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

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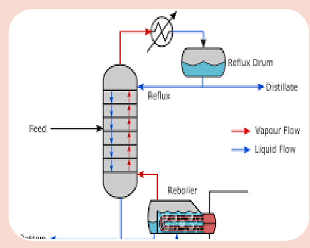
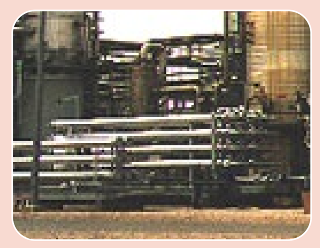
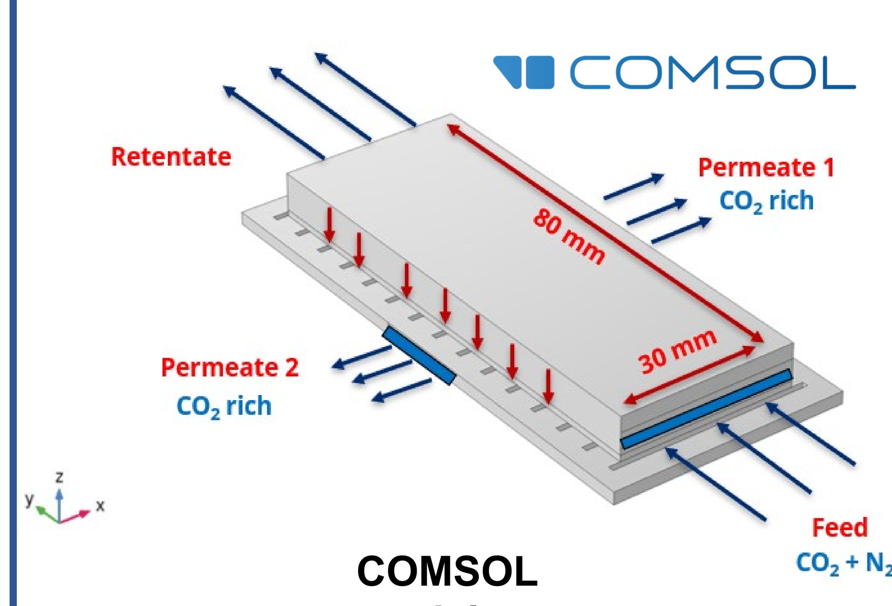
Motivation



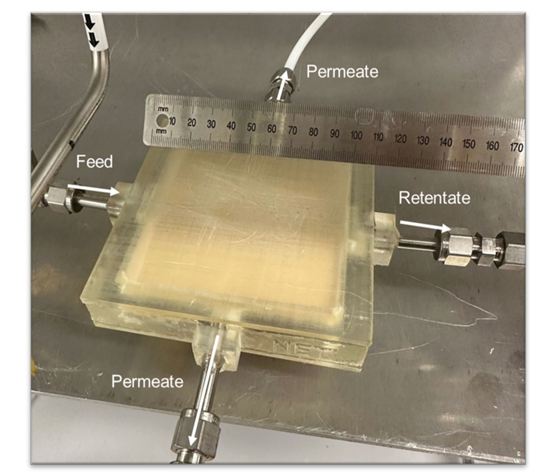



- **9.2 Gt** out of **36.8 Gt** of CO_2 in 2022
- **Net 0** emission by **2050** to limit temperature increase by 1.5 deg C
- Modeling speeds up lab work and scale-up
- Membranes are *modular*, have a *small footprint*, require *low maintenance*, and require much *less energy* than absorption and adsorption

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; Density; Diffusion coefficient; Fick's law

Diffusion on membrane boundary

$M_i [=] \frac{g}{gmol}$

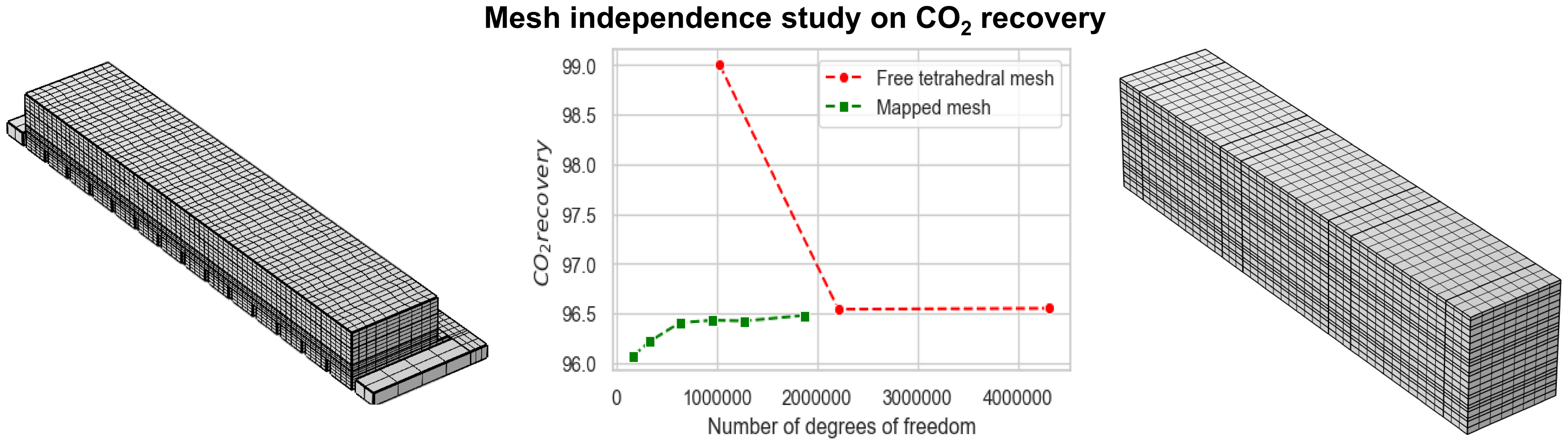
$$j_i [=] \frac{kg}{m^2\cdot s} \quad |J_i| = Q_i \cdot M_i \cdot (p_1 \cdot x_{w_{i_{feed}}} - p_2 \cdot x_{w_{i_{perm}}})$$

Molar mass; mole fraction feed side; mole fraction permeate side; Permeance; Pressure feed; Pressure permeate

$Q_i [=] GPU [=] 3.346\cdot 10^{-6} \frac{mol}{Pa\cdot s\cdot m^2}$ $\quad p [=] Pa [=] \frac{kg}{m\cdot s^2}$

Ensure Numerical Accuracy

Mesh independence study on CO_2 recovery



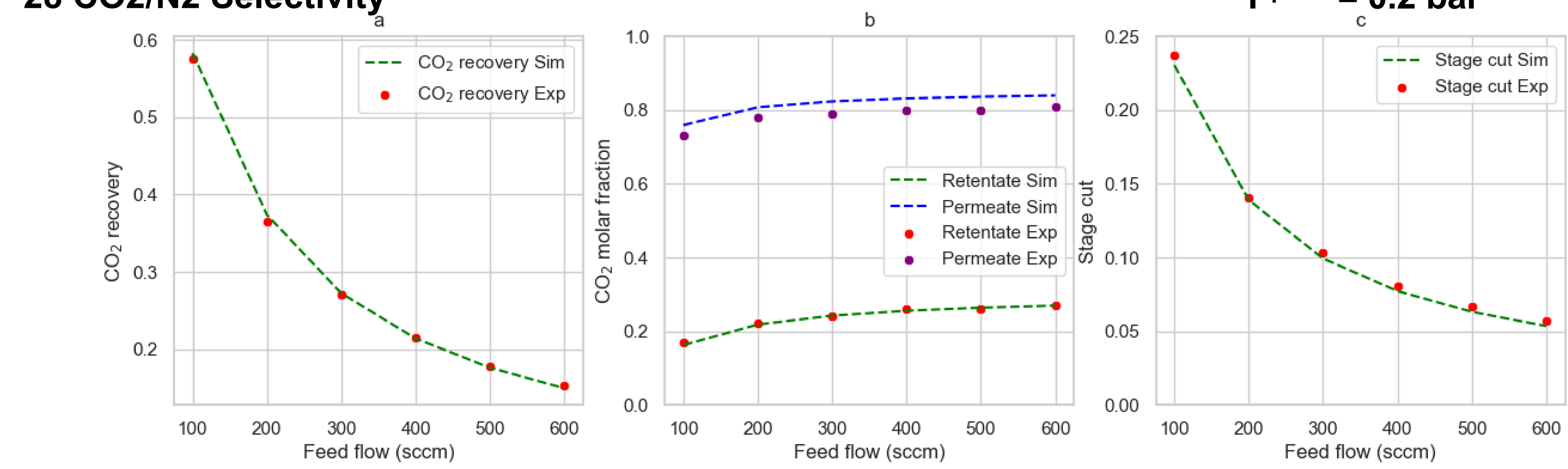
Optimized mesh for high accuracy and low number of degrees of freedom

Model is validated with experimental data

1600 CO2 GPU
28 CO2/N2 Selectivity

Feed concentration: 30% CO_2, 70% N_2

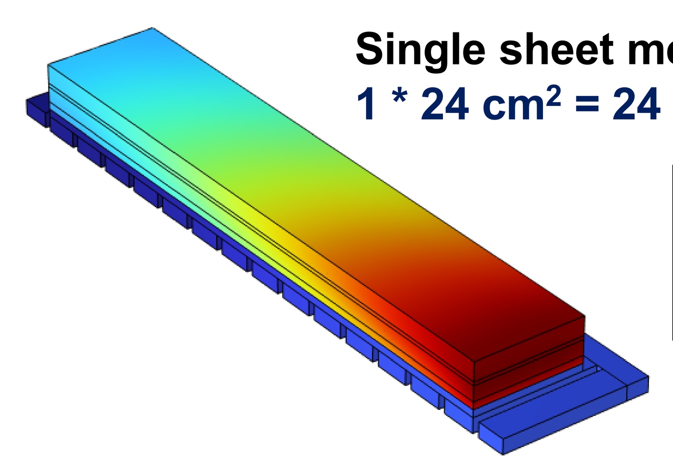
P^{feed} = 1.21 bar
P^{perm} = 0.2 bar



max error: 2.33%

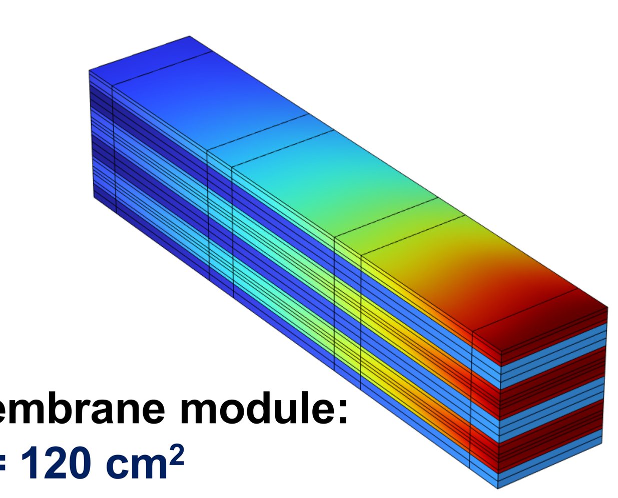
max error ret: 2.73%
perm: 4.5%

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

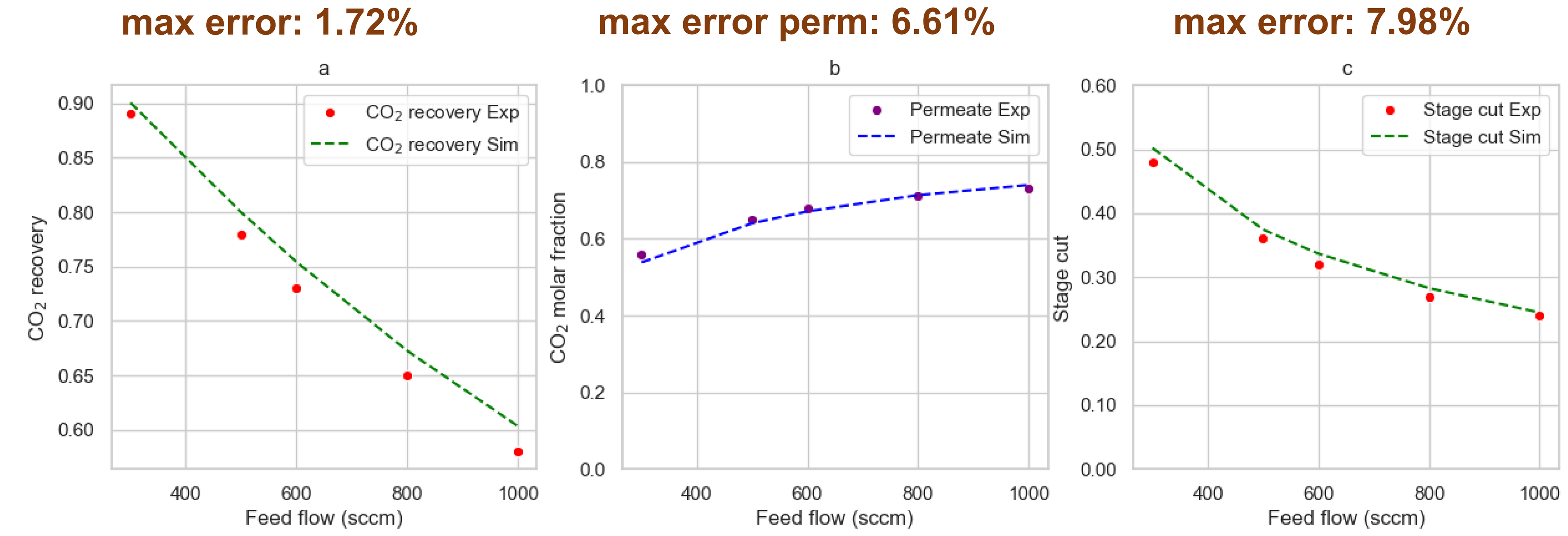
Feed concentration: 30% CO_2, 70% N_2

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

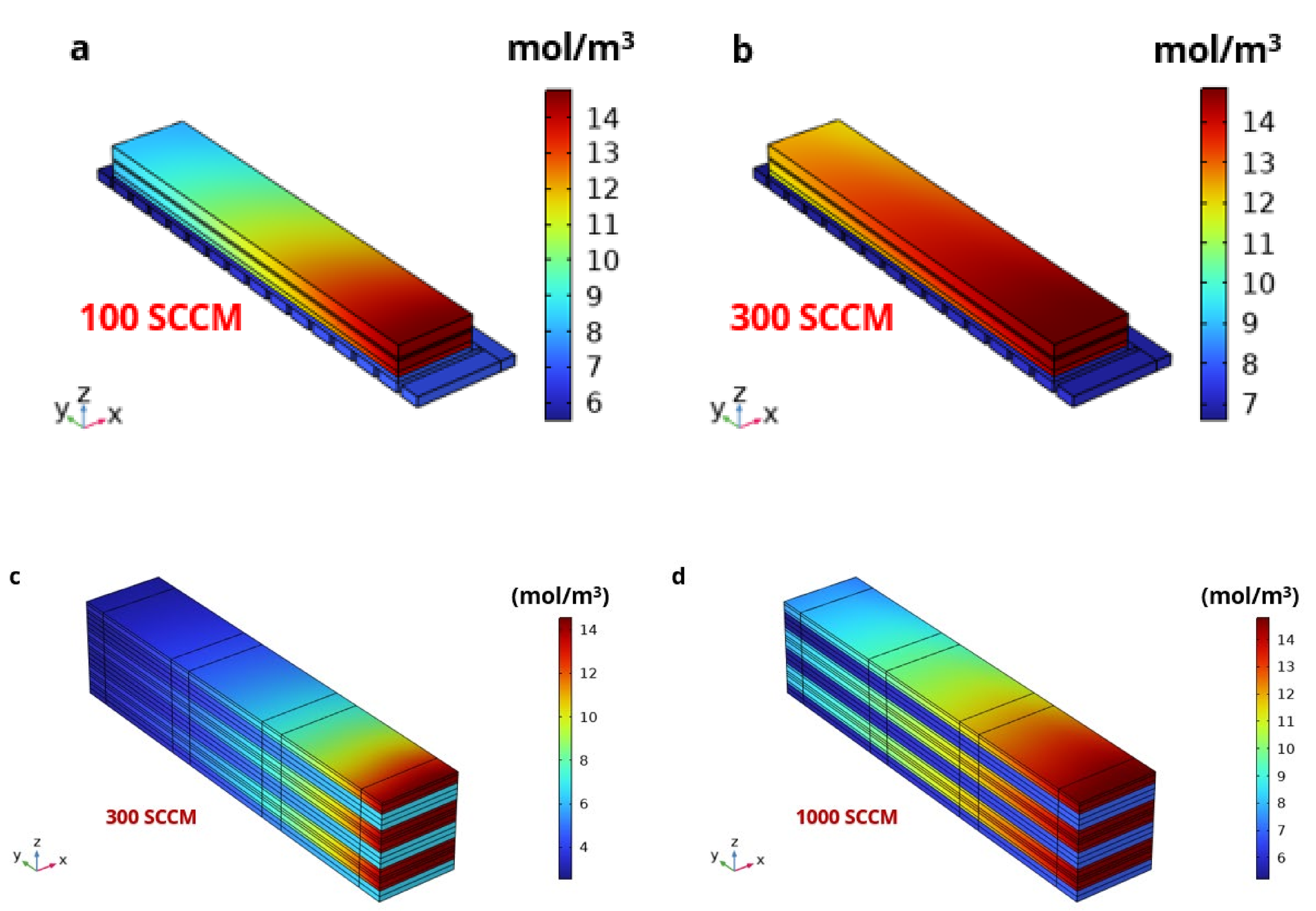
max error: 1.72%

max error perm: 6.61%

max error: 7.98%

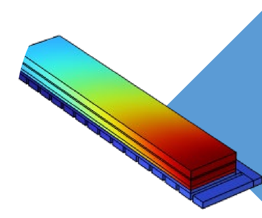


CO_2 concentration profiles (mol/m³)



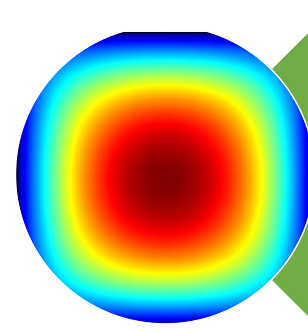
- Higher inlet flowrate → more uniform feed side concentration
- Uniform CO2 concentration on permeate side

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