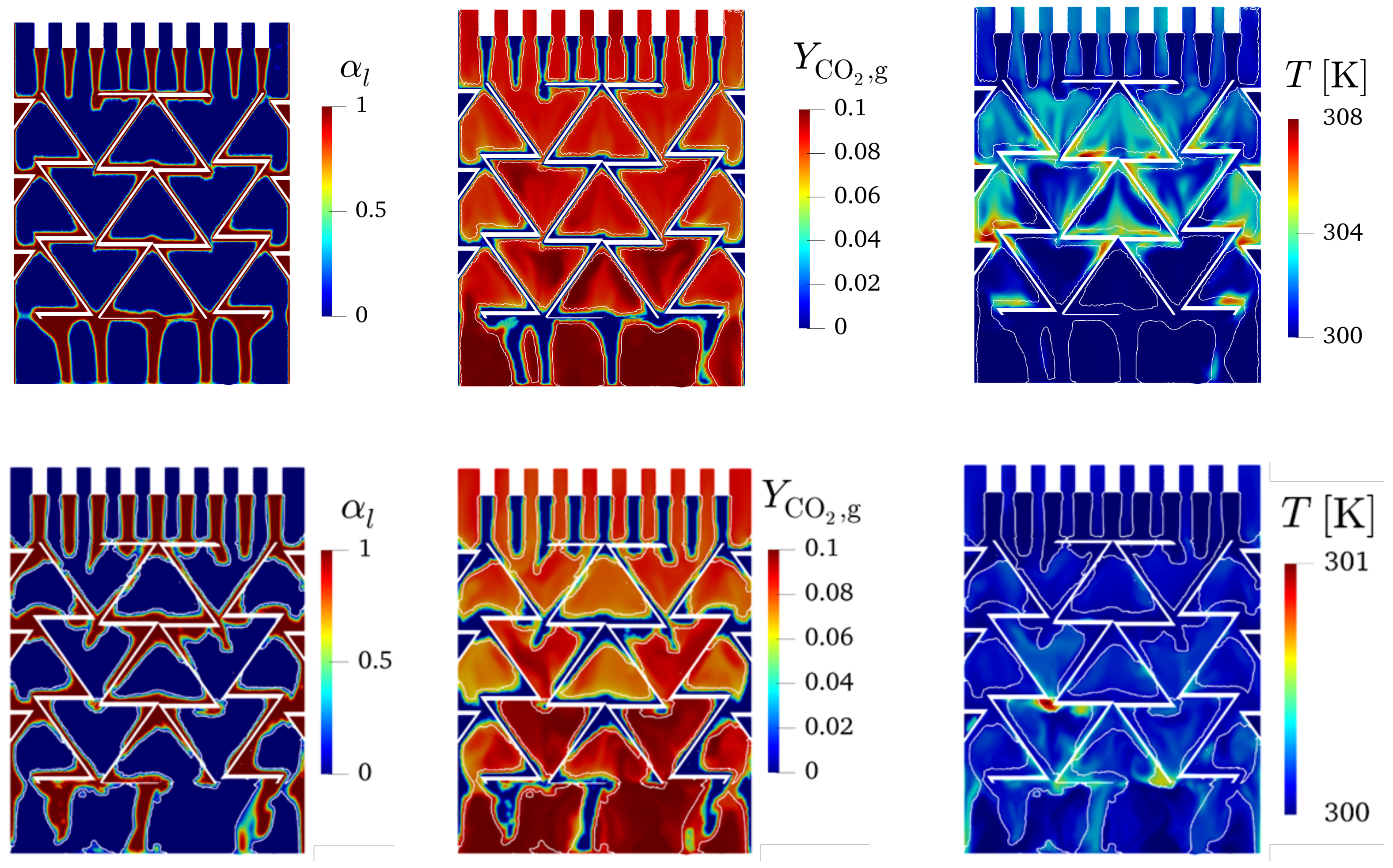
- Solvent: 30% MEA, 70% H_2O ($Ka \approx 1017$)
- Flue gas: 10% CO_2, 1.5% H_2O, 88.5% N_2
- Constant static contact angle of 40°

Liquid inflow velocity	T_{in} = 300 K	T_{in} = 343 K
0.1 m/s (Low)	Case 1A	Case 1B
0.3 m/s (High)	Case 2A	Case 2B

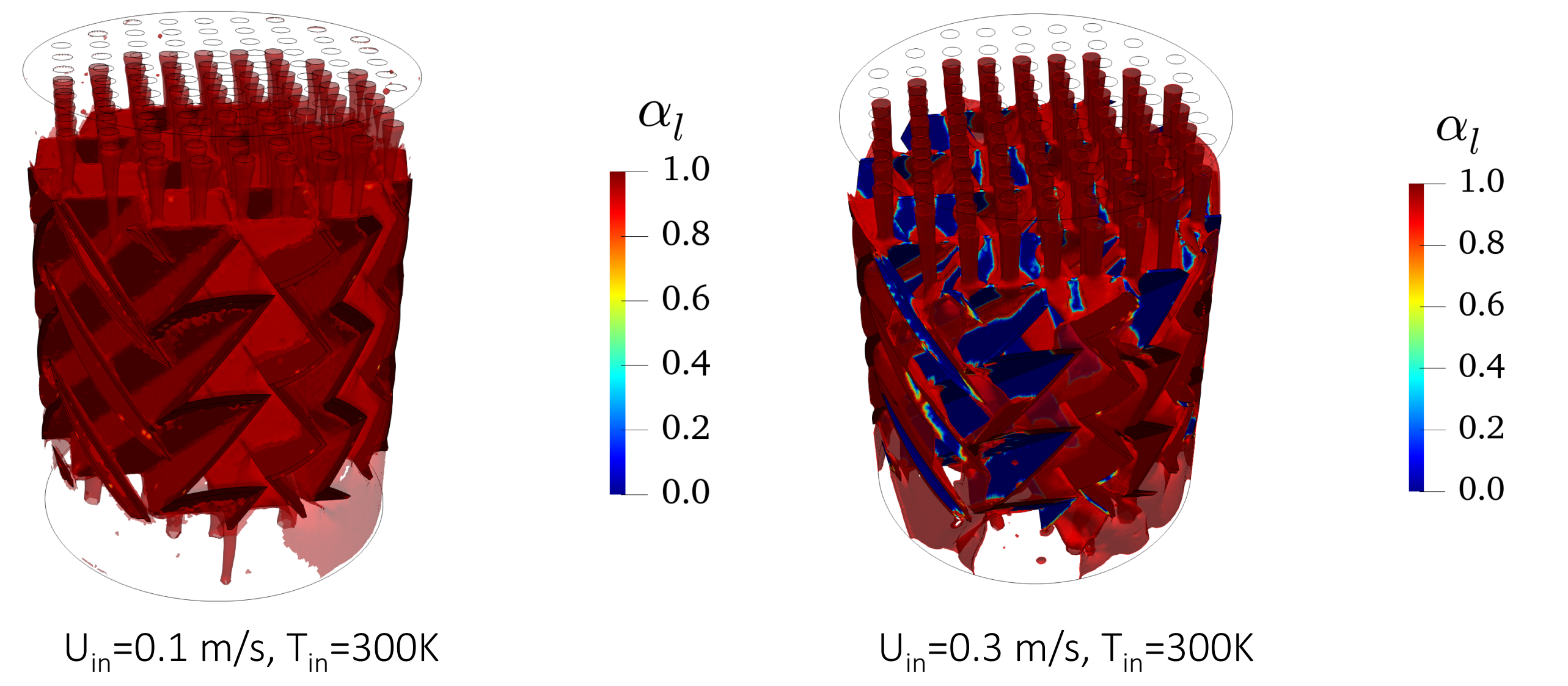




Preliminary Results



Distribution of liquid void fraction, CO_2 mass fraction and temperature in the column for liquid inflow velocity of $U_{in} = 0.1\ m/s$ and $U_{in} = 0.3\ m/s$ and temperature, $T = 300\ K$.

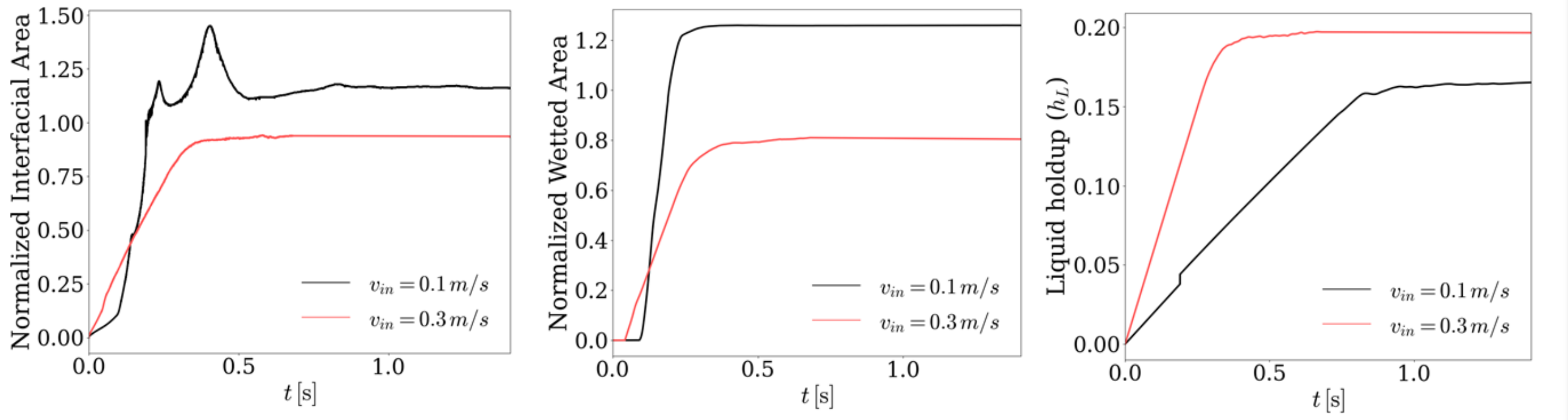


U_{in}=0.1 m/s, T_{in}=300K

U_{in}=0.3 m/s, T_{in}=300K

Distribution of the liquid void fraction α_l over the packing surface for Cases 1A (U_{in}=0.1 m/s, T=300K) and 2A (U_{in}=0.3 m/s, T=300K).

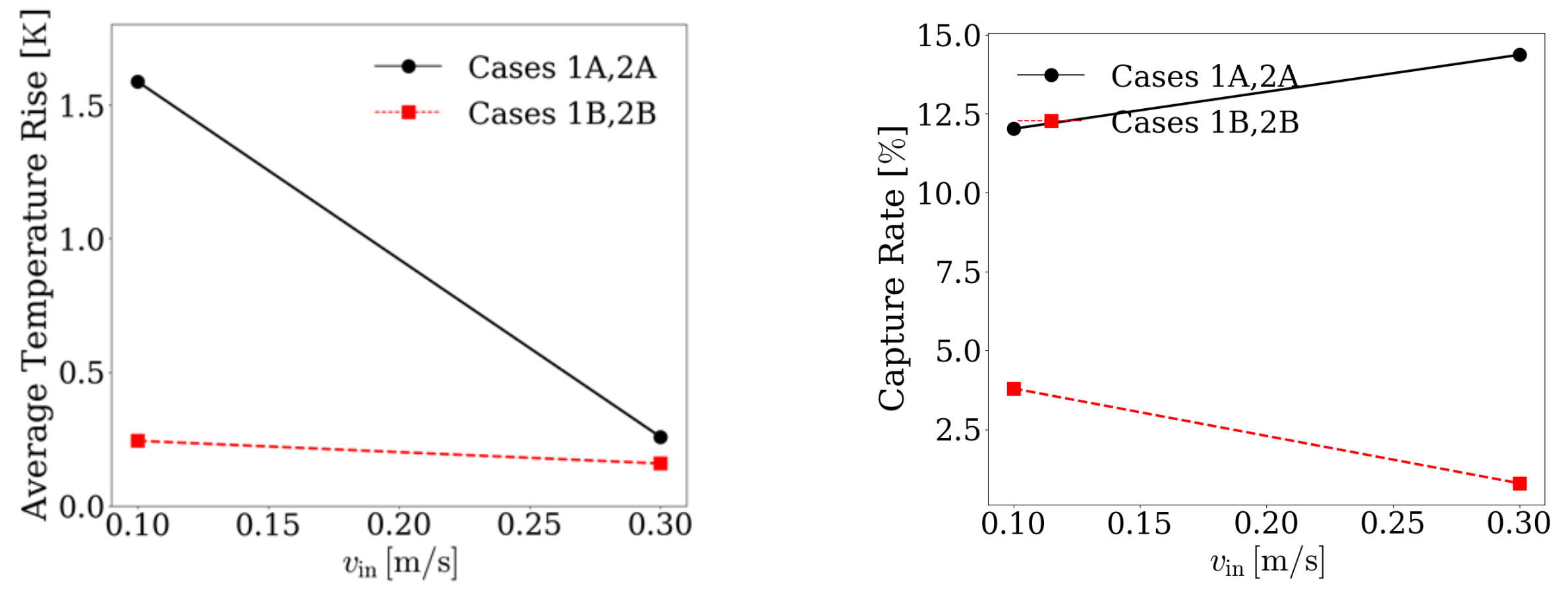
Column Performance Metrics



Normalized interfacial area (A_I/A_p) is $\approx$ 26% higher for case 1A at steady state.

Normalized wetted area (A_w/A_p) is $\approx$ 57% higher for Case 1A at steady state.

Liquid holdup is $\approx$ 17% higher for Case 2A at steady state.



Temperature rise is higher for case 1 (A and B) due to the higher A_I and flow residence time (τ_r).

Capture rate is higher for case 2A relative to 1A due to a lower temperature rise and τ_r.

Key quantities that impact the column performance: interfacial and wetted areas, liquid holdup, average temperature rise, and capture rate for different liquid loads.

Summary & Conclusions

- **First ever implementation of IDAES reaction dynamics and thermodynamics for an absorption CFD column.**
- **Unique, coupled multiphysics approach covering, mass, momentum and heat transfer.**
- **Locally and thermally dependent material properties.**
- CFD simulations were performed to model CO_2 absorption in a three-dimensional column for four different solvent inflow conditions.
- Trends in interfacial and wetted areas, and predicted rate of CO_2 absorption are found to be generally consistent with observations.
- Capture rate is higher in packed column at lower temperature ($T = 300\ K$) compared with that at $T = 343\ K$.
- Three-dimensional CFD modeling framework is shown to be a potential tool for predicting column performance trends in optimizing contactor designs. CFD predictions will further guide in improving existing process modeling frameworks for absorption columns.

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