CCSI^2
Carbon Capture Simulation for Industry Impact

Optimal Design of Intensified Towers for CO_2 Capture with Internal, Printed Heat Exchangers

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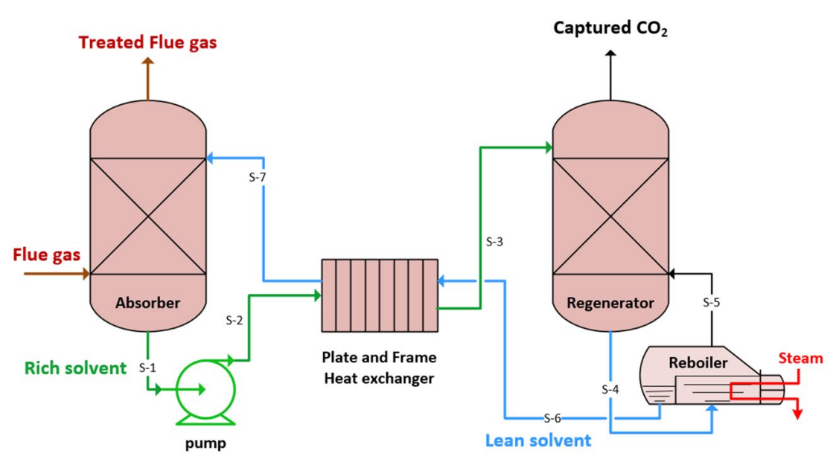
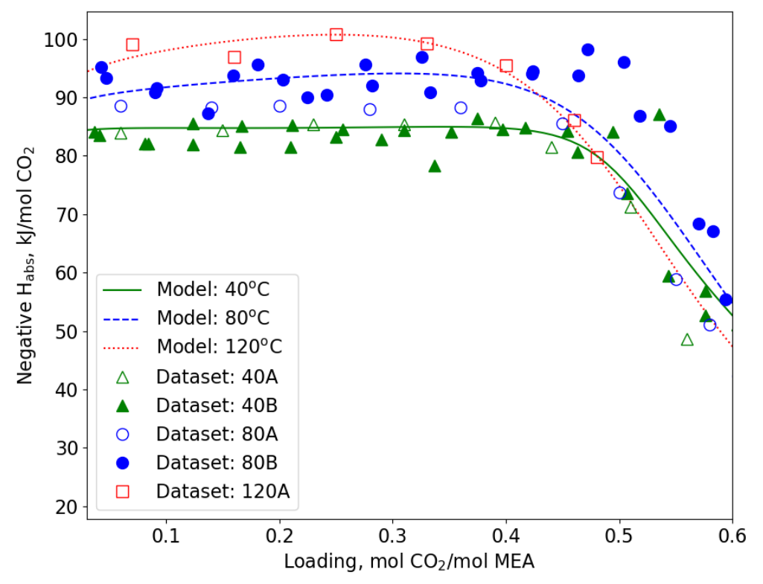
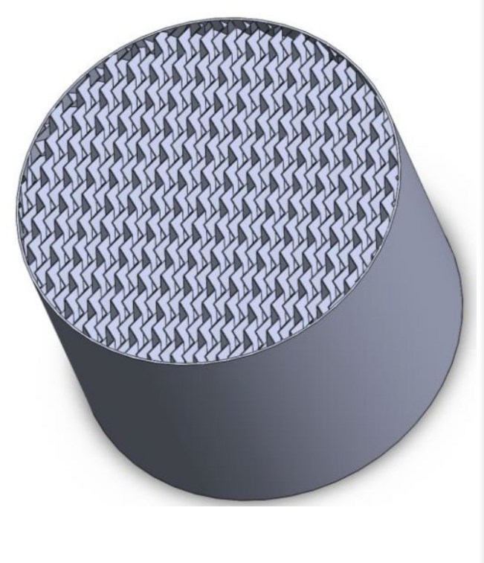
Motivation: Process Intensification of Packed Columns

- The temperature bulge in absorption towers as a result of exothermic reaction leads to lower mass transfer efficiency.
- Current solutions involve implementing intercoolers to remove heat at discrete locations of the tower but are unable to keep the process at the thermodynamic optimal conditions.
- Internal cooling with an embedded heat exchanger, made by 3D printing can aid in achieving a temperature profile which optimized performance.
- Increasing heat removal rate, however, has diminishing returns as available mass transfer area is reduced.
- The study seeks to answer questions like: Should such internal heat exchanger be placed all along the tower or should placement be varied spatially? How do the operating conditions affect the optimal placement? What are the optimal flow configurations for the cooling water?



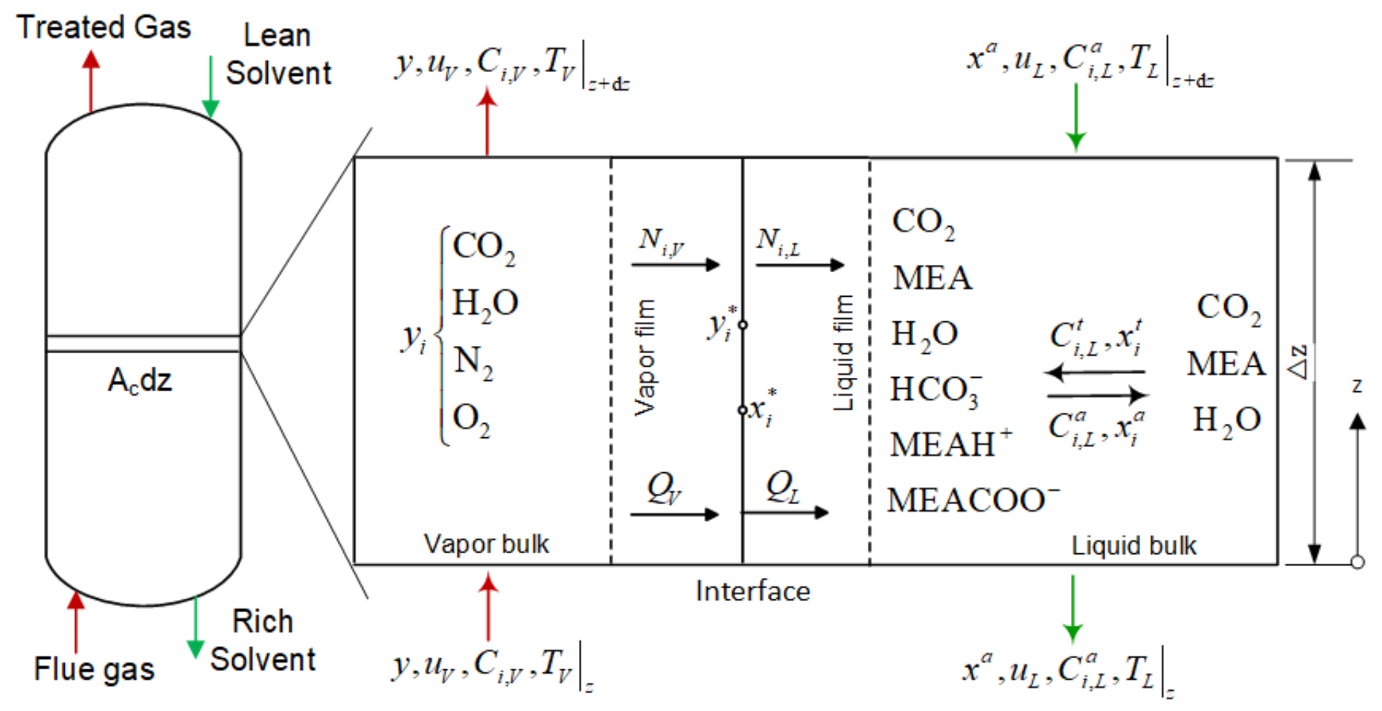


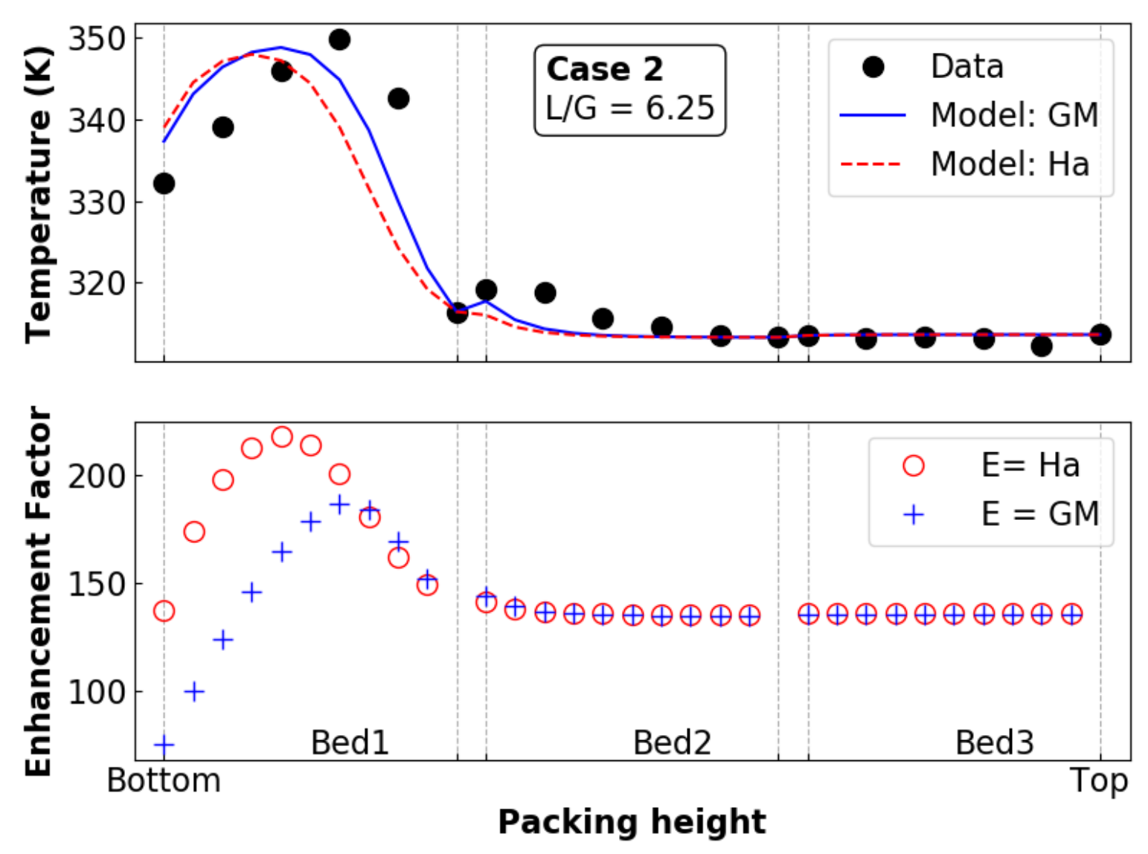


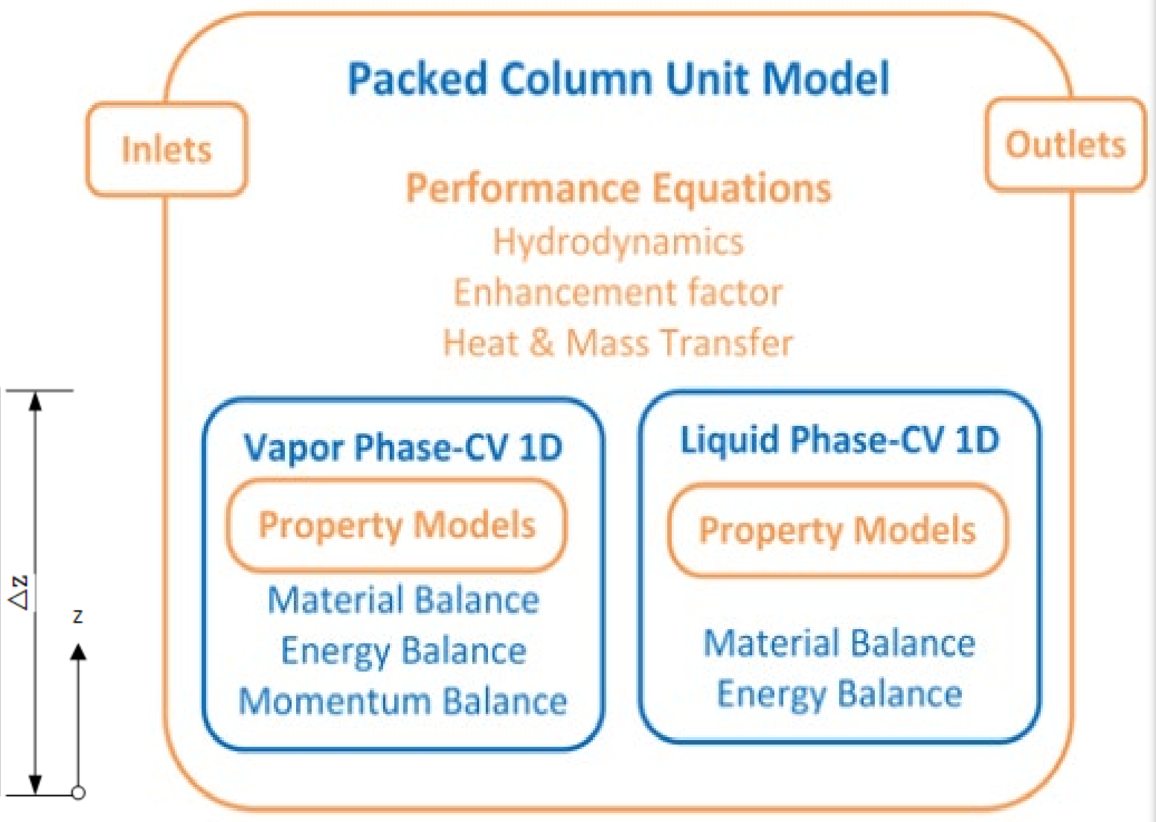
* Images are from Oak Ridge National Lab

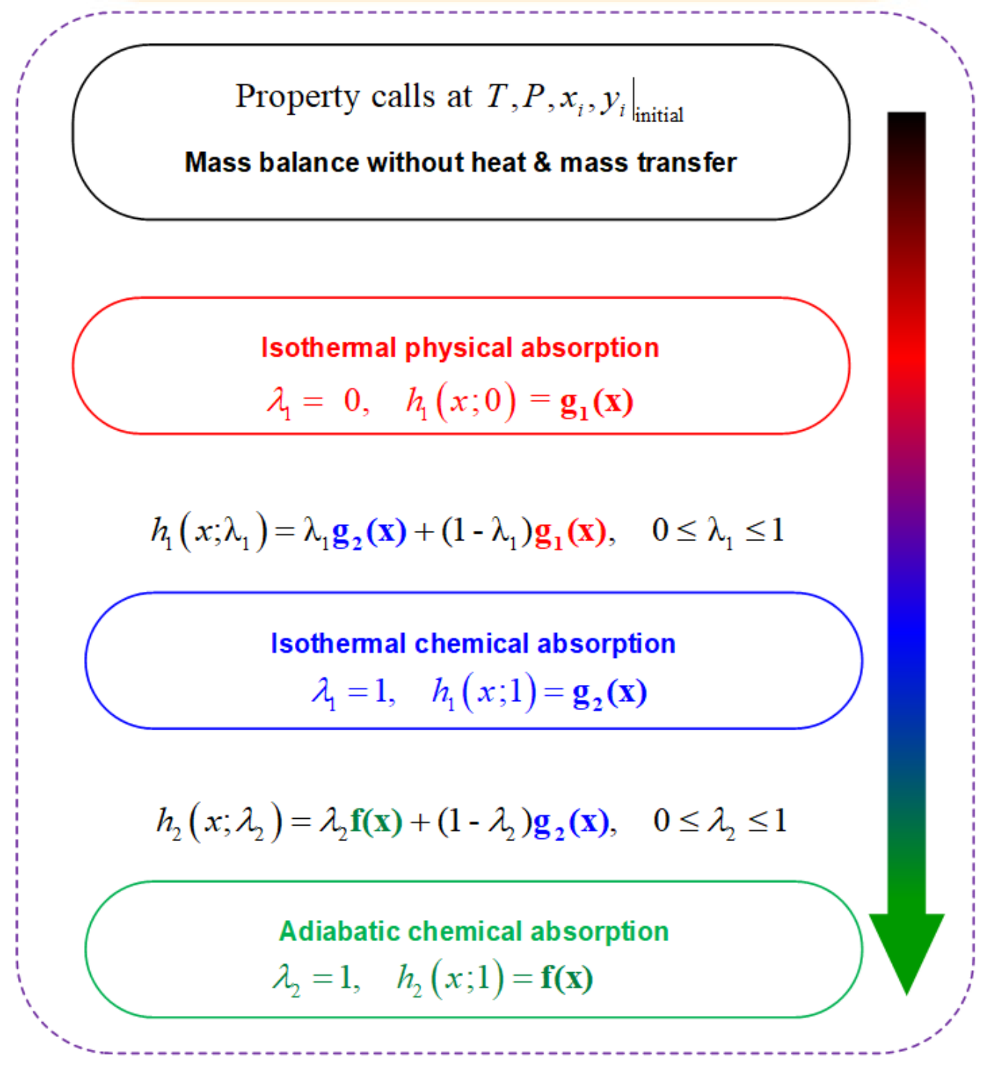
Tower Model Development and Validation[1,2]

- Two-film model with thermo-, chemistry, and properties models
- 1D in axial direction
- Validated using data from NCCC









References

[1] Akula, P, Lee, A, Eslick, J, Bhattacharyya, D, Miller, DC. Model Development, Validation, and Optimization of an MEA-Based Post-Combustion CO2 Capture Process under Part-Load and Variable Capture Operations. Ind. Eng. Chem. Res. 2021; 60(14).

[2] Akula, P, Lee, A, Eslick, J, Bhattacharyya, D, Miller, DC. A modified electrolyte non-random two-liquid model with analytical expression for excess enthalpy: Application to the MEA-H2O-CO2 system. AIChE J. 2023; 69(1).

[3] Moore, T, Nguyen, D, Iyer, J, Roy, P, Stolaroff, JK. Advanced absorber heat integration via heat exchange packings. AIChE J. 2021; 67(8).

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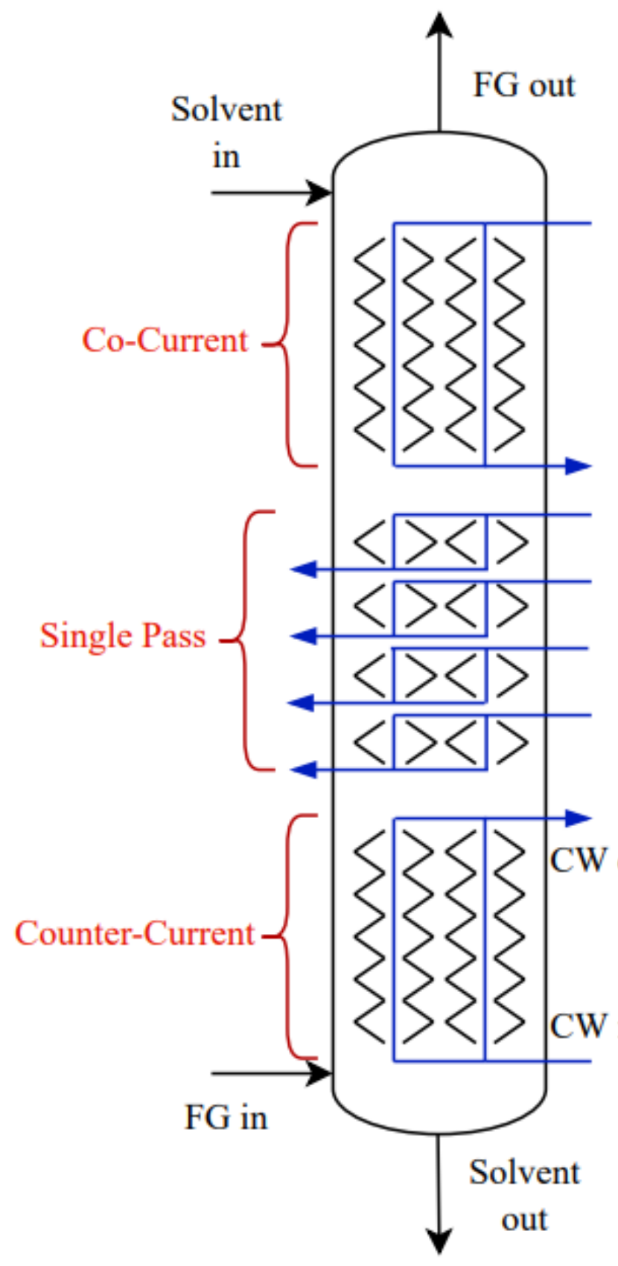
Internal Heat Exchanger Model

- Internal heat exchangers remove heat directly from liquid phase[3].
- Penalty to mass transfer area due to increase in the heat transfer area is accounted for.
- The model includes options for setting flow direction of cooling water and inlet and exit point of cooling water.

$$Q_i^{cw} = y_i U a_i \left(T_i^{cw} - T_i^L\right)$$
$$\varepsilon_i = \varepsilon^{\circ}{}_i - \varepsilon_i^{cw}$$



Model Setup

Software:

- Pyomo/IDAES
- IPOPT

Simulation conditions:

- Solvent: 30% MEA, 70% H_2O
- Flue gas: 4.2% CO_2, 5.4% H_2O, 13% O_2

Minimizing Emissions

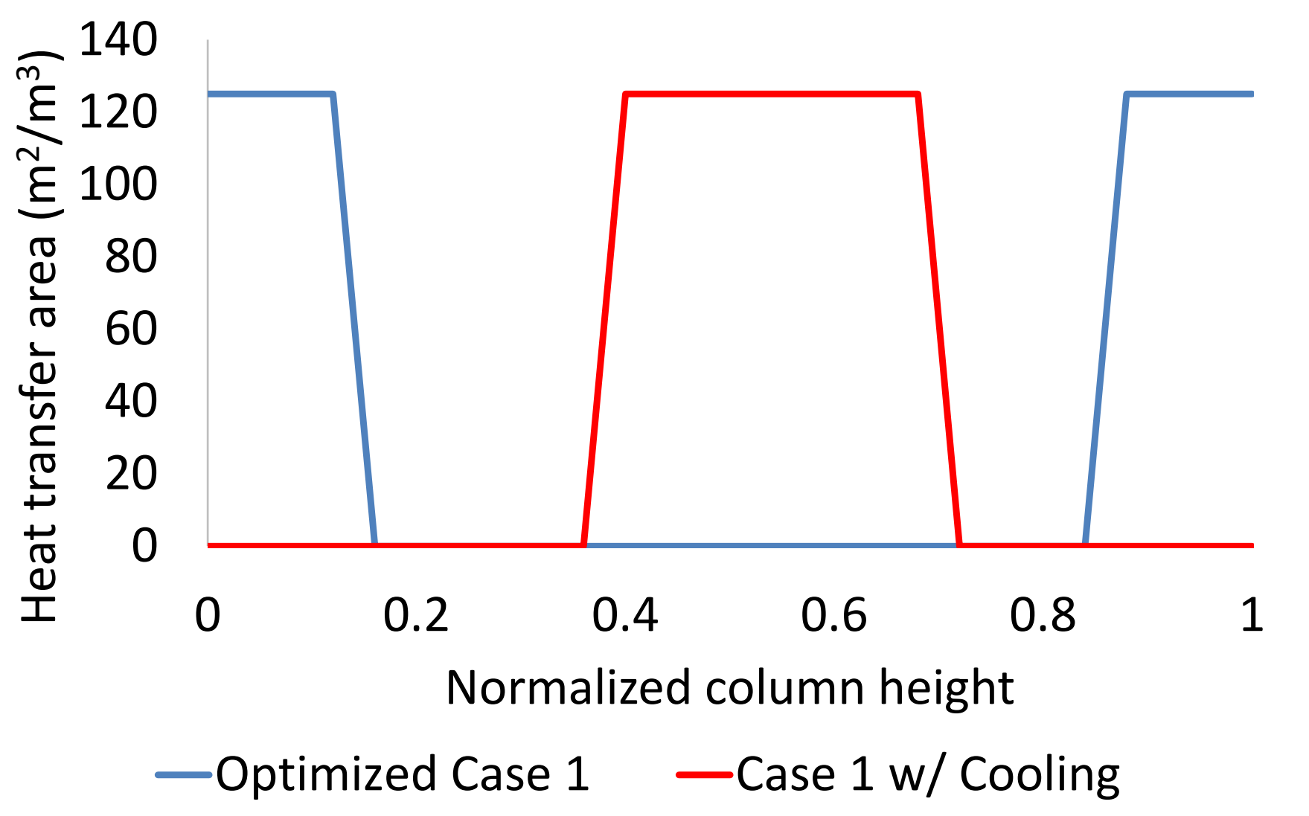
$$\min_{\varepsilon^{cw}, y, y^{start}, d} F^{V,out}_{CO_2}$$

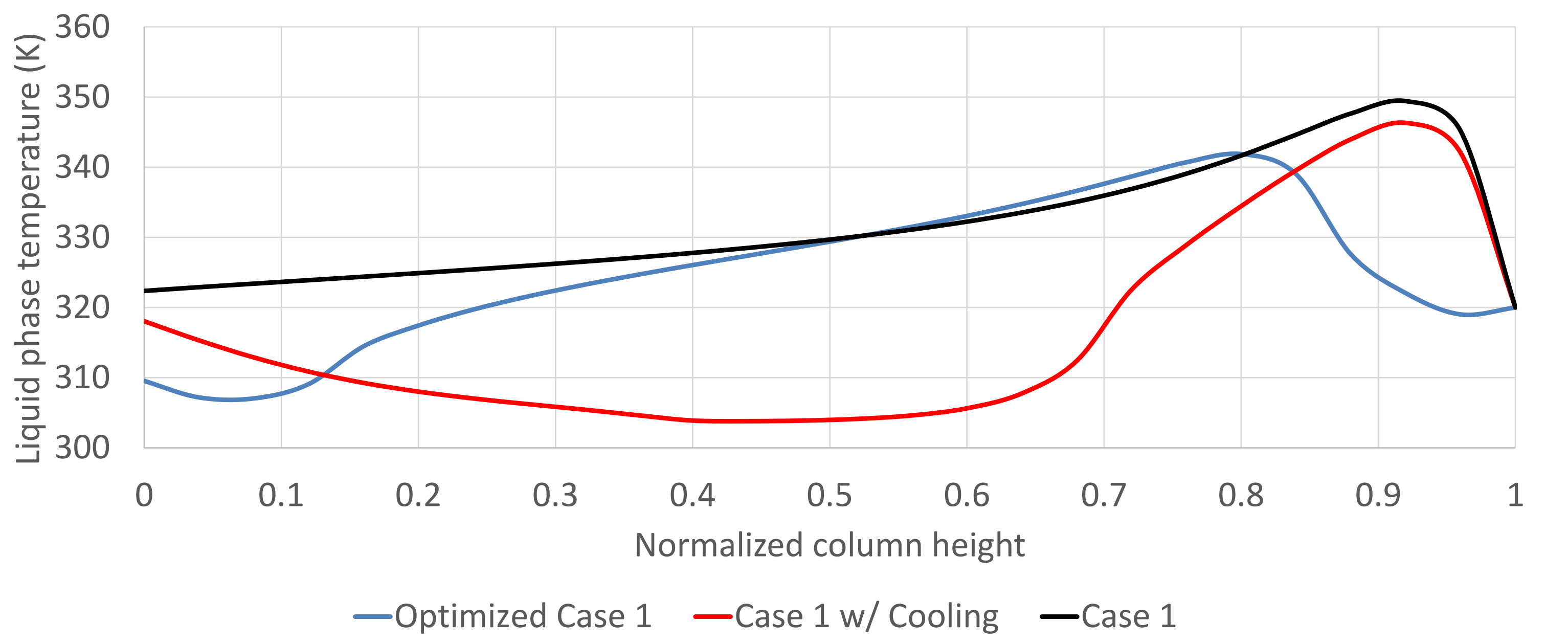
Tower Design and Operating Conditions

	Height (m)	Diameter (m)	$F^{V,in}$ (mol/s)	L/G	Lean Loading
Case 1 (Pilot Scale)	15	0.65	22	1.77	0.15
Case 2 (Process Scale)	20	12	12,000	1.83	0.22

* 0 and 1 indicate bottom and top of tower, respectively

Case	Capture percent
Case 1	72.46%
Case 1 w/ Cooling	75.63%
Optimized Case 1	76.94%



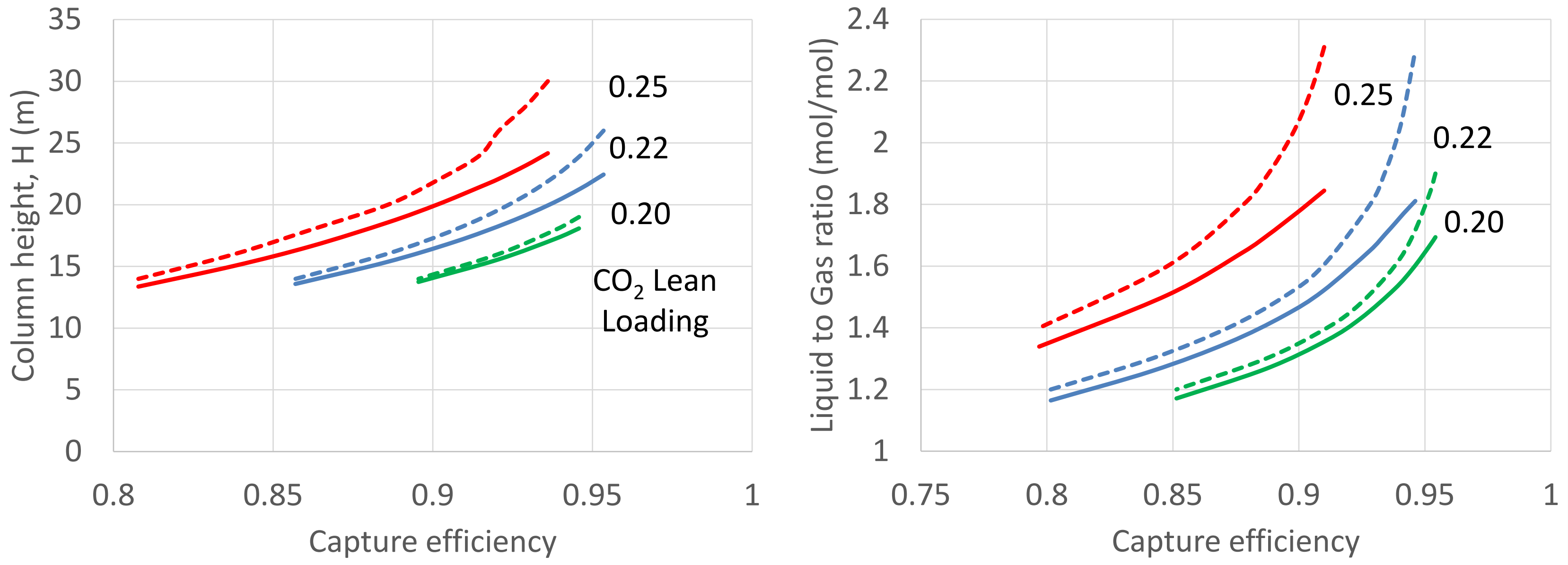


Optimization Case Studies

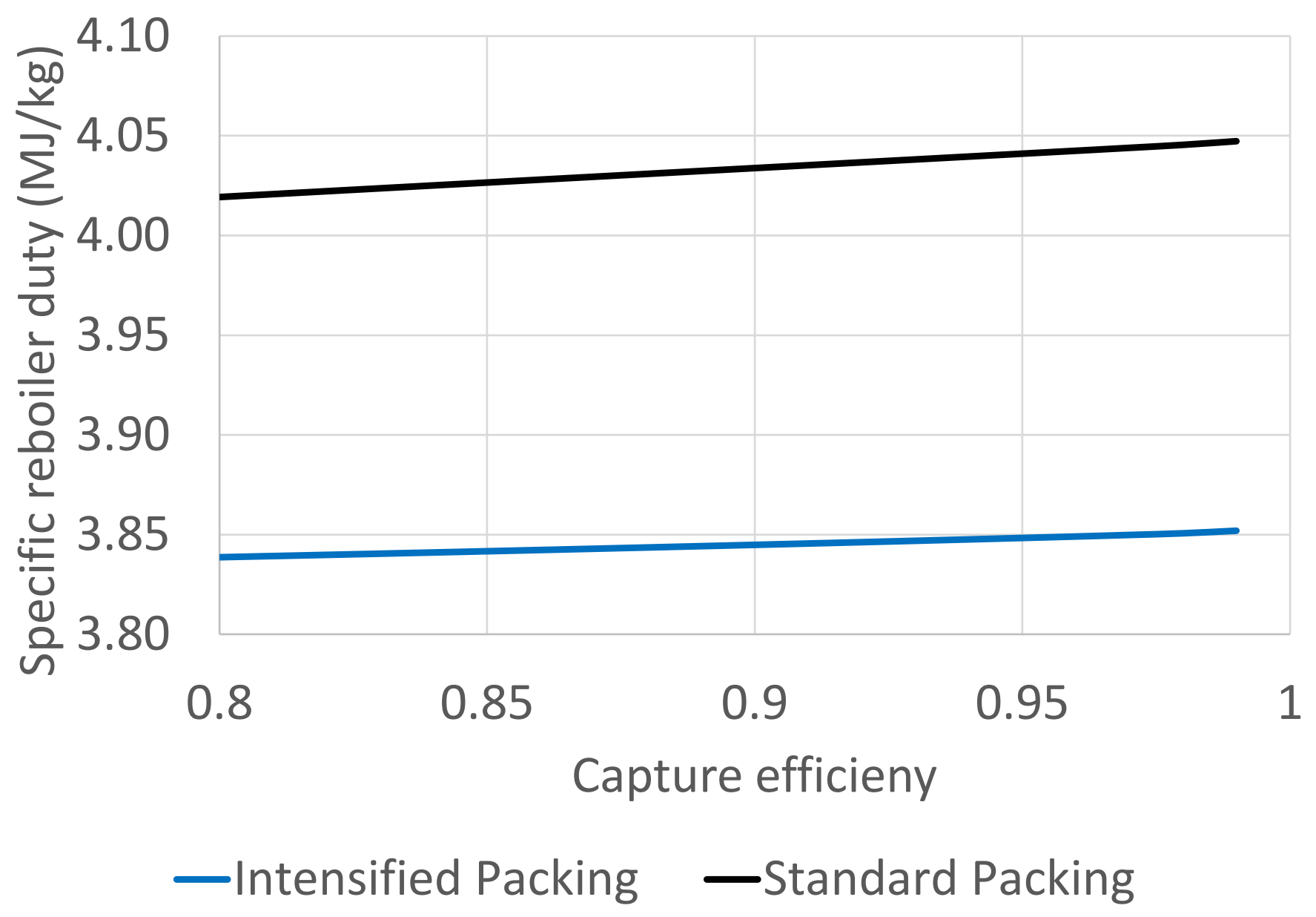
- Series of optimization studies are conducted at process scale (Case 2) absorber conditions.
- Minimizing column height and solvent flow rate have considerably implications to both capital and operating costs.
- As capture efficiency and lean loading increase, the benefit of internal heat exchanger application rises significantly.

Objective Functions

$$\min_{\varepsilon^{cw}, y, y^{start}, d} \mathrm{H} \qquad\qquad \min_{\varepsilon^{cw}, y, y^{start}, d} F^L/F^V$$
$$F^L/F^V = 1.83 \qquad\qquad H = 20m$$
$$s.t. \;\; \eta_{capture} \ge C$$



Both column height and solvent flowrate can have significant reductions, of up to 20%, while retaining capture efficiency due to optimally placed internal heat exchangers (**solid line**) compared to standard packing (**dashed line**), especially at higher capture rates



Increased efficiency from the internal heat exchangers allows energy penalties in other areas of the process to be reduced. Reboiler duty in the solvent regeneration process is decreased by as much as 5% when utilizing optimally placed internal heat exchangers compared to standard packing

Summary & Conclusions

- Placement of internal heat exchangers is optimal in regions which are thermodynamically limited by high temperatures or small concentration gradients.
- Relative improvement in capture is very high early on as the cooling water flowrate is increased and then beyond certain cooling water flowrate, there is hardly any improvement. Relative improvement with the change in the cooling water flowrate depends on the flow configuration.
- Optimal placement of the internal heat exchanger are found to result in considerable reduction in the tower height for a given L/G ratio or reduction in L/G ration for a given tower height when capture efficiency and CO_2 lean loading increase, which has significant implications for potential cost reductions.
- Future work will include economic optimization for varying flue gas loads.

Acknowledgements: The authors graciously acknowledge funding from the U.S. Department of Energy, Office of Fossil Energy and Carbon Management, through the Carbon Capture Program.