Electronic Supplementary Information

Are green solvents truly green? Integrating life cycle assessment and techno-economic analysis for sustainable membrane fabrication

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Table S1. The costs of raw materials and energy sources required to fabricate polyimide membranes. The quotations of chemicals, nitrogen, and electricity were obtained from Sigma Aldrich, Alpha Gas, and the average global electricity price, respectively.

Component	Quantity	Cost (USD)	Cost per unit (USD/unit)
6FDA	25 g	322.00	12.88/g
Durene	100 g	65.20	0.65/g
NMP	1 L	212.00	0.21/g
DMSO	1 L	336.00	0.31/g
EA	1 L	108.00	0.12/g
GBL	500 g	64.10	0.13/g
TEAm	100 mL	35.00	0.33/g
Ac_2O	25 g	38.30	1.53/g
Toluene	1 L	79.40	0.09/g
N_2	50 L	58.60	1.17/L
Methanol	200 L	2,260.00	11.30/L
Electricity	1 kWh	0.17	0.17/kWh

Table S2. The environmental impact scores for various membrane production routes at the midpoint level.

Route		R1	R2	R3	R4	R5
Impact category	Unit	Value				
Fine particulate matter formation (FPMF)	kg PM2.5-Eq	0.39	0.36	0.36	0.38	0.36
Fossil resource scarcity (FRS)	kg oil-Eq	80.92	73.89	74.75	76.43	74.41
Freshwater ecotoxicity (FET)	kg 1,4-DCB-Eq	7.61	7.09	7.16	7.41	7.19
Freshwater eutrophication (FEP)	kg P-Eq	0.09	0.08	0.08	0.08	0.08
Global warming potential (GWP)	kg CO_2-Eq	182.84	162.93	166.47	175.38	164.69
Human carcinogenic toxicity (HCT)	kg 1,4-DCB-Eq	503.05	458.84	466.14	489.74	464.85
Human non-carcinogenic toxicity (HNCT)	kg 1,4-DCB-Eq	37,439.89	32,908.49	33,488.27	35,534.94	33,229.27
Ionizing radiation (IR)	kBq Co-60-Eq	22.76	20.46	20.75	22.41	20.83
Land use (LU)	m^2 crop-Eq	2.46	2.00	2.12	2.38	2.03
Marine ecotoxicity (MET)	kg 1,4-DCB-Eq	47,000.53	41,468.82	42,175.86	44,676.35	41,886.38
Marine eutrophication (MEP)	kg N-Eq	0.07	0.07	0.07	0.07	0.07
Mineral resource scarcity (MRS)	kg Cu-Eq	0.28	0.23	0.24	0.26	0.24
Ozone depletion (OD)	kg CFC11-Eq	0.0001	0.0001	0.0001	0.0001	0.0001
Ozone formation, human health (OFH)	kg NO_x-Eq	0.40	0.36	0.37	0.39	0.37
Ozone formation, ecosystems (OFE)	kg NO_x-Eq	0.42	0.37	0.38	0.40	0.38
Terrestrial acidification (TA)	kg SO_2-Eq	0.68	0.59	0.61	0.65	0.60
Terrestrial ecotoxicity (TET)	kg 1,4-DCB-Eq	333.99	261.23	270.68	296.09	263.14
Water consumption (WCP)	m^3	2.31	1.41	1.47	2.24	1.42

Table S3. The environmental burden arising from the endpoint indicators of different membrane fabrication routes.

Route		R1	R2	R3	R4	R5
Damage category	Unit	Value				
Human health	points	57.10	50.59	51.51	54.50	51.12
Ecosystems	points	4.66	4.13	4.21	4.45	4.17
Resources	points	0.17	0.16	0.16	0.16	0.16
Total	points	61.93	54.87	55.87	59.11	55.44

Table S4. Comparison results of cumulative energy demand from various membrane preparation processes.

Route		R1	R2	R3	R4	R5
Energy demand	Unit	Value				
Non-renewable biomass	MJ	0.05	0.04	0.04	0.05	0.04
Fossil	MJ	3703.80	3381.82	3421.51	3498.61	3405.85
Nuclear	MJ	279.40	252.35	255.37	278.05	257.01
Biomass	MJ	34.35	26.69	28.99	33.94	26.98
Water	MJ	127.57	118.12	118.98	125.69	120.05
Wind, solar, geothermal	MJ	30.26	27.90	28.03	30.07	28.45

Table S5. Comparison data of ecological footprint involved in different membrane production routes.

Route		R1	R2	R3	R4	R5
Footprint	Unit	Value				
Carbon dioxide	m^2	475.15	423.03	432.29	455.71	423.03
Nuclear	m^2	54.75	49.45	50.04	54.48	49.45
Land occupation	m^2	10.23	8.33	8.83	9.96	8.33
Total	m^2	540.13	480.81	491.15	520.16	480.81

Table S6. The production costs incurred from different membrane fabrication routes.

Route		R1	R2	R3	R4	R5
Component	Unit	Value				
Monomers	USD	1170.35	1170.35	1170.35	1170.35	1170.35
Solvents	USD	658.81	972.53	376.46	407.84	972.53
Methanol	USD	414.71	414.71	414.71	414.71	414.71
Other materials	USD	91.82	91.82	91.82	91.82	15.80
Electricity	USD	18.80	18.80	18.80	18.80	19.24
Total	USD	2354.49	2668.21	2072.14	2103.51	2592.62

Table S7. The weighting factors and environmental costs for various membrane production routes at the midpoint level.

Route			R1	R2	R3	R4	R5
Impact category	Unit	Weighting factor (USD/unit)	Environmental cost (USD)				
FPMF	kg PM2.5-Eq	0.0325[a]	0.01	0.01	0.01	0.01	0.01
FRS	kg oil-Eq	0.0012[a]	0.10	0.09	0.09	0.09	0.09
FET	kg 1,4-DCB-Eq	0.0333[b]	0.25	0.24	0.24	0.25	0.24
FEP	kg P-Eq	0.1080[a]	0.01	0.01	0.01	0.01	0.01
GWP	kg CO_2-Eq	0.0077[a]	1.40	1.25	1.28	1.35	1.26
HCT	kg 1,4-DCB-Eq	0.0999[b]	50.25	45.84	46.57	48.92	46.44
HNCT	kg 1,4-DCB-Eq	0.0999[b]	3740.24	3287.56	3345.48	3549.94	3319.60
IR	kBq Co-60-Eq	3.3000[b]	75.10	67.51	68.47	73.95	68.75
LU	m^2 crop-Eq	3.0500[b]	7.49	6.11	6.46	7.27	6.18
MET	kg 1,4-DCB-Eq	0.0001[b]	5.22	4.60	4.68	4.96	4.65
MEP	kg N-Eq	0.1080[a]	0.01	0.01	0.01	0.01	0.01
MRS	kg Cu-Eq	0.0025[a]	0.0007	0.0006	0.0006	0.0006	0.0006
OD	kg CFC11-Eq	1.9800[a]	0.80	0.71	0.73	0.77	0.72
OFH	kg NO_x-Eq	1.9800[a]	0.82	0.73	0.76	0.79	0.74
OFE	kg NO_x-Eq	1.9800[a]	0.0002	0.0002	0.0002	0.0002	0.0002
TA	kg SO_2-Eq	0.0931[a]	0.06	0.06	0.06	0.06	0.06
TET	kg 1,4-DCB-Eq	0.0666[b]	22.24	17.40	18.03	19.72	17.53
WCP	m^3	0.2130[a]	0.49	0.30	0.31	0.48	0.30
Total	-	-	3904.51	3432.43	3493.18	3708.58	3466.59

[a] Obtained from Cao et al., 2015, [b] Estimated from Ecochain and US National Academy of Sciences.

Table S8. The deviations of endpoint impact scores obtained from the parameter sensitivity analysis.

Route		R1	R2	R3	R4	R5
Component	Unit	Value				
Monomers	%	8.9	10.0	9.8	9.3	9.9
Solvents	%	4.4	1.1	1.6	3.2	1.1
Methanol	%	3.0	3.3	3.3	3.1	3.3
Electricity	%	13.7	15.5	15.2	14.4	15.7

Table S9. The production cost variation resulting from the parameter sensitivity analysis.

Route		R1	R2	R3	R4	R5
Component	Unit	Value				
Monomers	%	14.9	13.2	16.9	16.7	13.5
Solvents	%	8.4	10.9	5.5	5.8	11.3
Methanol	%	5.3	4.7	6.0	5.9	4.8
Electricity	%	0.2	0.2	0.3	0.3	0.2