Validation Framework for Post-Combustion Carbon Capture CFD Simulations

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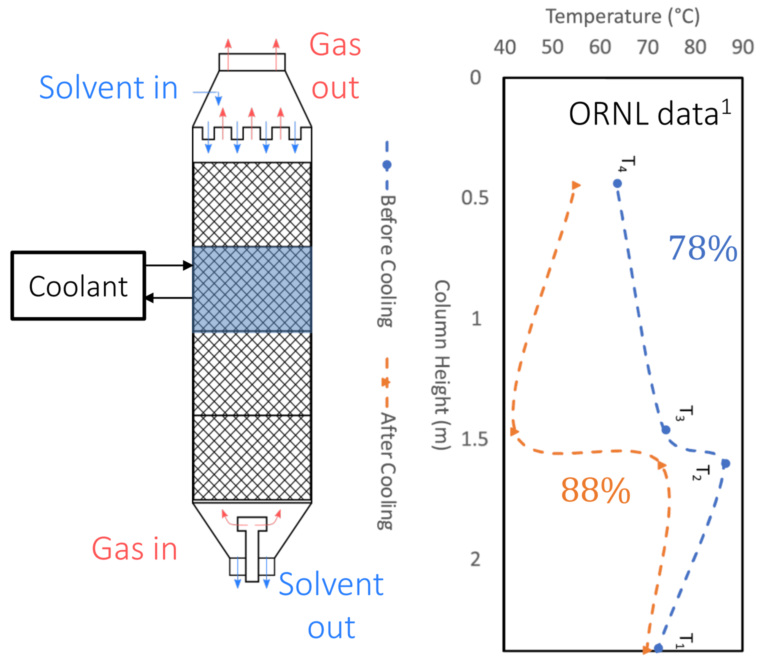
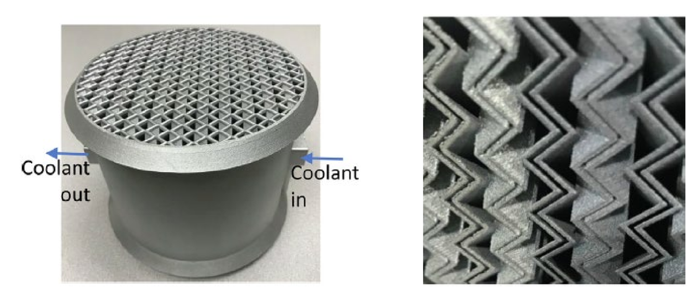
Motivation: Process Intensification of Packed Columns

- 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.

Longer-term Objective:

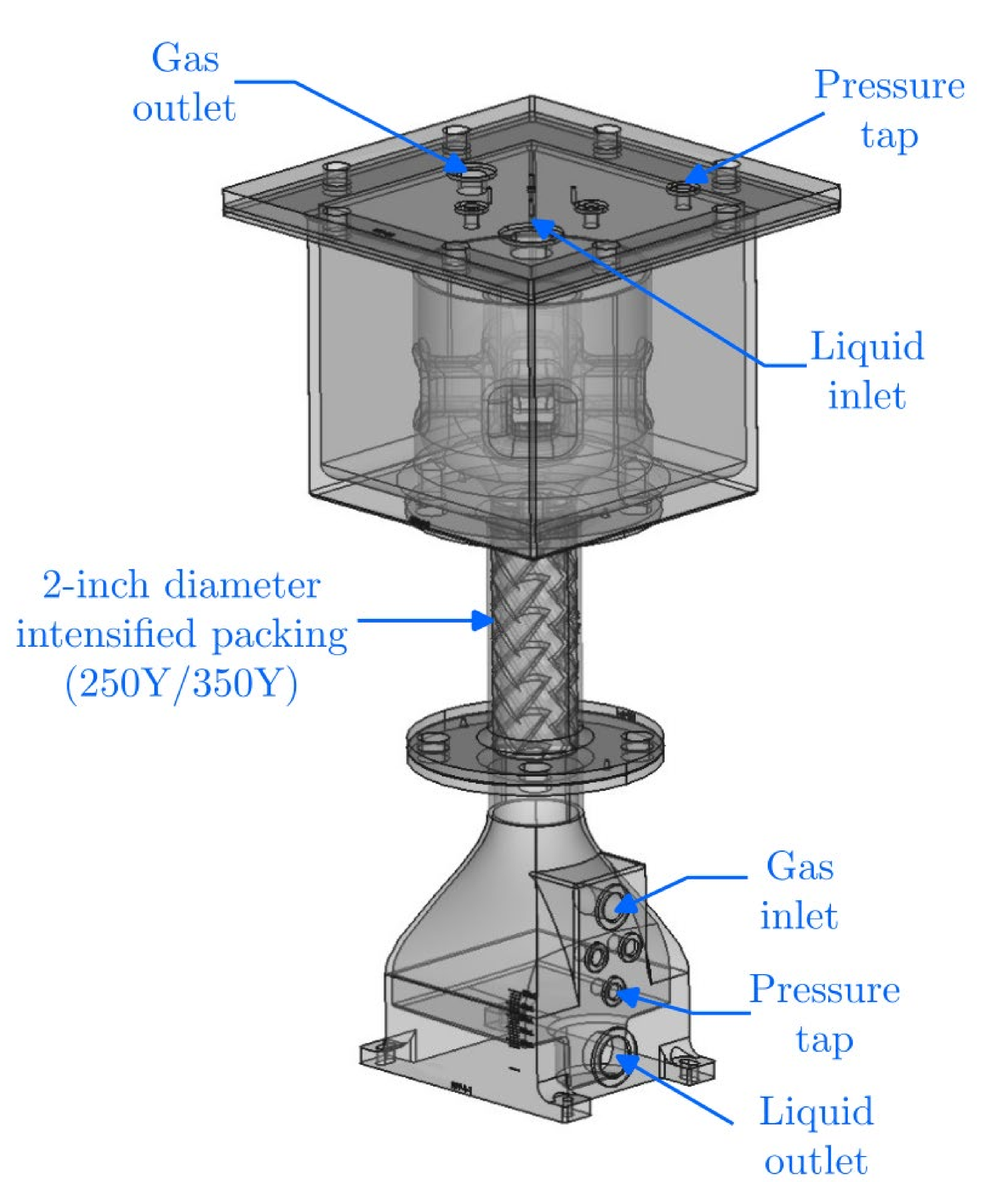
- Design structured packing to optimize carbon capture rate for given solvent and operating conditions.
- Develop a computational framework to map the geometrical features of the structured packing to column performance metrics.
- Create a computational tool for process optimization that can incorporate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





Intensified packing and coolant channels[2]

ORNL Packing Prototype Performance (PPP) Column



- A reduced-size 2-inch column with translucent walls was designed by ORNL to facilitate a more rigorous validation of the CFD model.
- The interior of the test section is illuminated to capture the dynamical evolution of the liquid/gas surface using high-speed (1000 fps) videography for different liquid and gas flow rates.
- Instantaneous pressure difference across the column is measured at the pressure taps at the bottom and top of the column using a differential transducer.
- A comprehensive dataset of pressure drop and liquid holdup is obtained for validation of CFD model/simulations.

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 CO_2 Absorption and Other Chemical Processes." Chemical Engineering Journal, 2020; 388, p. 124092.

[3] Plaza, J.M., Van Wagener, D. and Rochelle, G.T., "Modeling CO_2 capture with aqueous monoethanolamine." Energy Procedia, 2010; 1(1), pp.1171-1178.

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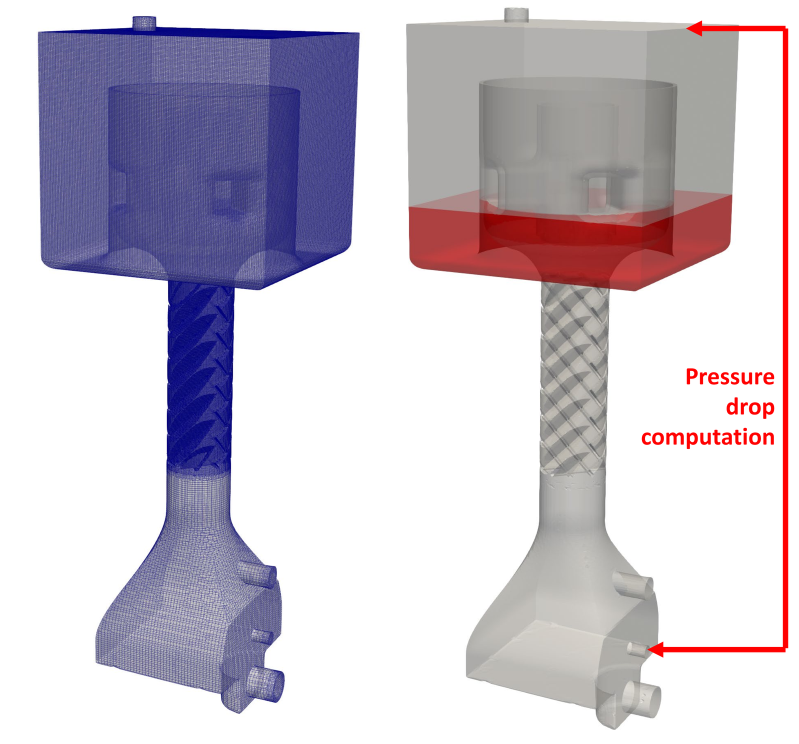
CFD Model and Simulation Setup

Numerical solver and algorithm:

- Multiphase flow solver: OpenFOAM
- Interface tracking: Geometric Volume of Fluid (VOF) method

Simulation conditions:

- 3 solvents: water (EG000), ethylene glycol (EG100), 50% (vol.) ethylene glycol solution (EG050) – viscosity range of all MEA operation states.
- 2 packing geometries: 250Y and 350Y.
- Simulations were performed using ORNL CADES and NETL Joule supercomputer.



Initial condition

Simulation Case Matrix

CFD simulations and experiments were performed for different liquid and gas flow rates determined from a sequential design of experiments (SDoE) procedure.

EG000: 250Y

Case	Liquid flow rate [LPM]	Gas flow rate [LPM]
A_1	3	25
A_2	6	50
A_3	6	0
A_4	4.7	38.1

EG050: 250Y

Case	Liquid flow rate [LPM]	Gas flow rate [LPM]
B_1	3	25
B_2	6	50
B_3	3.8	50
B_4	2.8	50
B_5	2.2	14.7
B_6	5.3	18

EG100: 250Y

Case	Liquid flow rate [LPM]	Gas flow rate [LPM]
C_1	3	25
C_2	6	30
C_3	0.6	7
C_4	6	20
C_5	2.1	33
C_6	3.7	13.3
C_7	4.5	46.1

EG000: 350Y

Case	Liquid flow rate [LPM]	Gas flow rate [LPM]
RA_1	3	25
RA_2	6	50
RA_3	3.6	45
RA_4	6	30
RA_5	4.1	16.5
RA_6	5.5	42.6

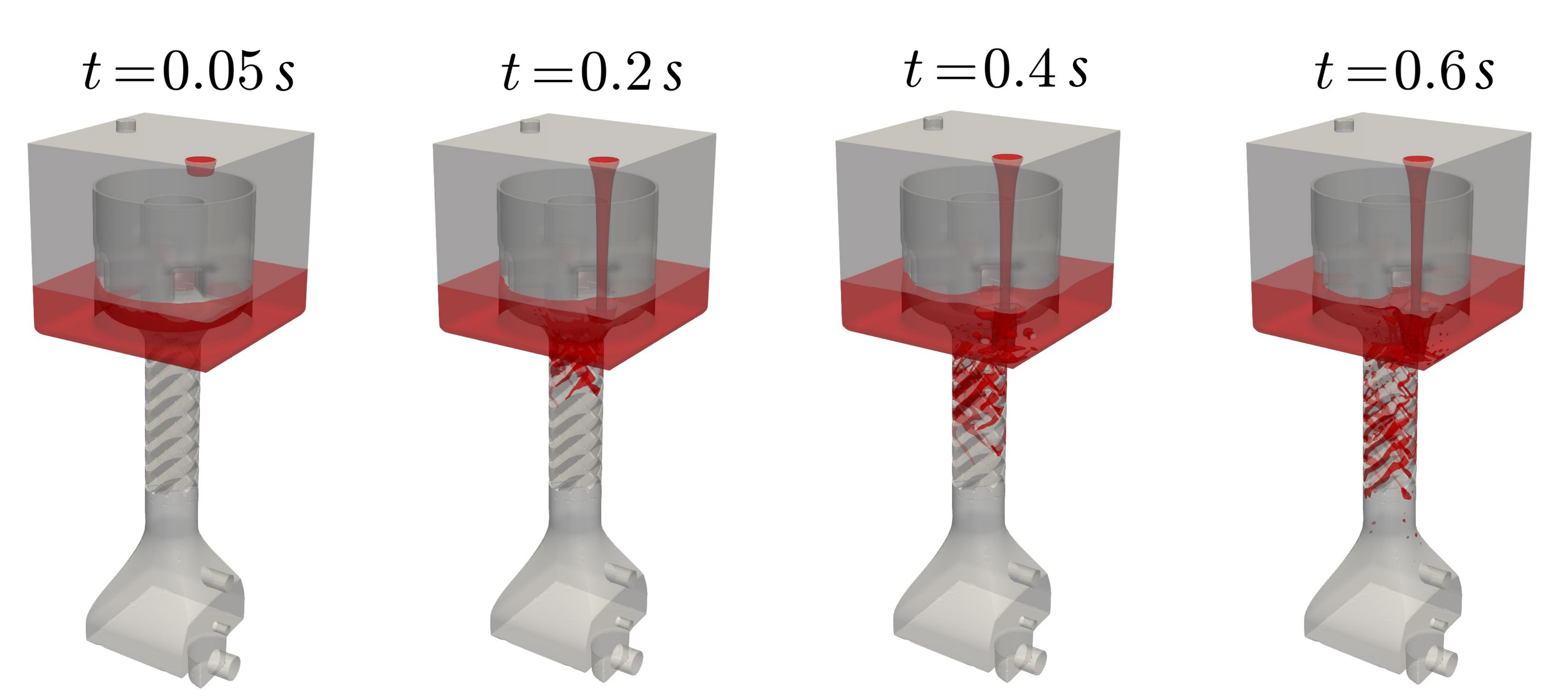
EG050: 350Y

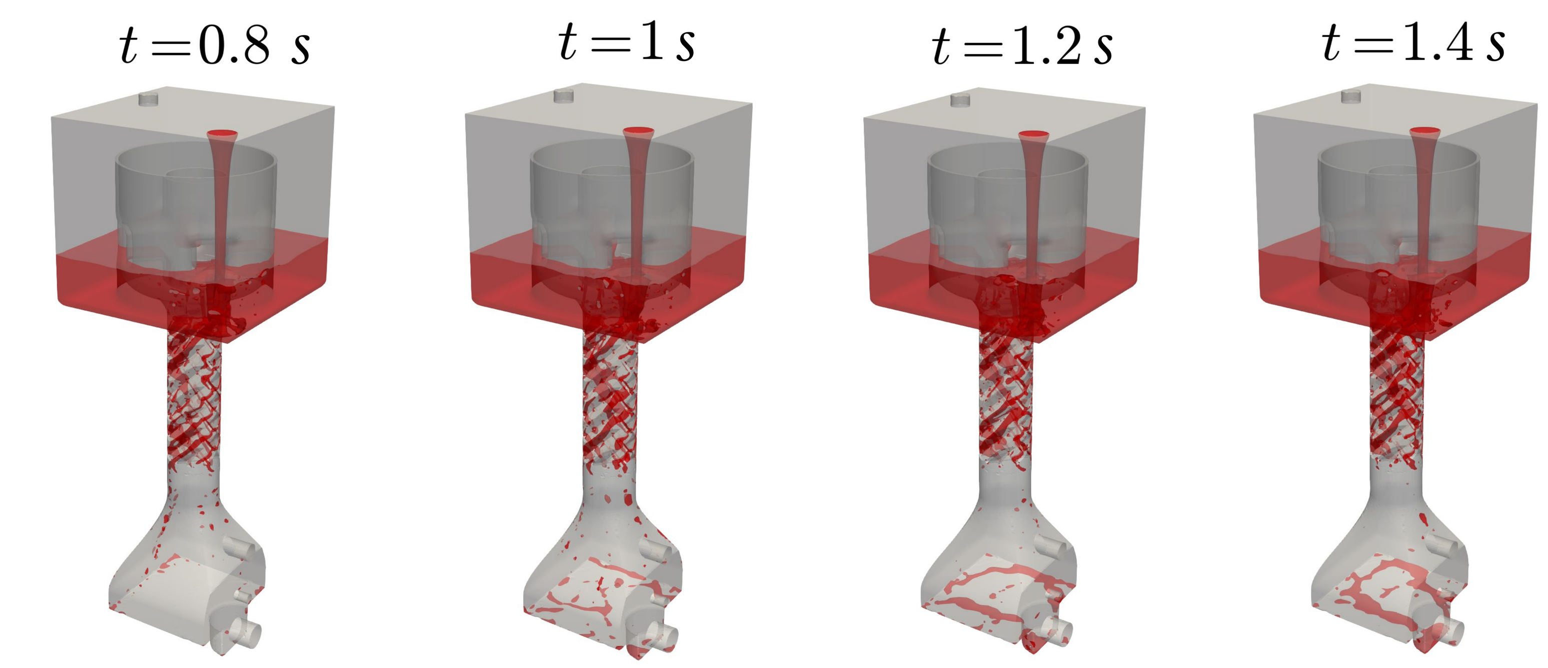
Case	Liquid flow rate [LPM]	Gas flow rate [LPM]
RB_1	3	25
RB_2	6	50
RB_3	2.4	50
RB_4	4.3	40.7
RB_5	4.9	12.1

EG100: 350Y

Case	Liquid flow rate [LPM]	Gas flow rate [LPM]
RC_1	3	25
RC_2	6	50
RC_3	9	50
RC_5	4.6	21.9
RC_6	5.2	35.4
RC_7	5.6	15

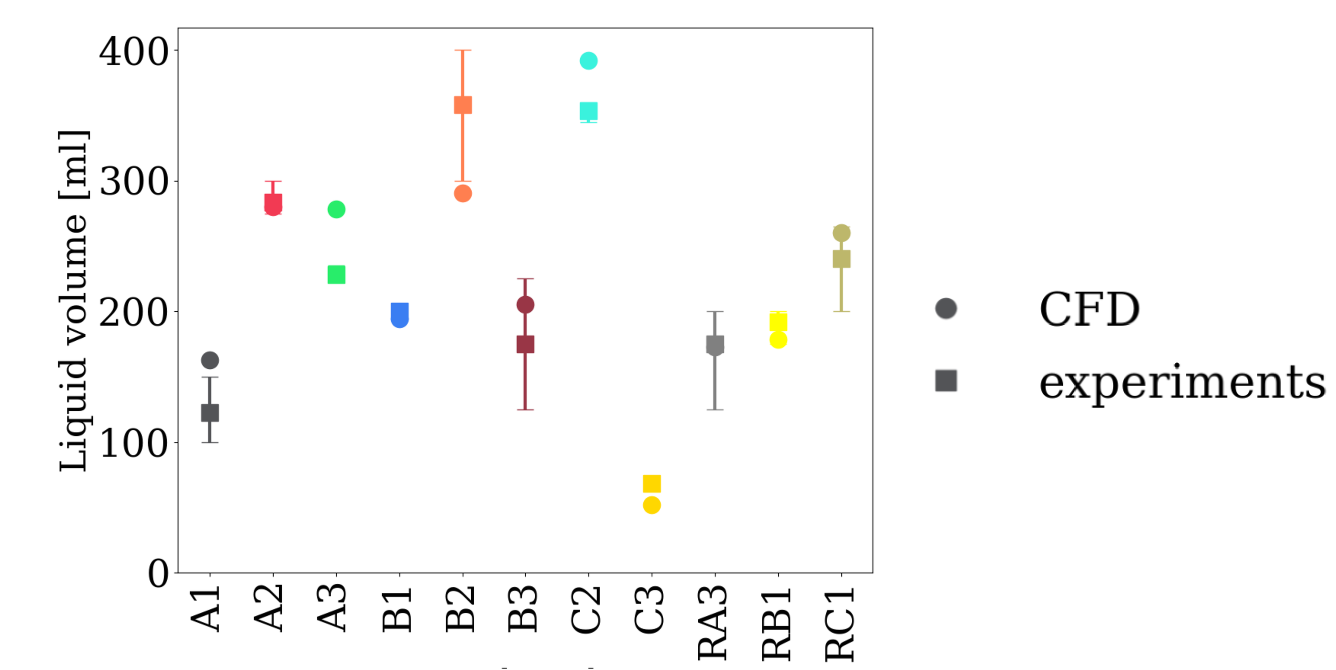
Evolution of Solvent–Gas Interface

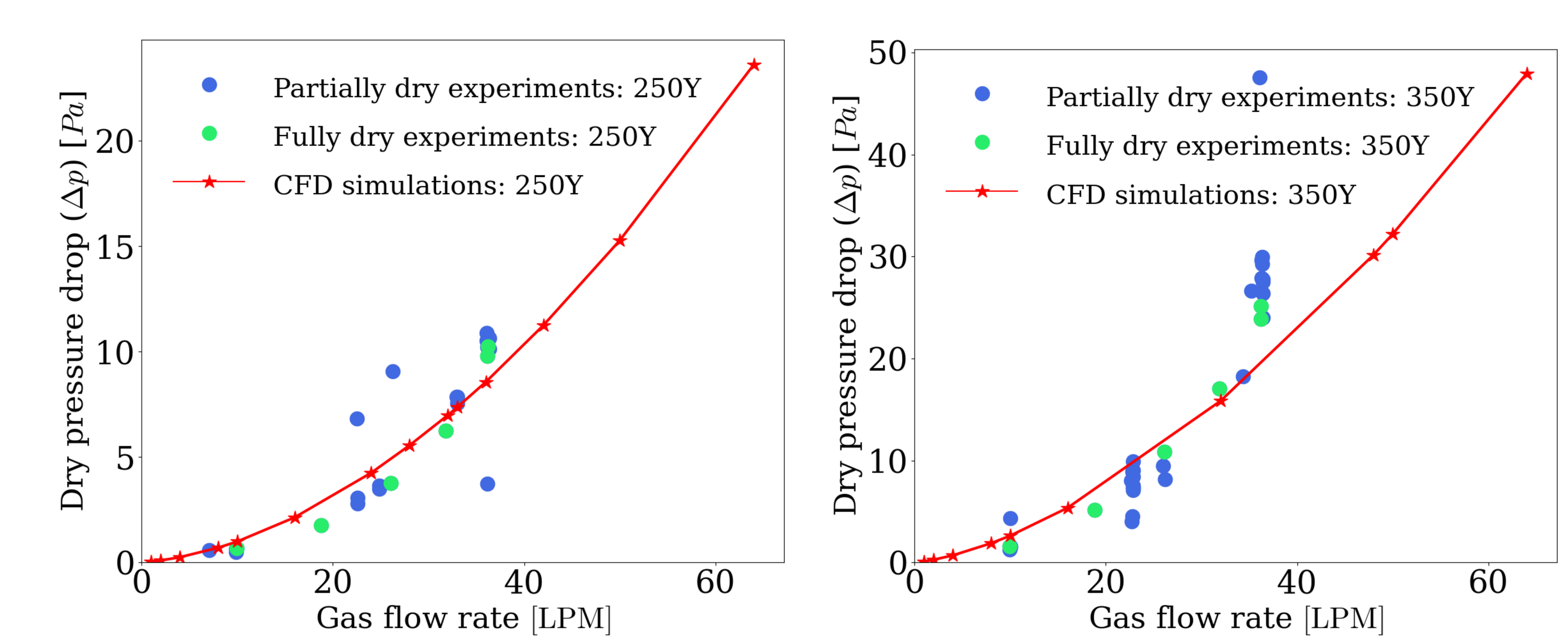




Time evolution of the solvent–gas interface for case B_2 using constant iso-surfaces of liquid volume fraction, $\alpha_l = 0.5$, highlighted in red. The simulations were performed to capture more than 10 seconds of flow time to ensure the dynamics have a statistically stationary state.

CFD Validation: Liquid Holdup and Dry Pressure Drop





- CFD predicted mean liquid volume at steady state is within 5% of the experimental variability for most cases.
- Trends in the CFD predicted dry pressure drop are shown to be in agreement with experiments for 250Y and 350Y geometries.

Summary & Conclusions

- Extensive validation campaign was performed with CFD simulations on a reduced-size 2-inch column for more than 40 cases comprising of three solvents, two packing geometries, and different liquid/gas flow rates.
- CFD predicted liquid holdup and dry pressure drop are shown to be in remarkable agreement with experiments for both geometries, suggesting that the proposed framework is capable of accurately predicting the underlying hydrodynamics.
- The CFD modeling approach is shown to be an effective tool in the future design and development of scaled-up intensified columns.

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