CFD Modeling of High-Flux Plate-and-Frame Membrane modules for industrial carbon capture

Cheick Dosso[a], Hector Pedrozo[a], Thien Tran[b,c], Lingxiang Zhu[b,c], Victor Kusuma[b,c], David Hopkinson[b], Lorenz Biegler[a], Grigorios Panagakos[a,b,c]

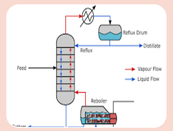
[a]Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA, USA 15213

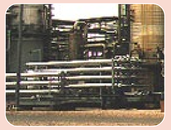
[b]National Energy Technology Laboratory, 626 Cochran Mills Rd, Pittsburgh, PA, USA 15236

[c]NETL Support Contractor, 626 Cochran Mills Rd, Pittsburgh, PA, USA 15236

Motivation





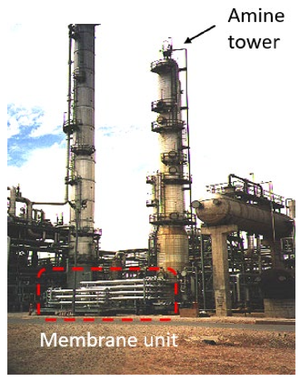


9.2 Gt out of 36.8 Gt of CO_2 in 2022

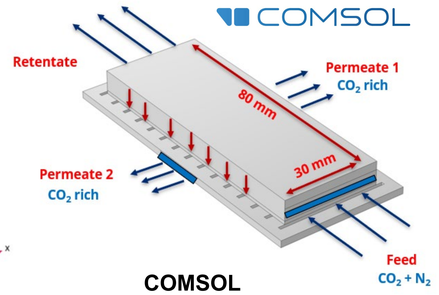
Net 0 emission by 2050 to limit temperature increase by 1.5 deg C

Modeling speeds up lab work and scale-up

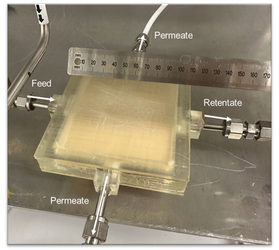
Membranes are *modular*, have a *small footprint*, require *low maintenance*, and require much *less energy* than absorption and adsorption



CFD Model



COMSOL model



Real membrane module

Fluid Flow and Diffusion

Physics of Transport in Feed and Permeate

Navier-Stokes: $(\boldsymbol{u}\cdot\nabla)\boldsymbol{u} = \nu\nabla^2\boldsymbol{u} - \frac{1}{\rho}\nabla p$ (Velocity; Kinematic viscosity; Pressure; Convective term; Diffusion term; Pressure gradient)

Convection-Diffusion: $\rho\boldsymbol{u}\cdot\nabla w_i = -\nabla\cdot\boldsymbol{j}_i = -\nabla\cdot(-\rho(D\nabla w_i))$ (Weight fraction; Diffusion; Diffusion coefficient; Density; Fick's law)

Diffusion on membrane boundary

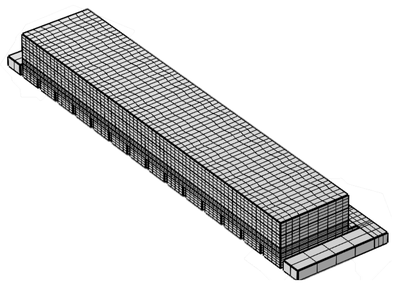
$|J_i| = Q_i \cdot M_i \cdot (p_1 \cdot x_{w_{i_{feed}}} - p_2 \cdot x_{w_{i_{perm}}})$

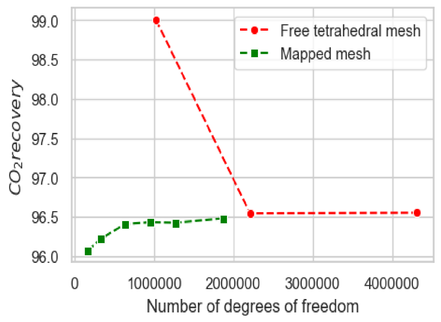
$M_i[=]\frac{g}{gmol}$ (Molar mass); $j_i[=]\frac{kg}{m^2\cdot s}$; mole fraction feed side; mole fraction permeate side; Permeance; Pressure feed; Pressure permeate

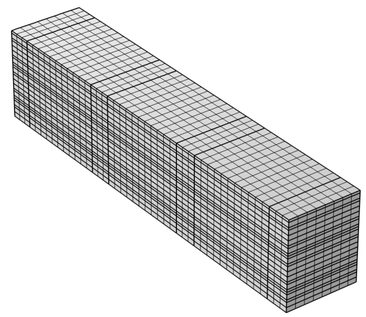
$Q_i[=]GPU[=]3.346\cdot10^{-6}\frac{mol}{Pa\cdot s\cdot m^2}$ $p[=]Pa[=]\frac{kg}{m\cdot s^2}$

Ensure Numerical Accuracy

Mesh independence study on CO_2 recovery







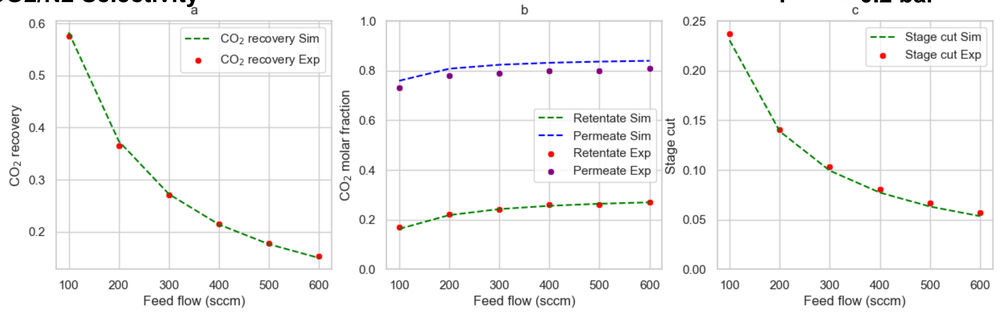
Optimized mesh for high accuracy and low number of degrees of freedom

Model is validated with experimental data

1600 CO2 GPU
28 CO2/N2 Selectivity

Feed concentration: 30% CO_2, 70% N_2

P^{feed} = 1.21 bar
P^{perm} = 0.2 bar

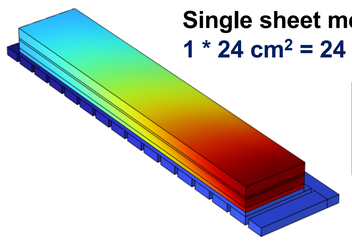


max error: 2.33%

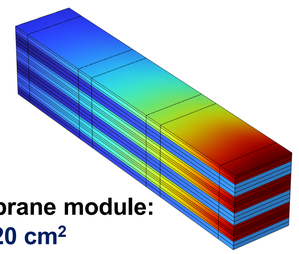
max error ret: 2.73%
perm: 4.5%

max error: 5.82%

Single sheet membrane module:
1 * 24 cm^2 = 24 cm^2



The CFD model is very reliable with small maximum relative errors!



Stacked membrane module:
5 * 24 cm^2 = 120 cm^2

3220 CO_2 GPU
23 CO_2/N_2 Selectivity

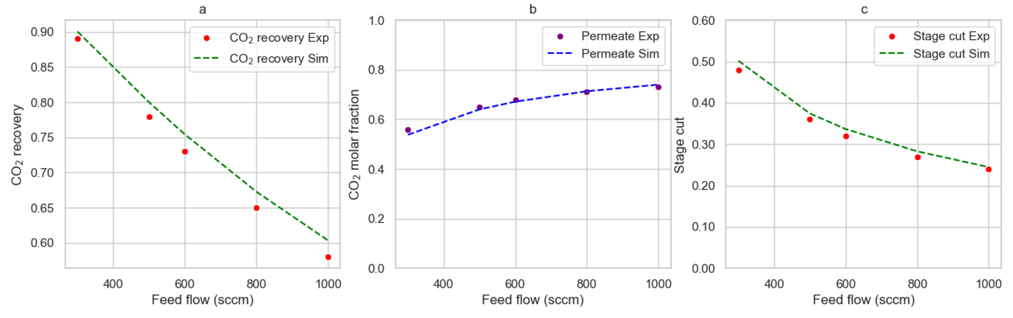
Feed concentration: 30% CO_2, 70% N_2

P^{feed} = 1.21 bar
P^{perm} = 0.2 bar

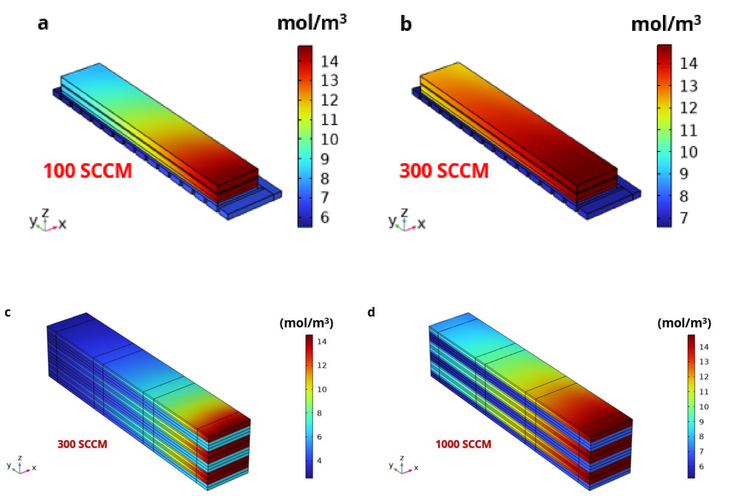
max error: 1.72%

max error perm: 6.61%

max error: 7.98%

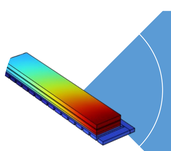


CO_2 concentration profiles (mol/m^3)



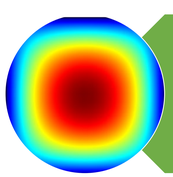
- Higher inlet flowrate → more uniform feed side concentration
- Uniform CO2 concentration on permeate side

Conclusions



Comprehensive model for fluid flow and diffusion

Validated bench scale model with low relative error compared to experimental



CFD is a powerful tool to gain insights on CO_2 capture systems