Optimization of Membrane-based Carbon Capture using Dimensional Analysis, CFD and Process System Engineering

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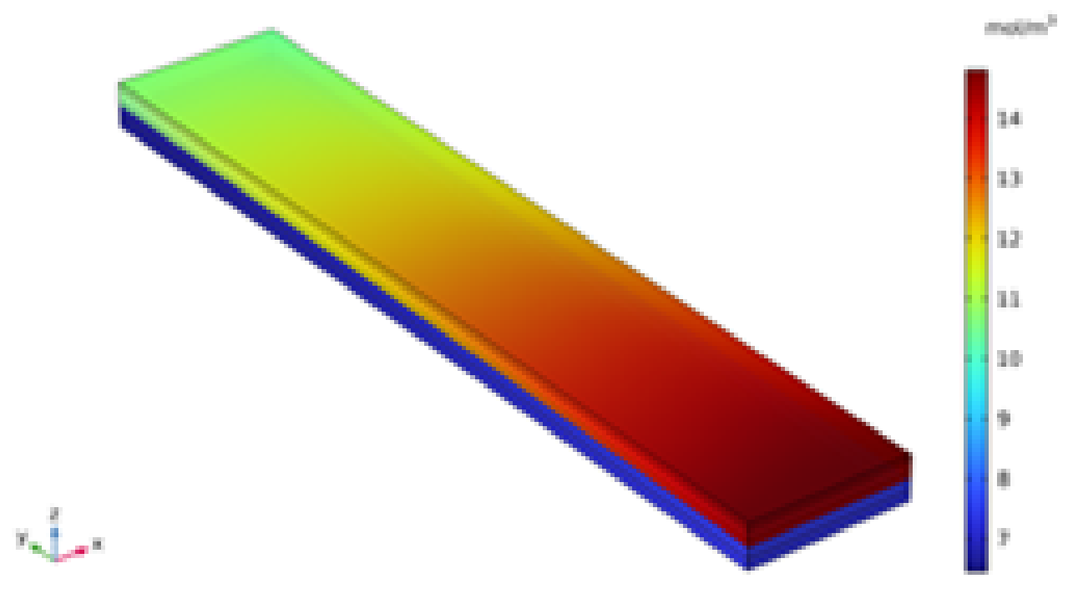
1 Introduction

- Carbon capture technologies based on polymeric membrane with high CO_2 permeance, high CO_2/N_2 selectivity, and stability can be competitive, if properly structured.
- Elucidation of transport mechanisms with Computational Fluid Dynamics (CFD) simulations can inform the design of modules and stacks of polymeric membranes under different conditions.
- Use of dimensional analysis to describe the physics of the processes, leading to simplified correlations and providing insights into the impact of different scaling parameters.
- Multi-stage membrane configurations are needed to achieve high capture rates and high purity simultaneously.
- Process superstructure exploits information from rigorous CFD models.
- Membrane Systems Engineering, based on surrogate models carrying the information from the rigorous CFD simulations, can reveal the true potential of this technology.

2 Membrane Designs

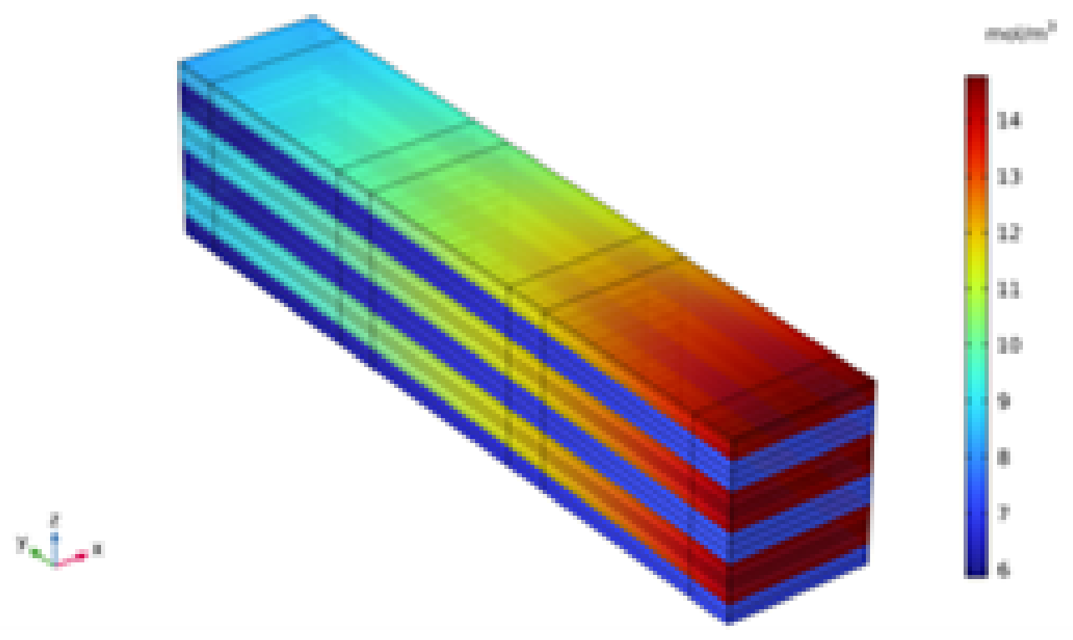
Design 1A

- Area per membrane sheet: 24 cm^2
- Number of sheets: 1
- Total area membrane: 24 cm^2
- CO_2 Permeance (GPU): 1600 and 3200
- Selectivity: 28 and 32



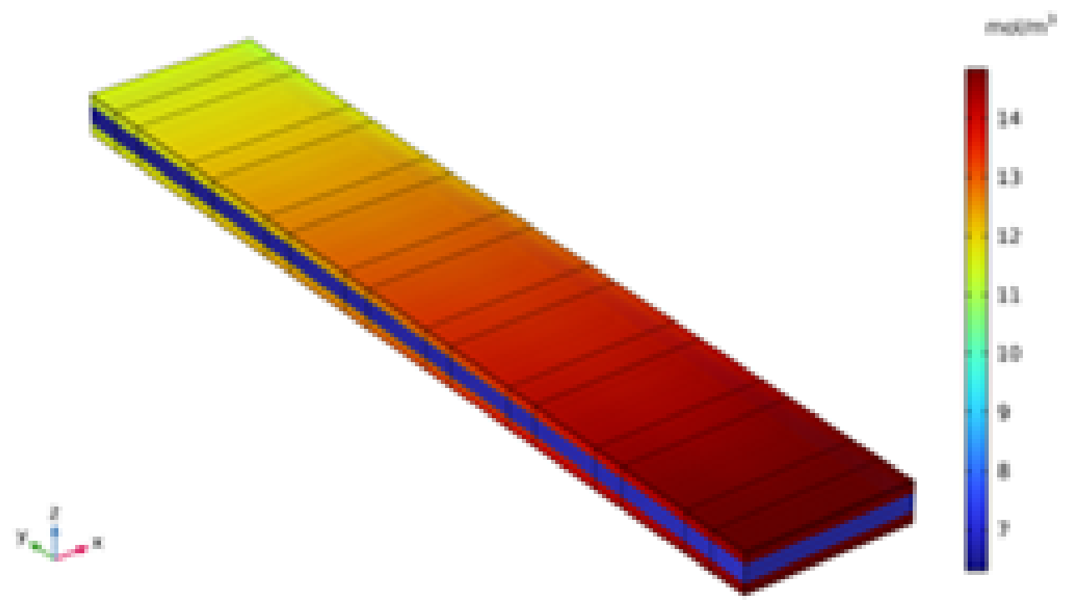
Design 1B

- Area per membrane sheet: 24 cm^2
- Number of sheets: 5
- Total area membrane: 120 cm^2
- CO_2 Permeance (GPU): 1600 and 3200
- Selectivity: 28 and 32



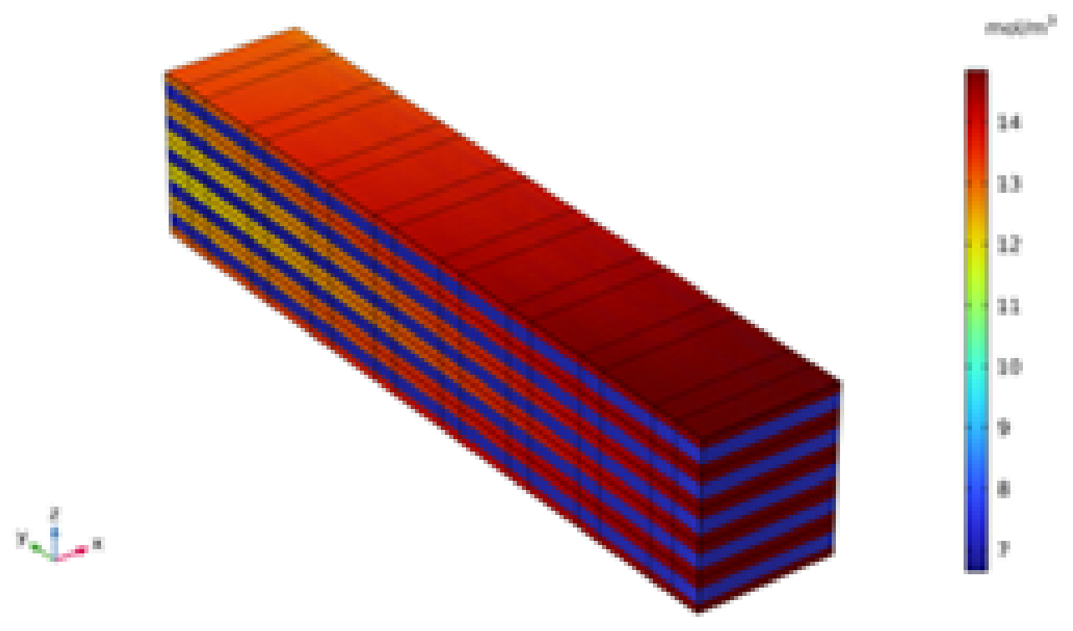
Design 2A

- Area per membrane sheet: 96 cm^2
- Number of sheets: 2
- Total area membrane: 192 cm^2
- CO_2 Permeance (GPU): 1600 and 3200
- Selectivity: 28 and 25



Design 2B

- Area per membrane sheet: 96 cm^2
- Number of sheets: 10
- Total area membrane: 960 cm^2
- CO_2 Permeance (GPU): 1600 and 3200
- Selectivity: 28 and 25



3 Dimensionless Numbers

Dimensionless feed flow $$F^d = \frac{N^{inlet}}{Q_{CO_2} A_M P^{feed}} = \frac{P^{feed}}{RT} U\, a\, b \frac{1}{Q_{CO_2} L a P^{feed}} = \frac{b/V_{CO_2}}{L/U} = \frac{\tau_m}{\tau_s}$$

Pressure ratio $$P^{ratio} = \frac{P^{feed}}{P^{perm}}$$

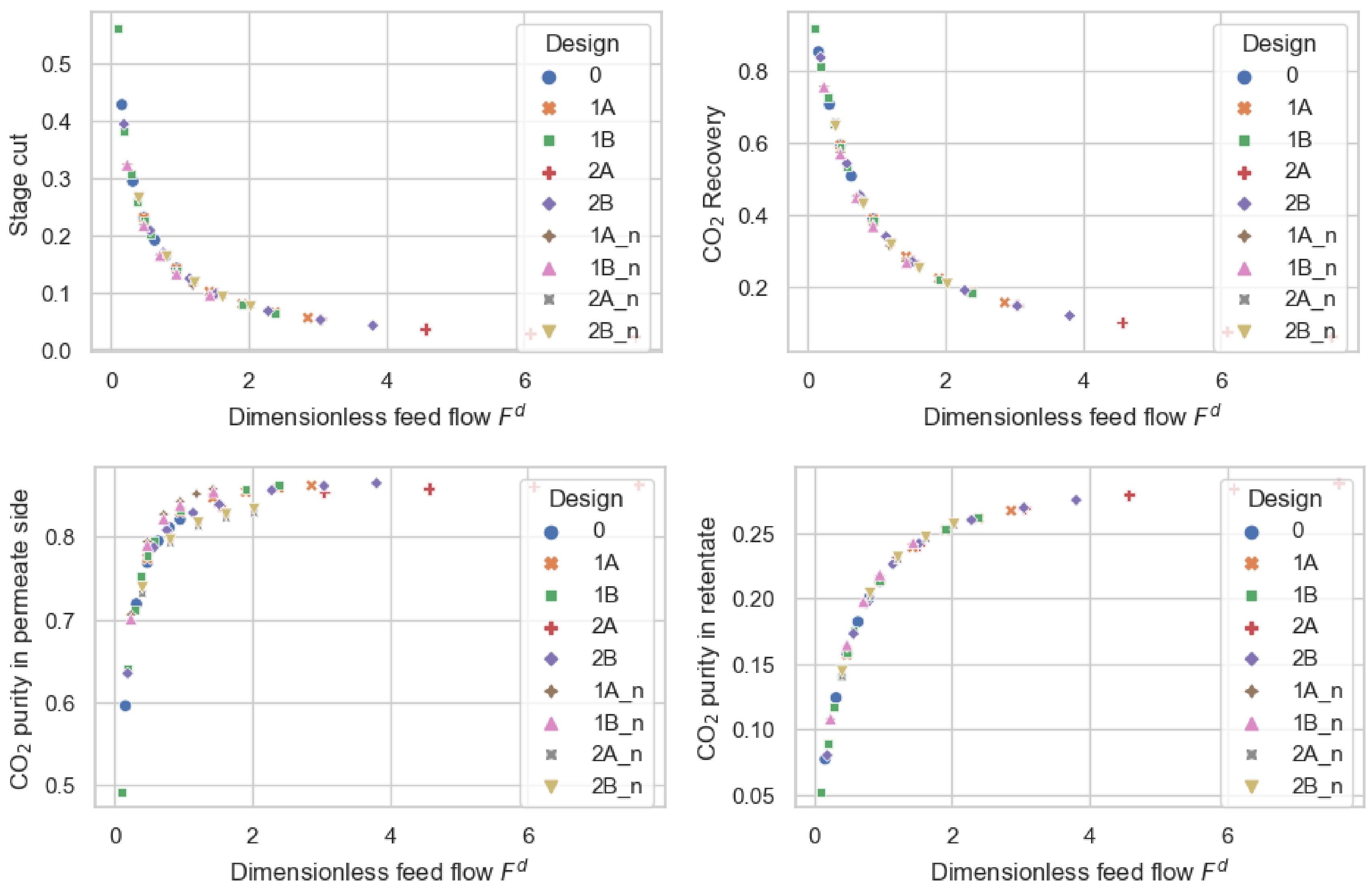
Selectivity $$Sel = \frac{Q_{CO_2}}{Q_{N_2}}$$

Inlet CO_2 concentration $$x_{CO_2}^{feed} = \frac{N_{CO_2}^{inlet}}{N^{inlet}}$$

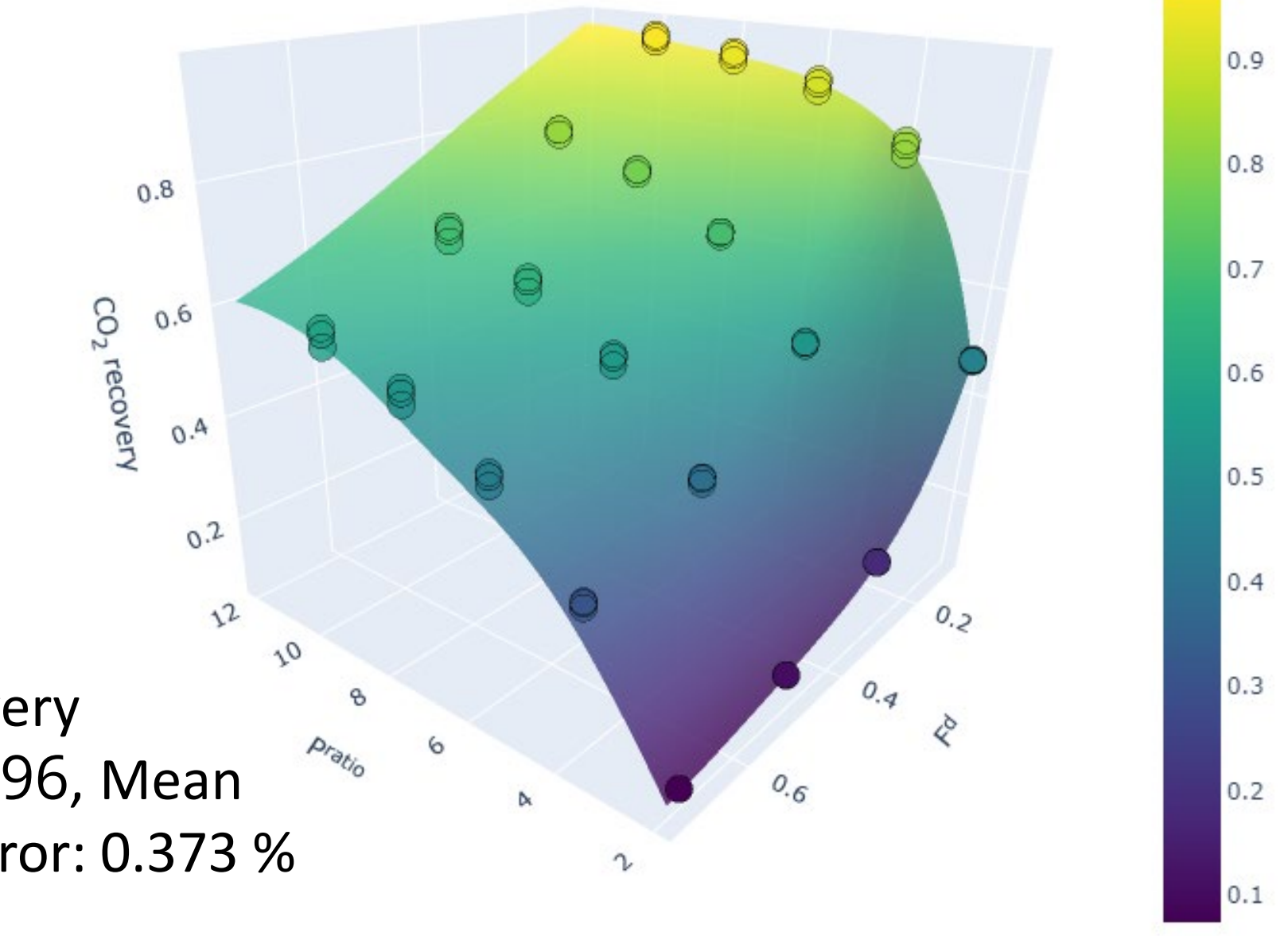
Process variables

a, b : width and height of the feed membrane side
L: membrane length
A_M: area of the membrane
$N^{inlet}, N_{CO_2}^{inlet}$: inlet total and CO_2 molar flows
P^{feed}, P^{perm}: feed and permeate pressure
Q_{CO_2},Q_{N_2}: permeances of i
U: gas superficial velocity CO_2, N_2
V_{CO_2}: mass transfer coefficient ($Q_{CO_2}RT$)
τ_m: time scale of mass transfer
τ_s: time scale of fluid to exit the feed

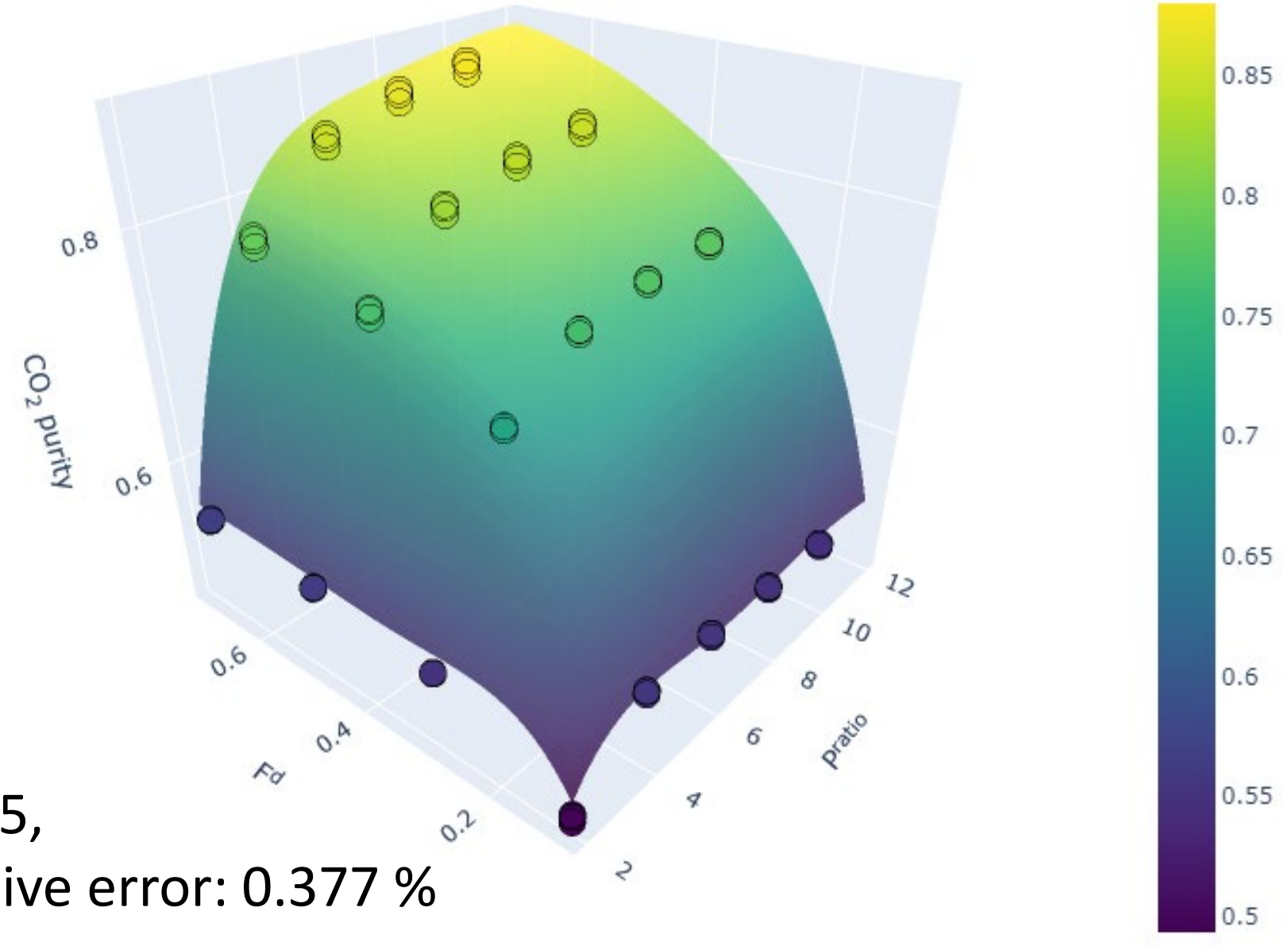
4 F^d to predict the separation performance



5 Kriging-based models



CO_2 recovery
R^2: 0.99996, Mean relative error: 0.373 %



CO_2 purity
R^2: 0.99985,
Mean relative error: 0.377 %

6 Process System Engineering approach

$$\min_x f(x) \rightarrow CapCost = \frac{\gamma CAPEX + OPEX + M_{REP}}{F_{CO_2}}$$

$$s.t.\ h(x) = 0$$

- Kriging models for membranes
- Mass balances
- Units equipment models
- Cost correlations

$$g(x) \leq 0$$

- Pressure drop constraints
- Min. purity target
- Min. CO_2 recovery target
- Min. ΔT in heat exchangers

$$x^L \leq x \leq x^U$$

- Pressure limits
- Mass flowrate per module
- CO_2 concentrations

Optimal operating conditions for the membrane stages

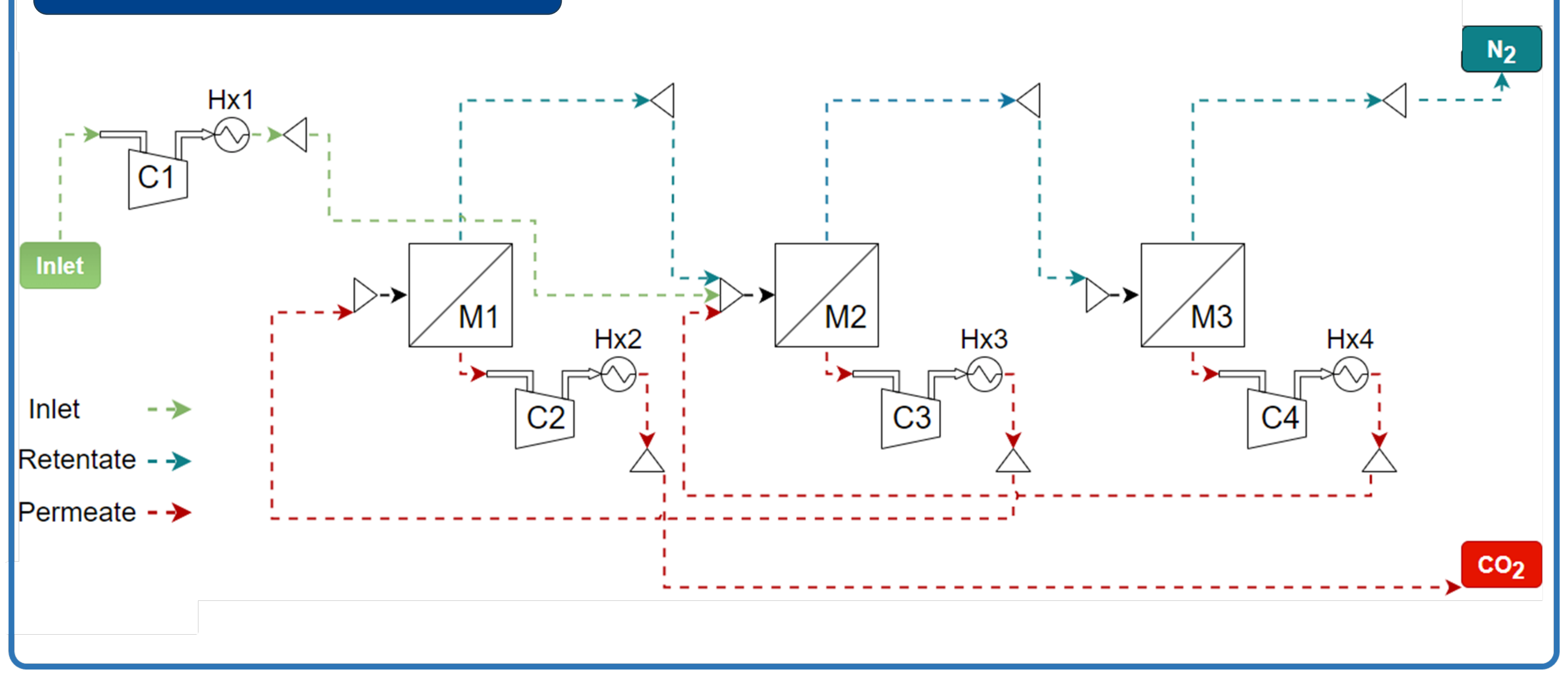
Input variables	M1	M2	M3
Dimensionless feed flow (F^d)	0.21	0.41	0.29
Inlet CO_2 molar fraction	0.73	0.31	0.12
Pressure ratio (P^{ratio})	2.42	8.65	11.90
Selectivity	33.02	37.39	35.61
CO_2 recovery	0.813	0.715	0.709
CO_2 purity	0.950	0.839	0.510

Process metrics

Capture cost: 23.62 \$/t-CO_2

- CO_2 purity: 95 %:
- CO_2 recovery: 90 %
- Capital cost: 26.31 MM$
- Operating cost: 2.68 MM$/y

Optimal scheme



7 Conclusions

- CFD model for **fluid flow** and **diffusion**
- **Validated** bench scale model
  - **low** relative error compared to experimental
- **Dimensional Analysis (DA)** can provide **four** dimensionless variables for the membrane separations: F^d, P^{ratio}, Sel, $x_{CO_2}^{feed,initial}$
- The dimensionless feed flow presents a relevant **physical meaning** associated with the time scales of mass transfer through the membrane and time scale of fluid to exit the feed side
- **Kriging-based surrogate models** were built to determine the CO_2 recovery and CO_2 purity in the retentate for a given combination of dimensionless variables
- Optimal design with three membrane stages shows a capture cost of 23.62 \$/t-CO_2