



Supplementary Information

Experimental, Modeling and AspenPlus Simulation of Different Configurations of Membrane Separation Systems for Highly Loaded CO₂ Selective Pebax 1657-ZIF-8 Membrane

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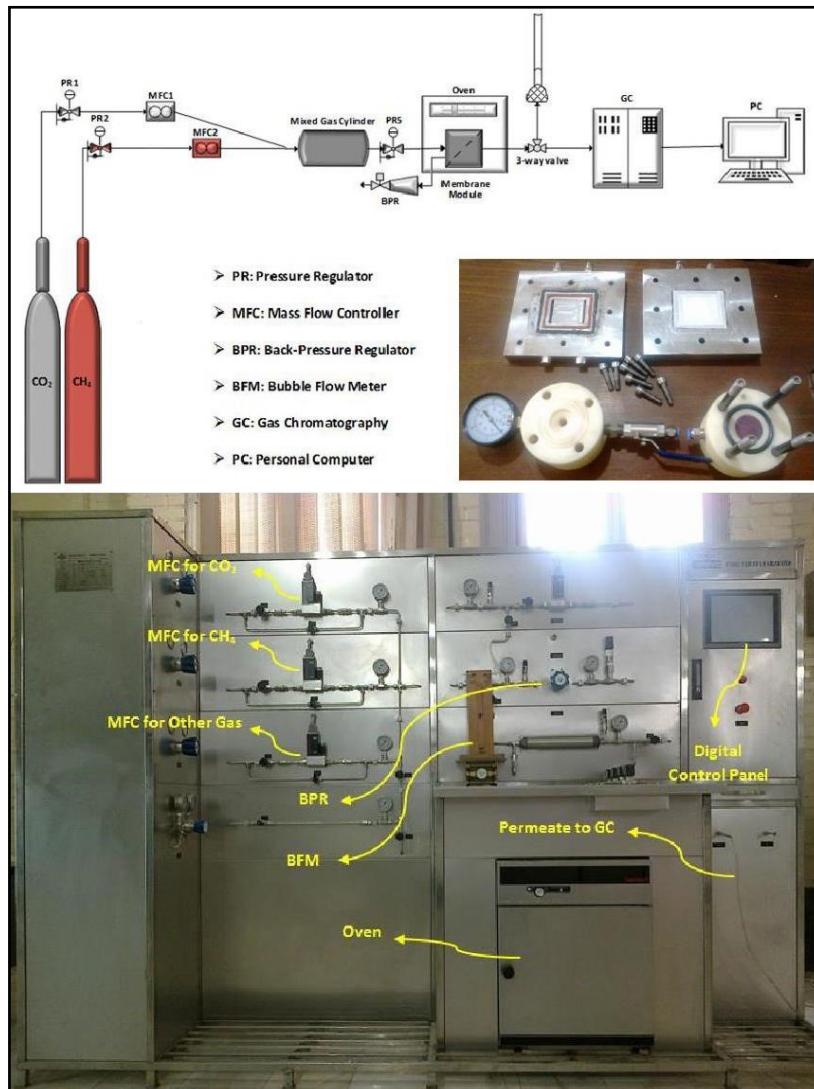


Fig. S1. Schematic diagram and image of applied gas permeation set-up with an embedded image of utilized membrane modules.

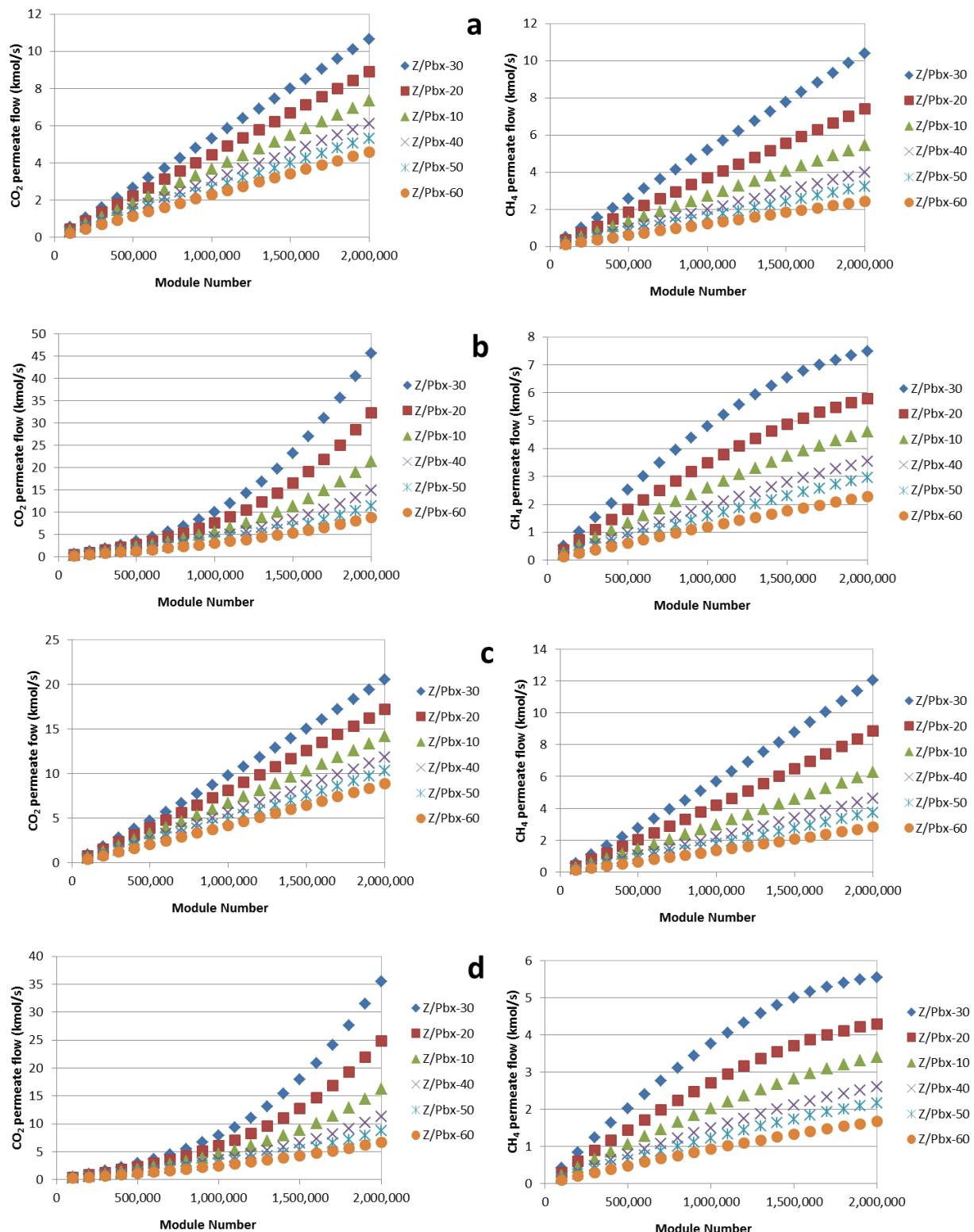


Fig. S2. The simulated effect of module number on CO₂ and CH₄ permeate flow rates in a) SiS, b) SiSRP, c) DoSRP and d) DoSRR membrane system configurations for all synthesized MMMs.

Table S1

Types, names and values of variables defined in Aspen Plus membrane model.

Variables type	Variable Name	Default Value
Real	Module Area	0.0125 m ²
	Selectivity	Depends on MMM
	Effective Thickness	0.00001 m
	Delta P	1,900,000 Pa
	CH ₄ feed composition	0.9
	Temperature	298.15 K
Integer	Module Number	1,000,000

Table S2¹³C NMR chemical shifts referenced to tetramethylsilane for all different investigated samples.

Sample	Chemical shifts (ppm)									
	Pebax 1657	174.26	171.11	72.35	62.12	47.14	36.41	30.03	27.56	19.08
DBMF	145.29	122.43	47.37	30.31	19.89	14.05				
ZIF-8	145.12	122.20	14.3							
UZ/Pbx-10	174.26	171.14	145.12	122.21	72.33	62.10	47.12	36.51	30.00	
	27.52	19.15	14.32							
Pbx	174.20	171.14	14.33	125.20	122.50	72.37	62.82	47.43	47.14	
	36.54	30.31	30.05	27.55	23.71	20.13	19.92	14.12		
Z/Pbx-10	174.23	171.18	145.36	145.17	125.23	122.53	122.21	72.32	62.81	
	47.48	47.17	36.56	30.34	30.01	27.52	23.63	20.12	19.92	
	14.32	12.51								

Table S3CO₂ and CH₄ permeances (GPU) in different MMMs at different temperatures.

Temperature (K)	Z/Pbx-10		Z/Pbx-20		Z/Pbx-30		Z/Pbx-40		Z/Pbx-50		Z/Pbx-60	
	CO ₂	CH ₄										
303	61.3	3.7	73	5.03	85	7.08	52.2	2.7	46.1	2.2	40.5	1.66
313	74	4.1	87	6	102	8.9	55	3.2	49	2.4	44	1.75
323	75	5.1	95	7.1	115	10.5	62	3.6	54	2.9	47	2.10

Table S4Calculated CO₂ and CH₄ activation energy of permeation for synthesized MMMs.

MMM samples	E _P (kJ/mol) for CO ₂	E _P (kJ/mol) for CH ₄
Z/Pbx-10	8.27	13.12
Z/Pbx-20	10.75	14.02
Z/Pbx-30	12.32	16.05
Z/Pbx-40	6.97	11.72
Z/Pbx-50	6.42	11.19
Z/Pbx-60	5.99	9.50