# Optimal Design and Operation of a Solvent-Sorbent Hybrid Capture Process for Minimizing the Cost of High Capture

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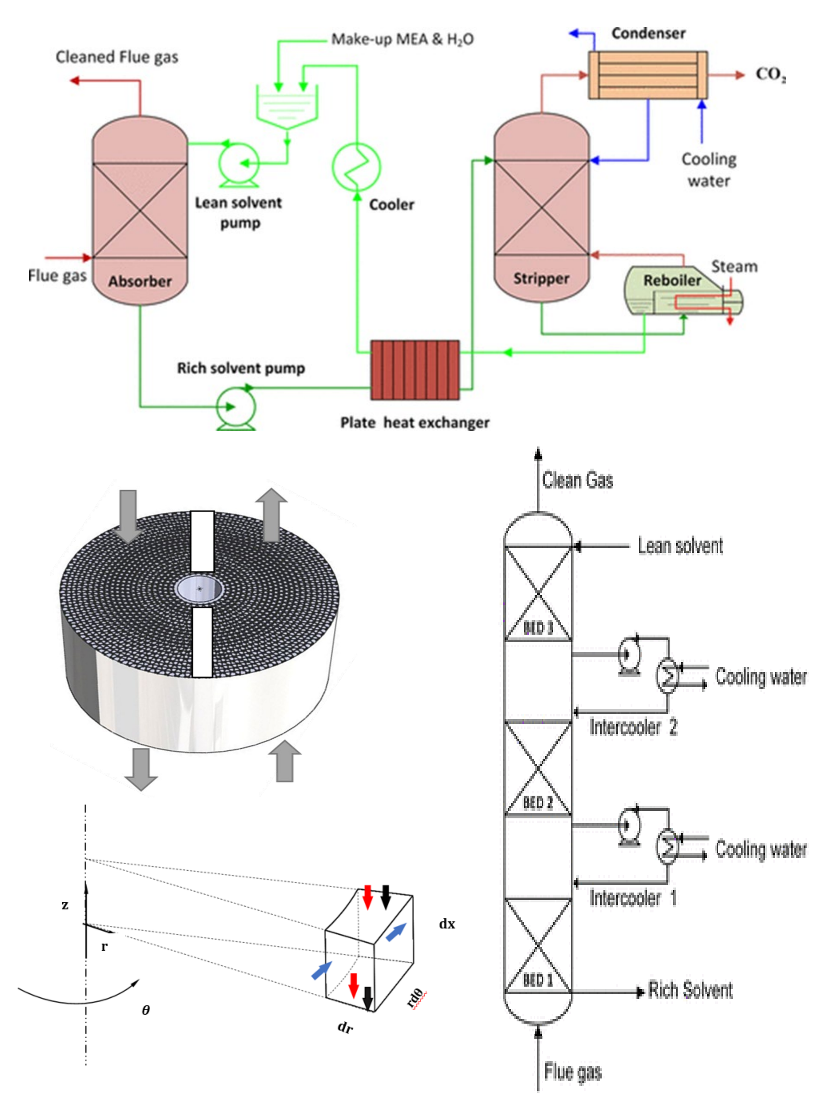
CCSI[2] Carbon Capture Simulation for Industry Impact

## Motivation: Hybrid Technology[1,2]

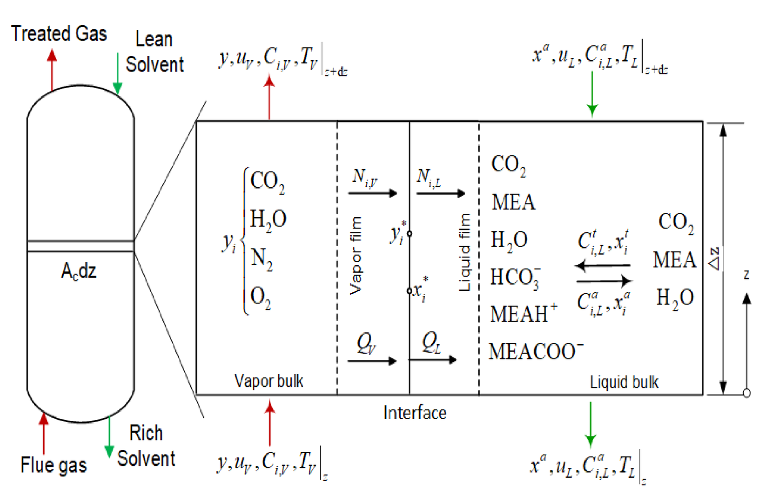
- **Steep Increase in Cost at High Capture:** High capture can cause a significant increase in energy penalty if the appropriate technology/technologies are not utilized.
- **Hybrid Technology for Improved Energy Efficiency:** The optimal technology for bulk capture is not necessarily the optimal technology for polishing capture (i.e., high extent of capture from the flue gas with very low partial pressure of $CO_2$). This work investigates the use of MEA for bulk capture with the polishing capture being accomplished by a functionalized metal organic framework (MOF).
- **Key Questions:** What should be the optimal bulk capture by the solvent and polishing capture by the sorbent? What are the optimal design and operating conditions for the desired capture by the solvent and sorbent systems?

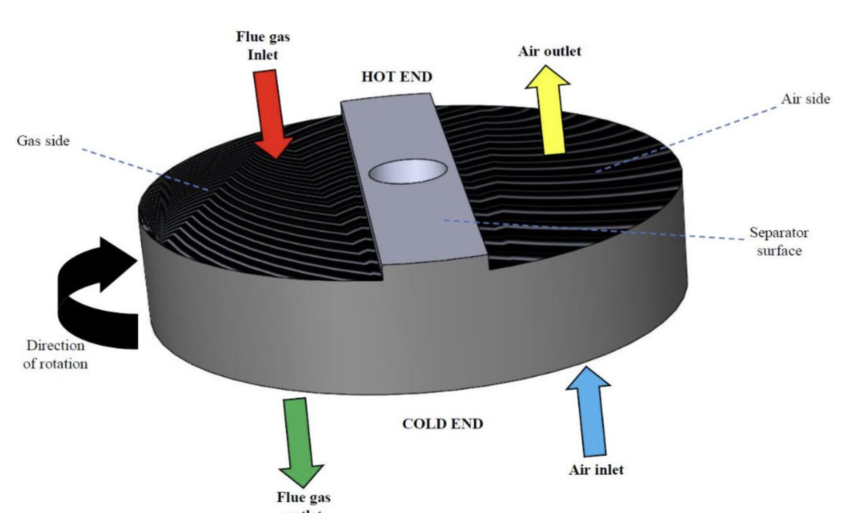


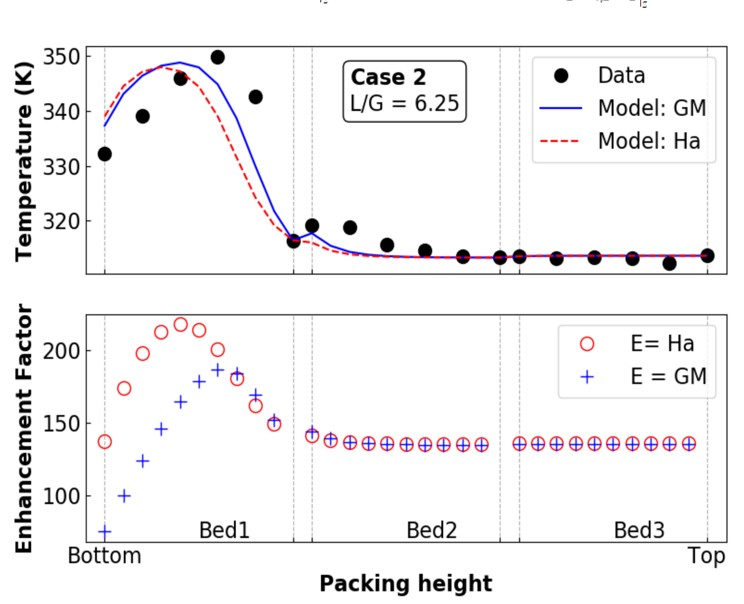

## Model Development[1,3]

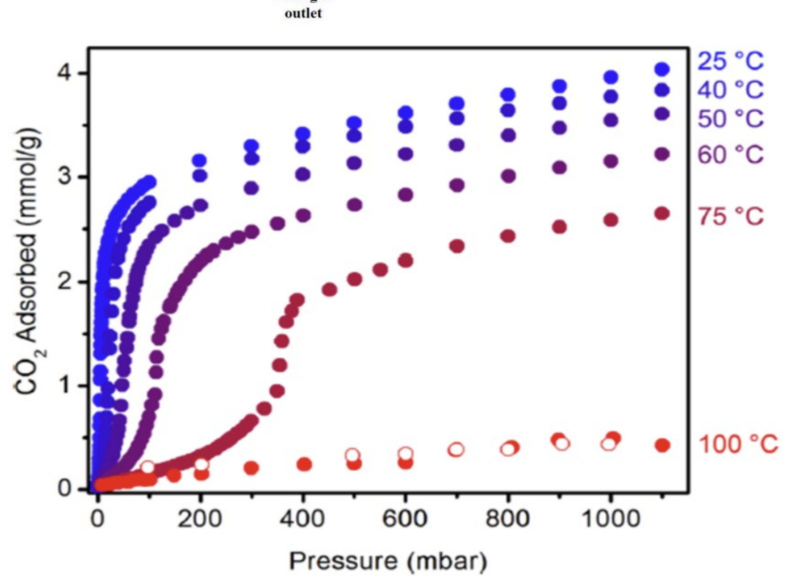
- Two-film model with thermo, chemistry, and properties models
- 1D in axial direction
- Validated using data from NCCC

- RPB model is 2d considering variation in axial and angular directions
- Utilizes a chemistry-based isotherm model for predicting adsorption behavior





### References

[1] Akula, P., Eslick, J., Bhattacharyya, D., & Miller, D. C. (2021). Model Development, Validation, and Optimization of an MEA-Based Post-Combustion CO 2 Capture Process under Part-Load and Variable Capture Operations. Industrial & Engineering Chemistry Research, 60(14), 5176–5193.

[2] Hughes, R., Kotamreddy, G., Bhattacharyya, D., Parker, S. T., Dods, M. N., Long, J. R., Omell, B., & Matuszewski, M. (2024). Development of a chemistry-based isotherm model and techno-economic optimization of a moving bed process for CO2 capture using a functionalized metal-organic framework. Chemical Engineering Science, 287, 119679.

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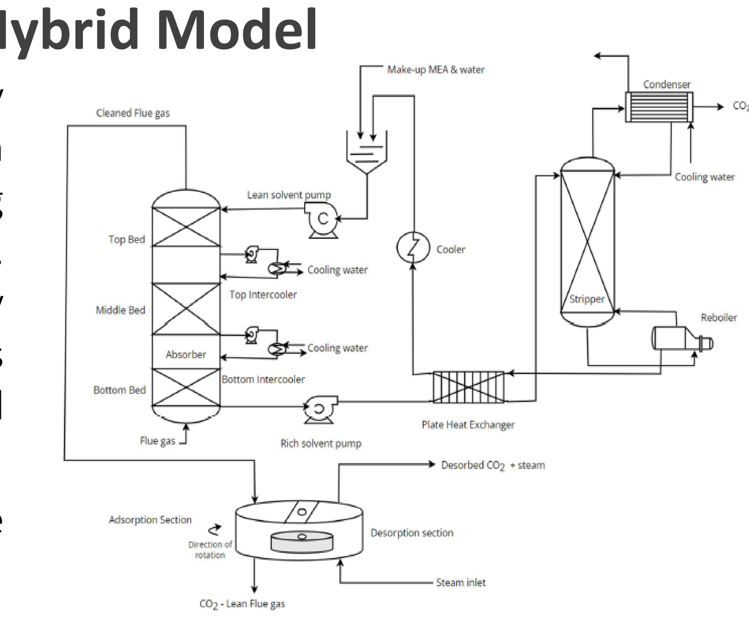
## Solvent-Sorbent Hybrid Model

- With the increase in the extent of capture by the solvent system, partial pressure of $CO_2$ in the sorbent-based capture keeps decreasing even for the same overall extent of capture. However, the respective increase in the energy requirement in the sorbent system is much less steep than the solvent system for similar level of capture from the lean flue gas.
- The polishing step by the MOF helps to reduce the capital costs for the capture system.



## Model and Optimization Setup

Software:

- Pyomo/IDAES
- IPOPT

Simulation conditions:

- Solvent(wt%): 30% MEA, 66% $H_2O$, 4% $CO_2$
- Flue gas(mol%): 5% $CO_2$, 5% $H_2O$, 78% $N_2$ , 12% $O_2$

**Solvent-based capture**

Objective Function:
Minimize specific heat duty

Decision variables:

- Solvent recirculation rate
- L/G ratio
- Reboiler duty
- Intercooler return temperature

Constraints:
Other than equality constraints, minimum approach temperature for the intercooler is considered to be 10 °C, and the approach temperature for the lean/rich heat exchanger is set at 5 °C

**Sorbent-based capture**

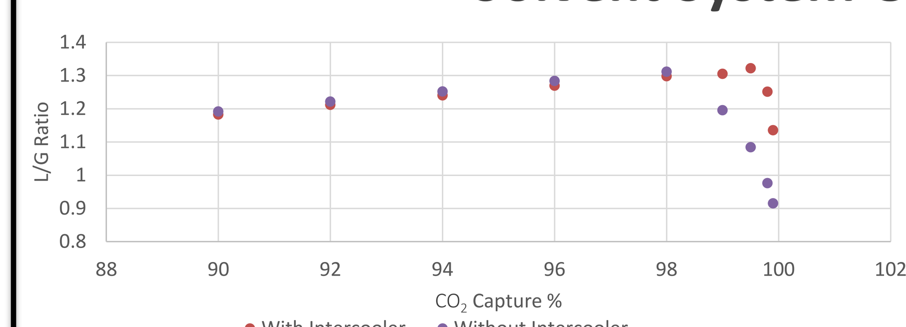
Objective Function:
Minimize specific heat duty

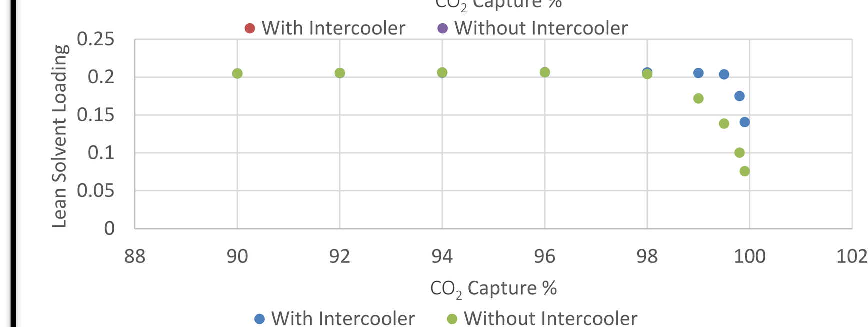
Decision variables:

- Bed length
- Bed rotational speed
- Adsorber bed fraction
- Sweep steam flow rate
- Adsorption cooling temperature
- Desorption heating temperature

Constraints:
Other than equality constraints, bound constraints for the decision variables

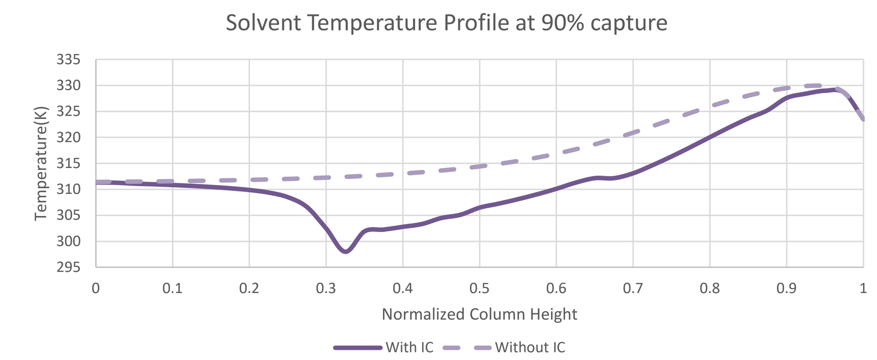
## Solvent System Optimization

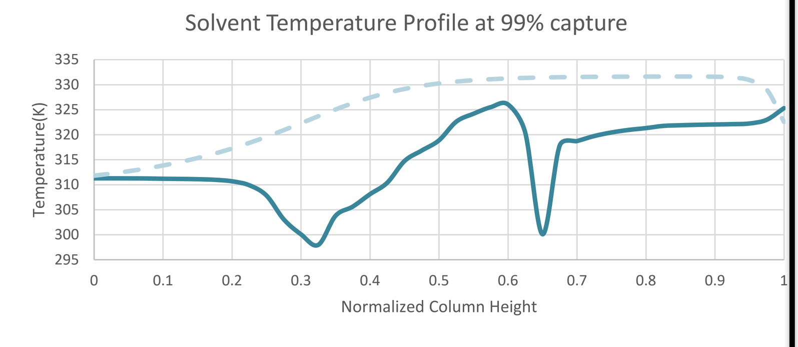


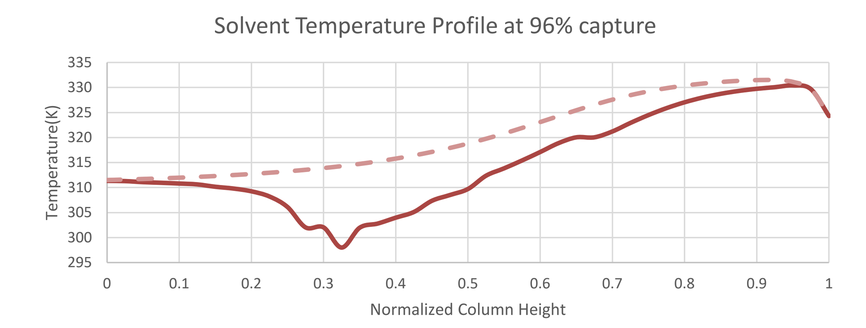



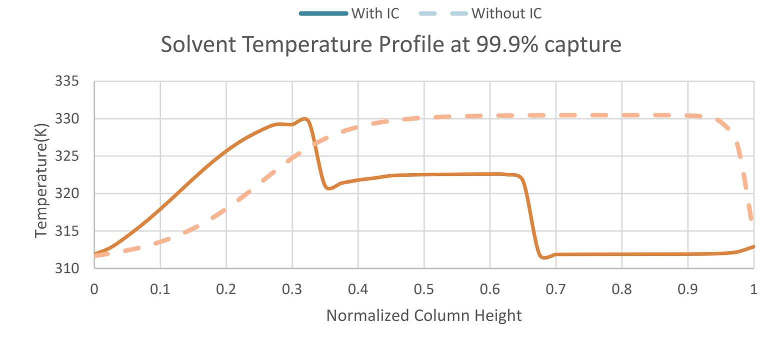

| CO2 Capture (%) | SRD with Intercooling (MJ/kg) | SRD without Intercooling (MJ/kg) |
|---|---|---|
| 90 | 4.096 | 4.104 |
| 92 | 4.102 | 4.113 |
| 94 | 4.109 | 4.123 |
| 96 | 4.117 | 4.134 |
| 98 | 4.134 | 4.173 |
| 99 | 4.168 | 4.811 |
| 99.5 | 4.219 | 6.477 |
| 99.8 | 4.869 | 10.959 |
| 99.9 | 6.627 | 16.288 |

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

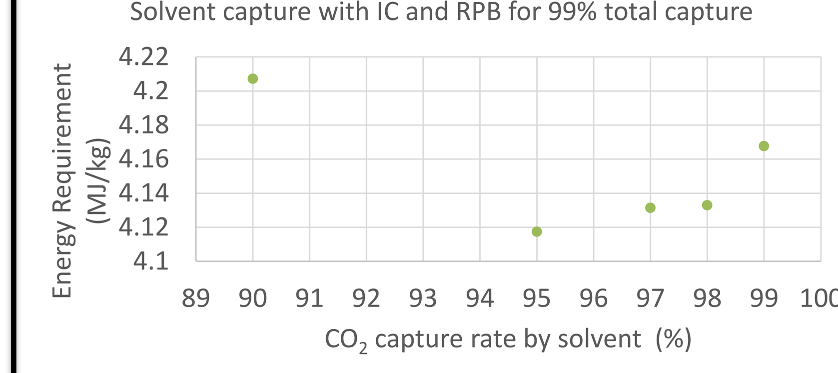


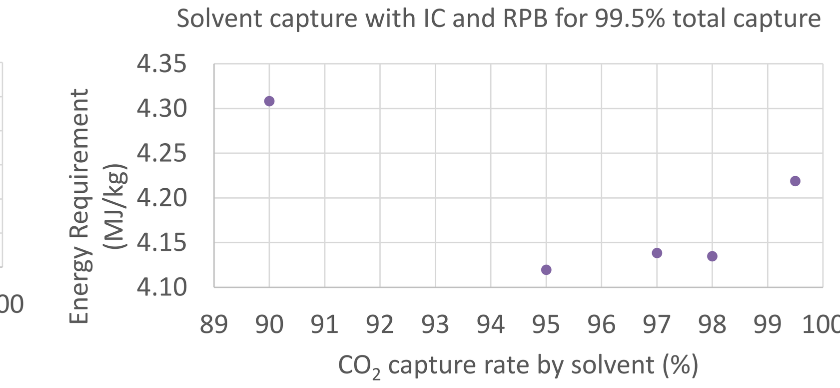



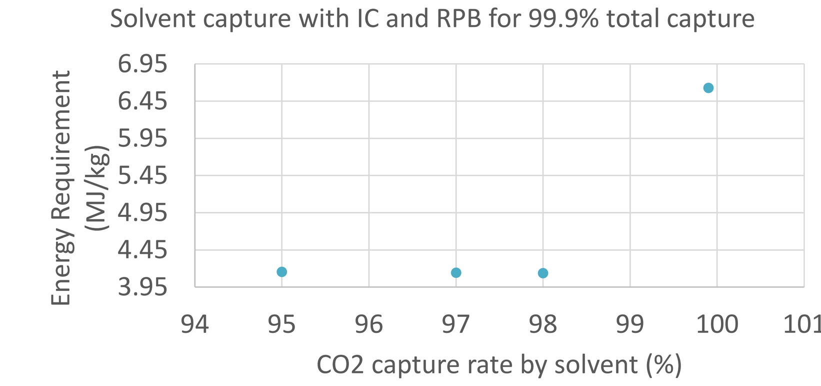




## Hybrid System Optimization




**Optimal Values of decision variables for high capture**

| Total Capture | 99% | 99.5% | 99.9% |
|---|---|---|---|
| **Captured by Solvent** | **95%** | **95%** | **98%** |
| L/G ratio | 1.255 | 1.255 | 1.298 |
| Reboiler duty (MW) | 101.73 | 101.73 | 105.46 |
| Intercooler 1 return temperature (K) | 318.17 | 318.17 | 327.42 |
| Intercooler 2 return temperature(K) | 298 | 298 | 298 |
| | | | |
| **Captured by Sorbent*** | **80%** | **90%** | **95%** |
| Bed length(m) | 3.221 | 3.878 | 6.466 |
| Adsorber bed fraction | 0.712 | 0.791 | 0.922 |
| Sweep steam flow rate (mol/sec) | 2.436 | 2.704 | 1.269 |
| Adsorption cooling temperature (K) | 298 | 298 | 304.33 |
| Desorption heating temperature (K) | 433 | 433 | 432.86 |

* Rotary Packed Bed (RPB) diameter is fixed at 10m

## Summary and Conclusions

- Intercoolers within the absorption tower can offer a reduction in energy consumption compared to the base case without intercooling, with the reduction in energy being steeper at higher capture rates.
- While the energy requirement for MEA-based capture steeply increases at high capture, the energy penalty of the solid sorbent system remains reasonably flat even at high capture. The steep increase in the energy requirement by the MEA system is due to the required low $CO_2$ loading of the lean solvent for achieving high capture.
- Integrating a functionalized MOF-based RPB for polishing capture from the flue gas from the solvent-based capture unit can considerably reduce the energy penalty at high capture rates.
- The optimal capture split between the solvent and RPB units depends on the target capture rate. The solvent unit is found to be energetically efficient for bulk capture while the sorbent capture is found to be comparatively much more energy efficient than the solvent system at very high capture, especially approaching net-zero and net-negative capture rates.
- Future work will include development of the economic model of the solvent and sorbent systems and economic optimization of the integrated process.

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