CFD Modeling of Hollow Fiber Membrane Contactor for Post-Combustion CO_2 Capture

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Outline

- Introduction
  - Mass Transfer in a gas/liquid membrane contactor
- Development of CFD model
- Results and discussion
  - Characterization of Liquid/gas film resistance
  - Influence of membrane to overall mass transfer
  - Influence of chemical reaction to overall mass transfer
- Conclusions

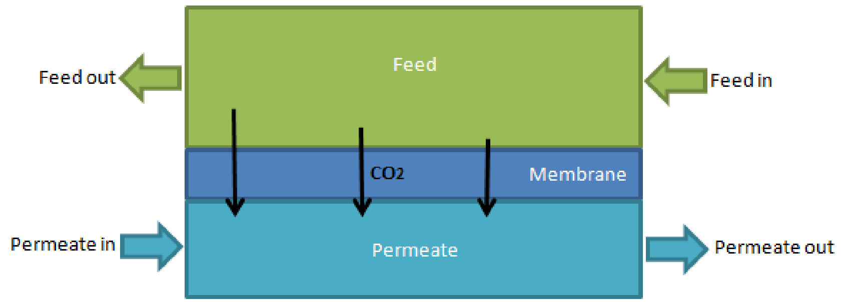
Introduction

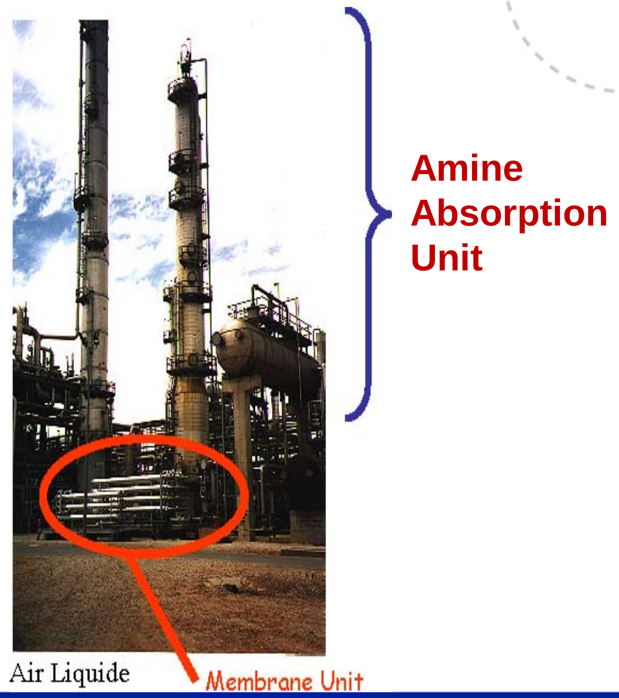
Membrane contactor; a hybrid technology

❑ Compared to absorption columns

- Larger sp. surface area, linear scale-up, modular design, flexible operation

Contractors	Sp surface area (m^2/m^3)	Reference
Free dispersion column	1-10	Reed et al. (1995)
Mechanically agitated column	50-150	Westerterp et al. (1984)
Packed column	100-800	Reed et al. (1995)
Membrane contactor	1500-3000	Kumar et al. (2002)

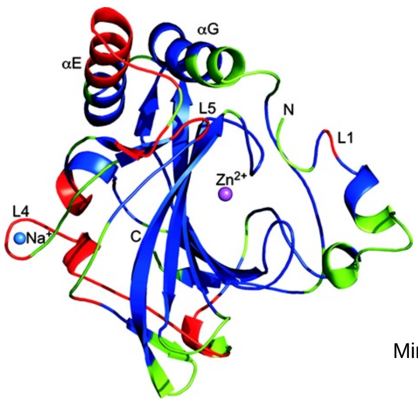




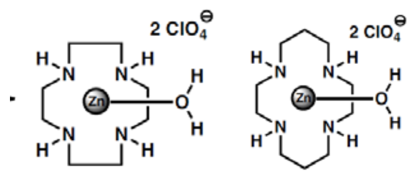
Introduction

❑ Membrane contactor for flue gas treatment

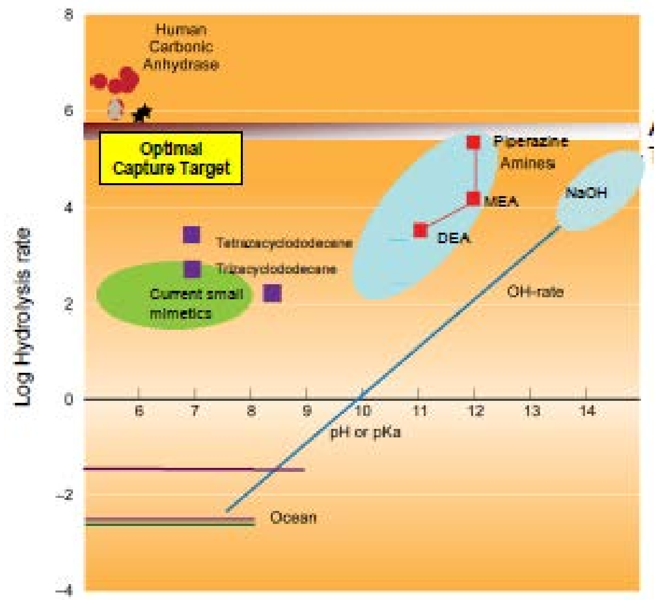
- High and non dispersive contact offers efficient mass transfer
- Highly reactive Carbonic anhydrase (CA) and mimic CA with reaction rate 4000 times faster than MEA to account for low mass transfer driving force



Carbonic Anhydrase Molecular structure



Mimic Carbonic Anhydrase Molecular structure



Hydration rate of CO2 by various absorbents.
Aines R. H Lawrence Livermore National Laboratory

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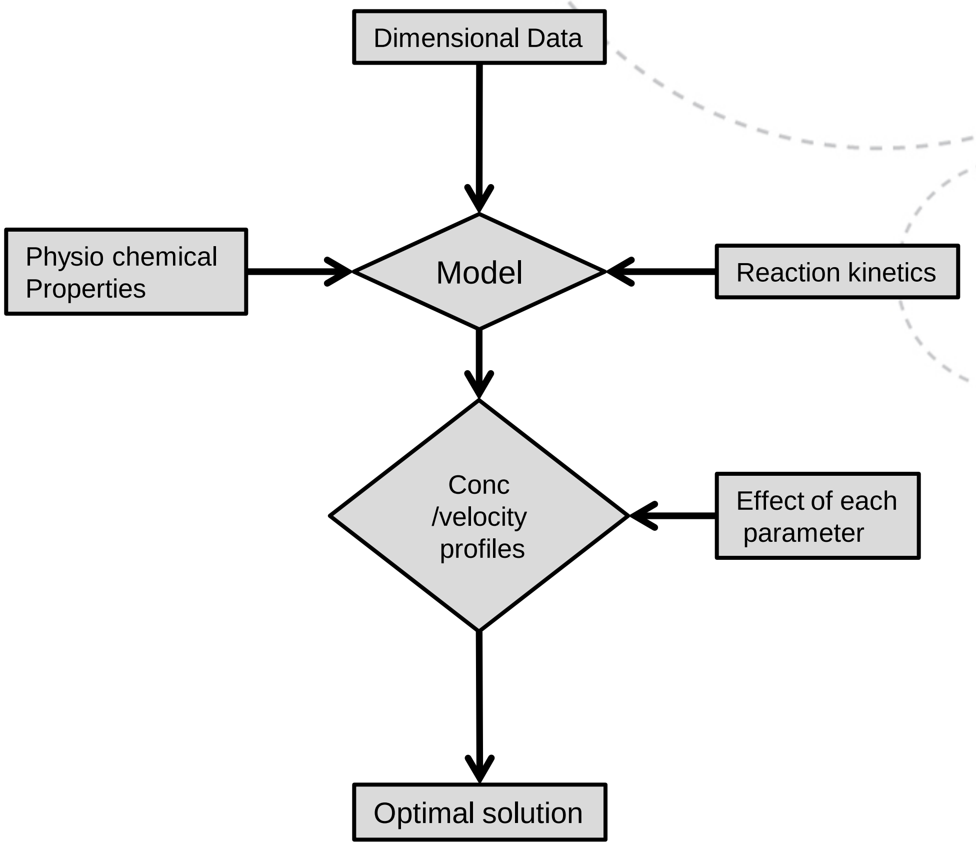
Scope

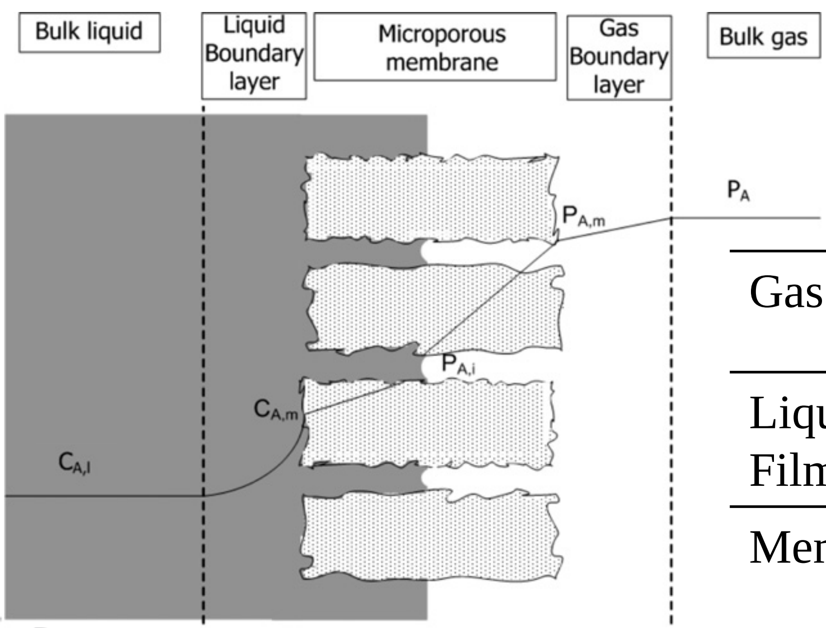
This work

- CFD model of a membrane contactor with physical and chemical absorption by using **Multi physics COMSOL**
- Carbonic anhydrase (CA) and mimic CA for reactive absorption of CO_2
- Mass transfer through a micro porous, hydrophobic membrane
- Developed model to suggest an optimal set of parameters for designing operations of a membrane contactor.



Mass Transfer in Membrane Contactor

- Overall mass transfer in a membrane contactor is analogues to heat transfer and can be exemplified by resistance in series model.

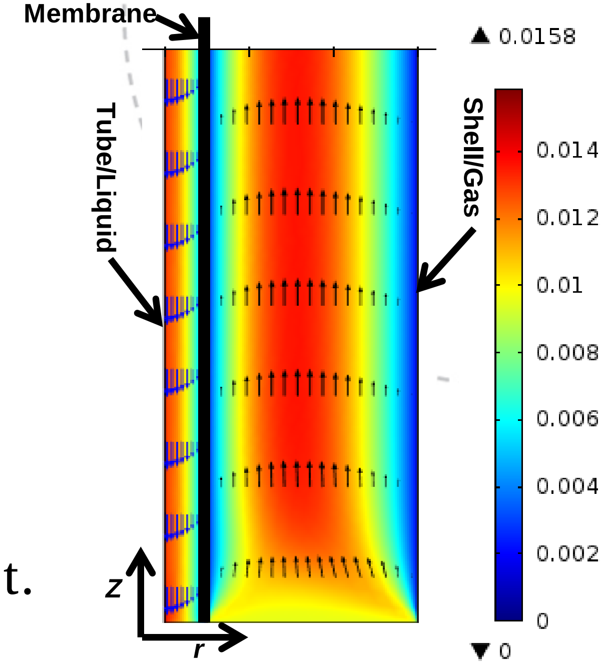


$$\frac{1}{K_{ov}} = \frac{1}{k_l} + \frac{1}{k_m} + \frac{1}{k_g}$$

Gas Film	$u\frac{\partial C_A}{\partial z} = D_{Ag}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r.\frac{\partial C_A}{\partial r}\right)\right]$
Liquid Film	$v\frac{\partial C_A}{\partial z} = D_{AL}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r.\frac{\partial C_A}{\partial r}\right)\right] - R_A$
Membrane	$D_{Am}\left[\frac{\partial^2 C_A}{\partial r^2} + \frac{1}{r}\left(\frac{\partial C_A}{\partial r}\right) + \frac{\partial^2 C_A}{\partial z^2}\right] = 0$

CO_2 concentration profile in a membrane contactor adapted from **Journal of Membrane Science 380 (2011) 21– 33**

Model development



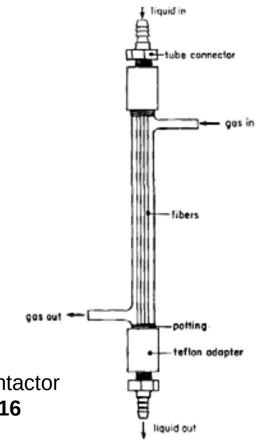
Velocity profile in gas/ liquid phase

❑ Assumptions

- Regular and uniform pores
- Hydrophobic membrane
- First order reaction between CO2 and catalyst.

❑ Model Basis

- Velocities are adjusted to maintain a laminar regime
- Flue gas containing 10% CO2 at 1 bar and 25^{o}C.
- Carbonic Anhydrase (CA) and mimic CA catalyst to promote the absorption in liquid



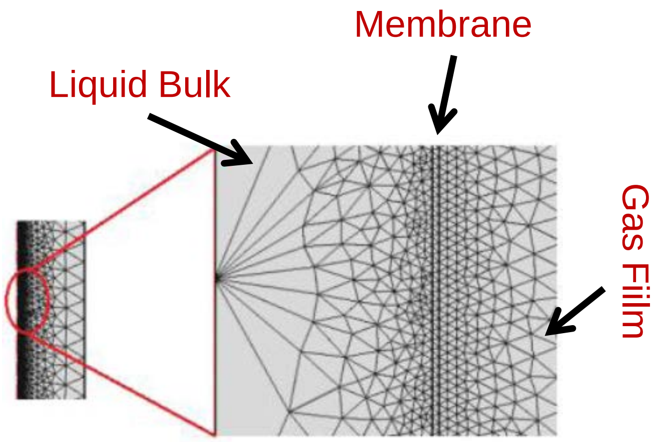
Longitudinal hollow fiber membrane contactor
AIChe Journal 1986,32,11 1910-16

Model development (cont…)

Basis for model geometry

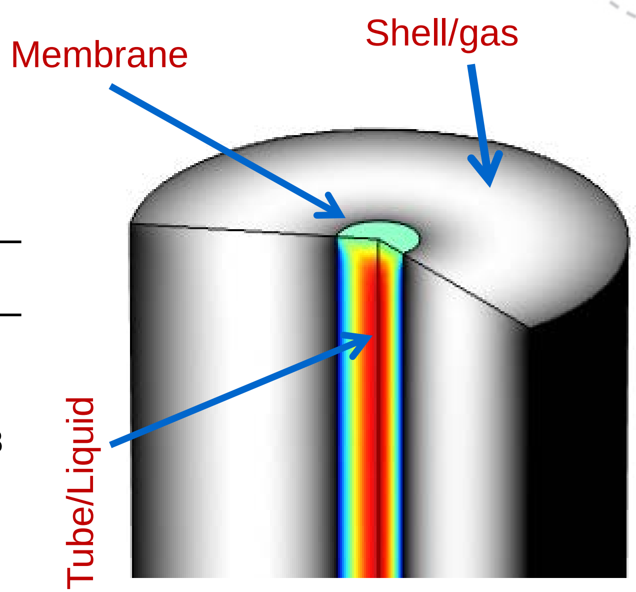
Parameter	Symbol	Value
Length	L	100mm
Radius of membrane	R_1	1 mm
Radius of shell	R_2	6mm
Porosity	P_{or}	0.7
Tortuosity	T_{or}	2
Conc. in gas phase	C_o	10 %

- In this work Finite Element Method is used for calculations.



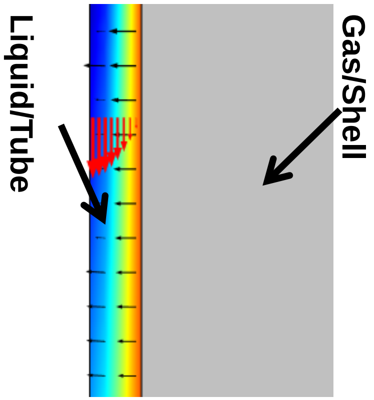
Finite element with physics controlled size

Literature	Value	Source
Diffusivity in Shell	1.5 x 10^{-5} m^2/S	Reid, R. C.; Prausnitz, 1986
Diffusivity in water	1.92 x 10^{-9} m^2/S	Chem. Eng. Comm., 1996, 144,113-158
Partition coefficient	1.205 x 10^{-2}	J. Chern. Eng. Data, 1988, 33, 29-34,
Reaction rate of MEA	5920 (1/s)	Chem Eng. Sci. 2007,39,207-25

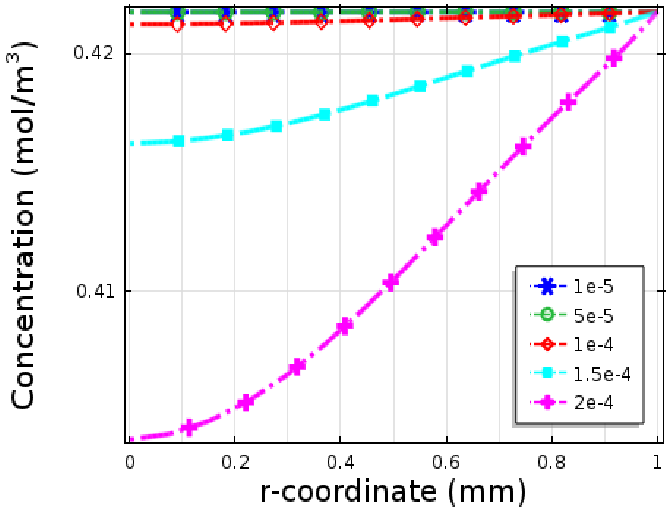


Results and Discussion

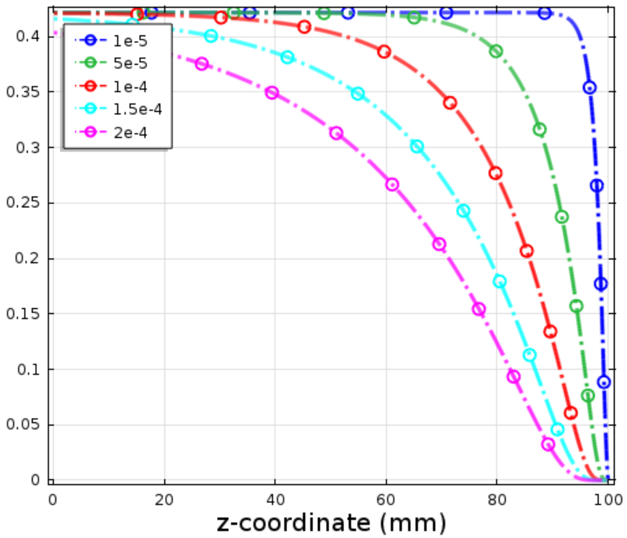
- Physical absorption of CO2 in liquid



Concentration profile of CO_2 in tube/Liquid



Radial concentration profile in liquid phase



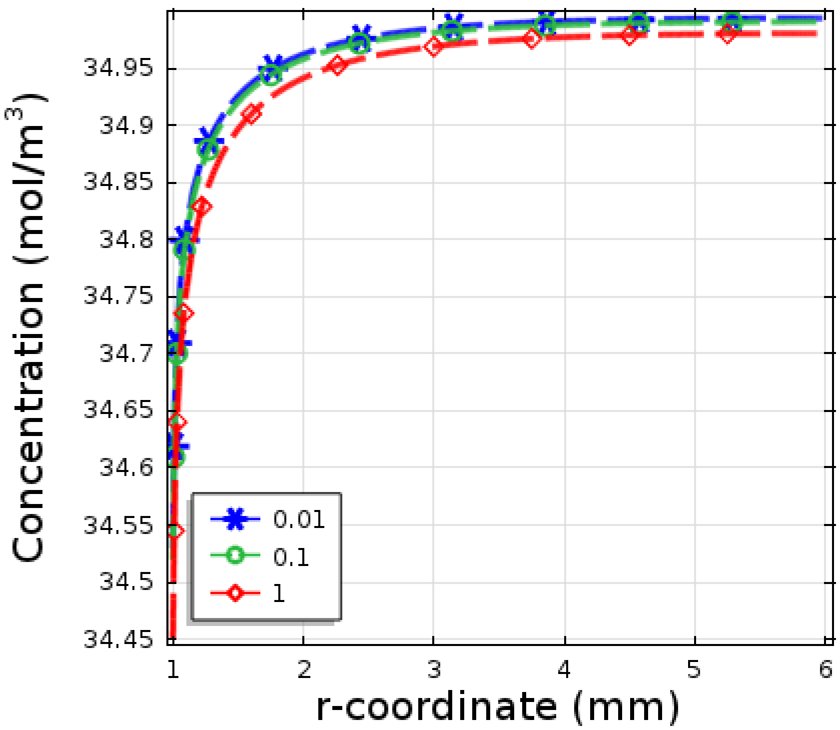
Liquid phase bulk concentration along the length of contactor.

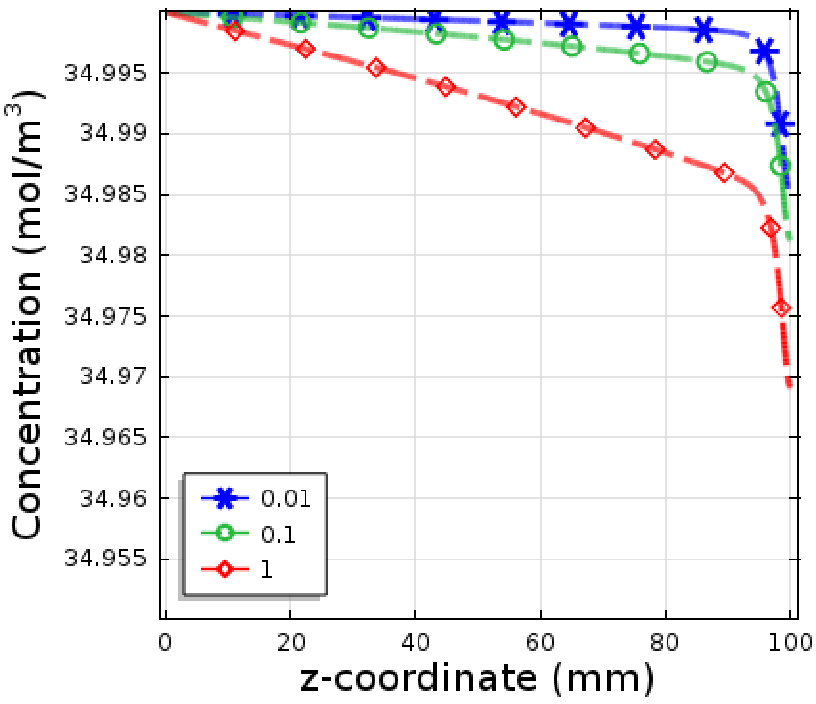
Liquid velocity changing from 1e-5 to 1 m/s

Appreciable effect on liquid loading.

Results and Discussion

❑ Physical absorption of CO2 in liquid

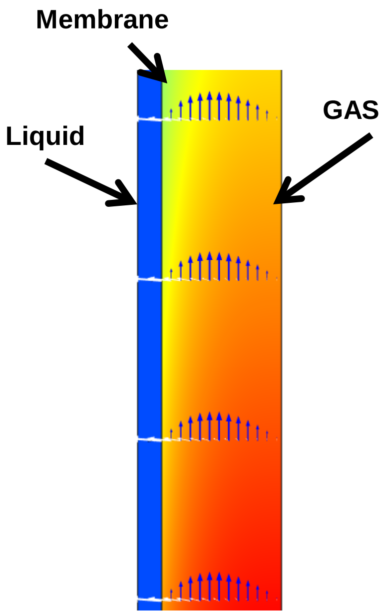




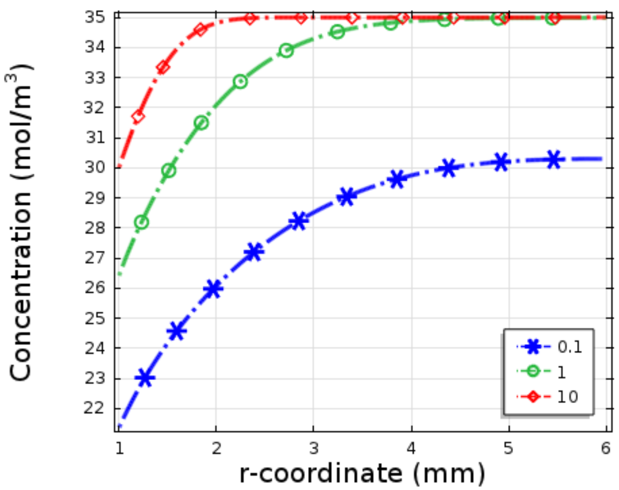
- **Appreciable effect on liquid loading. However, no significant effect on gas phase**

Results and Discussion

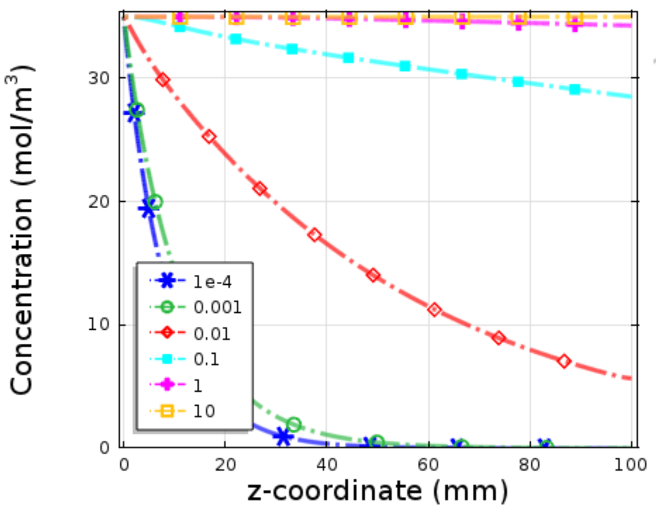
❑ Characterization of Gas film resistance



Concentration profile of CO_2 in shell and tube



Radial concentration profile in gas



Gas phase concentration along the length of contactor

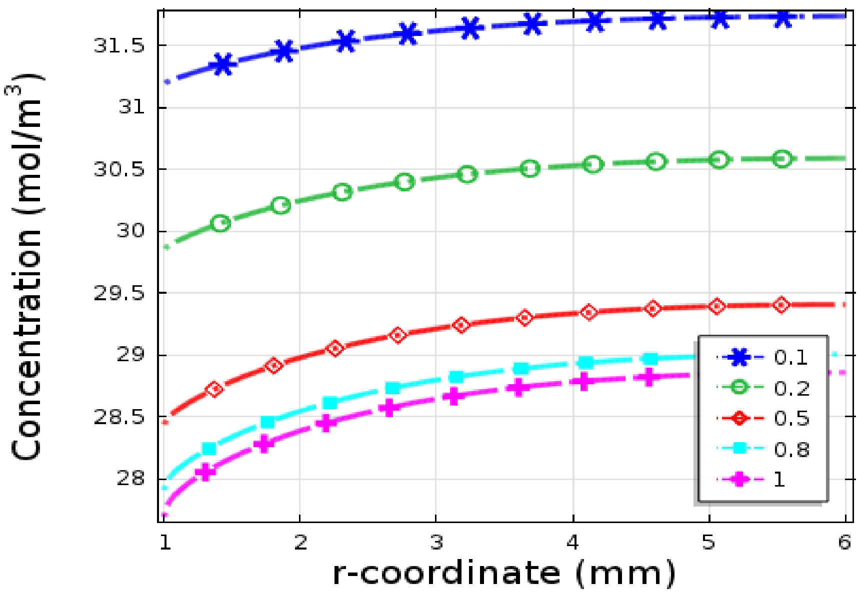
Investigated gas velocity: 1e-4 to 10 m/s

Appreciable effect of gas velocity at interfacial concentration shows that mass transfer limitation has now moved from liquid film to gas film/membrane.

Results and Discussion

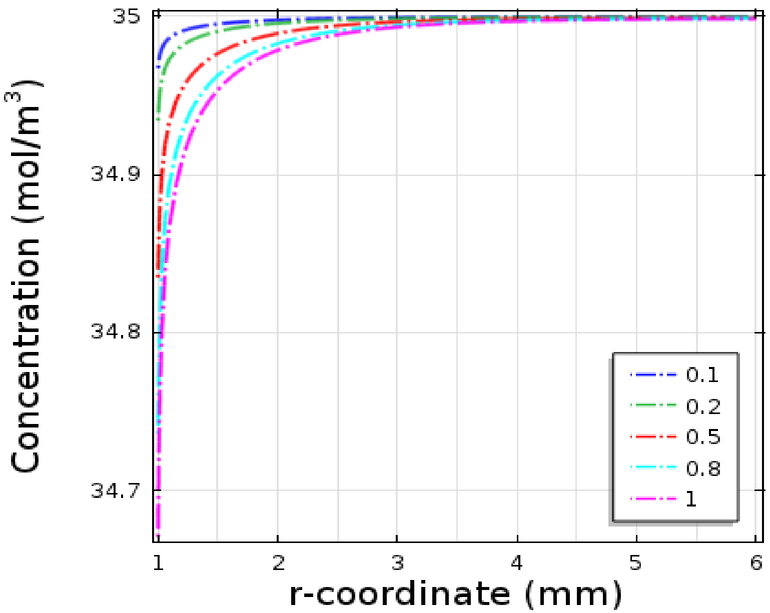
- Influence of porosity

Chemisorption



Gas phase radial concentration. porosity

Physical absorption



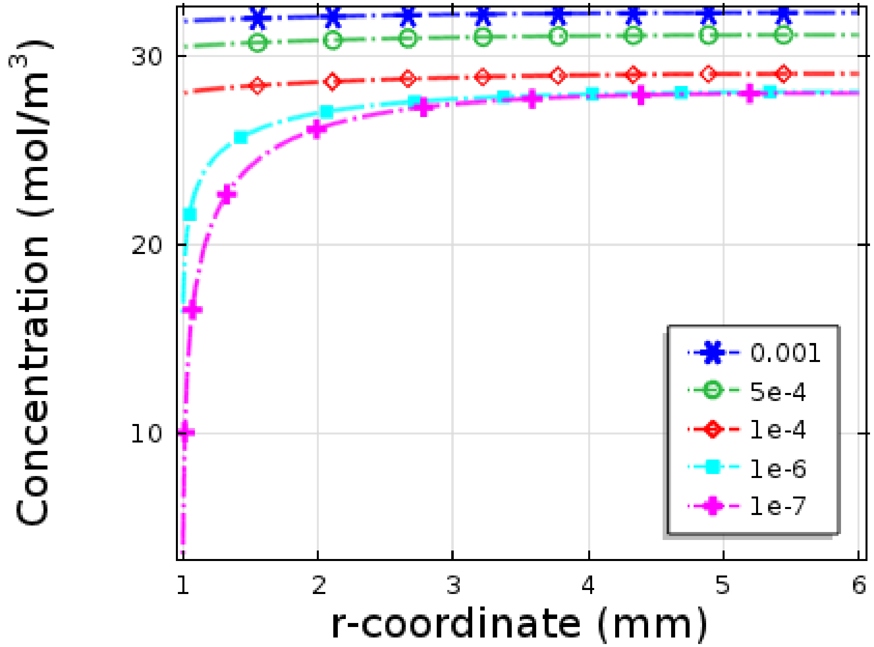
Gas phase radial concentration. porosity

Porosity of membrane varied from 0.1 to 1.

Membrane resistance has significant contribution to mass transfer in chemical absorption .

Results and Discussion

❑ Influence of membrane thickness



Gas phase radial concentration at varies membrane thickness

- Thickness of membrane was varied between 1 mm and 1e-4 mm.
- Thickness of membrane does have a significant effect on mass transfer but developing a self supported membrane of 1e-4 mm is challenging.

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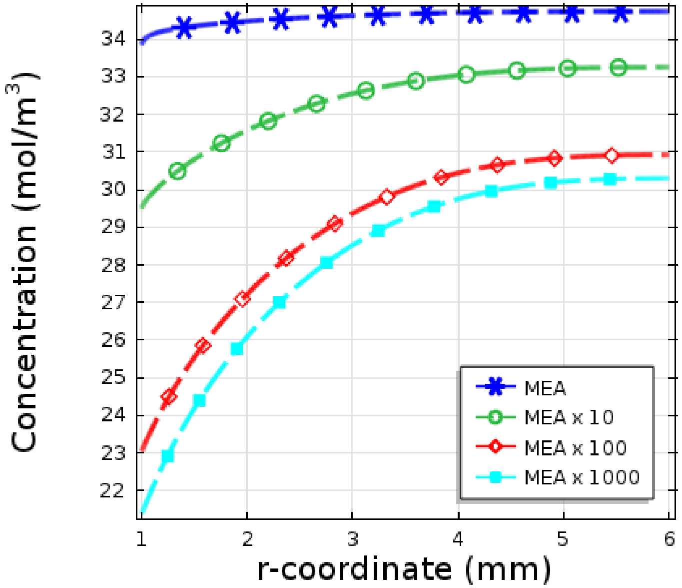
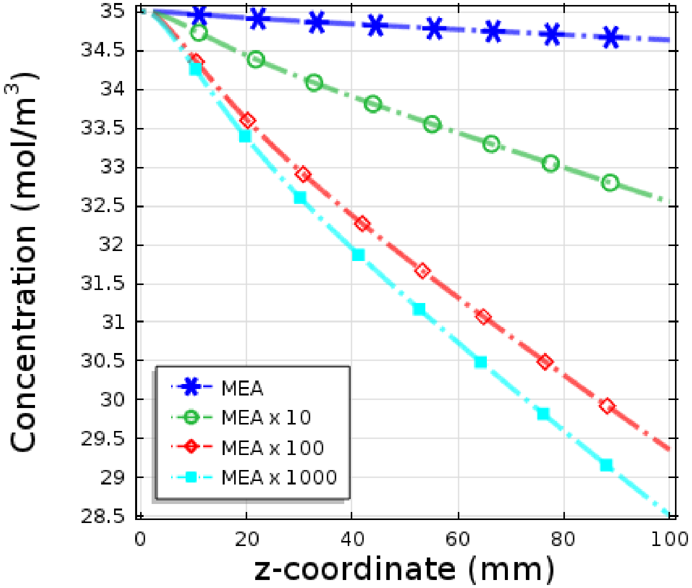
Results and Discussion

❑ Influence of Reaction



Gas phase radial concentration at various reaction rates



Gas phase axial concentration at various reaction rates

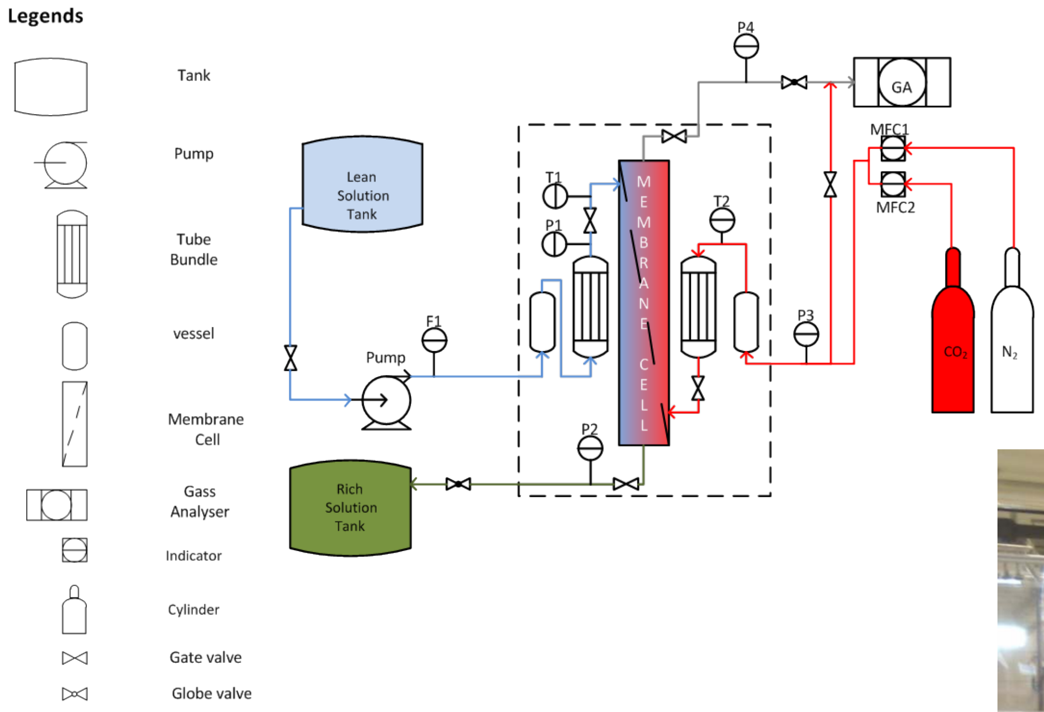
Reaction rate varied 10, 100 and 1000 times that of MEA.

With increase in reaction rate, a significant increase in efficiency is observed

Conclusions

- For Physical absorption, liquid film resistance is the limiting factor to mass transfer.
- For Chemisorption mass transfer resistance shifts to membrane and gas film.
- Membrane porosity and thickness contributes significantly to mass transfer in chemical absorption.
- This work is a guideline to design a membrane contactor operating with and without chemical reaction.

Validation


Legends
Tank
Pump
Tube
Bundle
vessel
Membrane
Cell
Gass
Analyser
Indicator
Cylinder
Gate valve
Globe valve
Lean
Solution
Tank
Rich
Solution
Tank
Pump
F1
P1
P2
P3
P4
T1
T2
MEMBRANE CELL
GA
MFC1
MFC2
CO2
N2

PCCC2 Post Combustion Capture Conference

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Thank you for your attention!

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