Supporting Information

Cradle-to-Gate Life Cycle Assessment of Zeolite-Modified PAN/PVDF Electrospun Composite Membranes for Cationic Dye Removal: Parametric Analysis of Natural Zeolite Loading

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Contents

Auto-population: Numerical tables below are populated by running the value-population script after the five analysis notebooks (01–05) have executed. Unpopulated cells display as red [TBD: ...].

S1 Foreground Life Cycle Inventory

Table S1 lists the foreground life cycle inventory per 1 membrane ($50 \times 50\ \mathrm{mm}^2$) for each of the five scenarios Ze0–Ze5, under base-case assumptions (DMF recovery = 0%, lifetime = 5 cycles, literature-default equipment powers documented in Section S8).

Table S1: Foreground LCI per 1 membrane ($50 \times 50\ \mathrm{mm}^2$). Inputs required to produce one reference membrane. Values from Values correspond to those reported in the main text Methods section.

Process	Flow	Ze0	Ze1	Ze2	Ze3	Ze5	U
Polymer dissolution	PAN (Mw 150,000)	1.00	1.00	1.00	1.00	1.00	
Polymer dissolution	PVDF (Mw 534,000)	0.25	0.25	0.25	0.25	0.25	
Polymer dissolution	DMF (solvent)	10.0	10.0	10.0	10.0	10.0	[illegible]
Polymer dissolution	Stirring (400 W, 60 °C)	4	4	4	4	4	
Electrospinning	Applied voltage	10	10	10	10	10	
Electrospinning	Tip–collector	10	10	10	10	10	
Electrospinning	Feed rate	0.7	0.7	0.7	0.7	0.7	m
Electrospinning	Duration	8	8	8	8	8	
Electrospinning	Electrical energy (150 W)	1.20	1.20	1.20	1.20	1.20	k
Zeolite deposition	Natural zeolite	0.00	0.01	0.02	0.03	0.05	
Zeolite deposition	Deionised water	0	200	200	200	200	[illegible]
Zeolite deposition	Ultrasonication (100 W)	0	1	1	1	1	
Zeolite deposition	Vacuum filtration (200 W, 0.5 bar)	0	0.5	0.5	0.5	0.5	
Membrane drying	Oven drying (500 W, 60 °C)	1	1	1	1	1	
DMF emission (airborne)	Direct NMVOC (0% recovery)	9.44	9.44	9.44	9.44	9.44	

Notes on assumptions. Membrane dimensions $50 \times 50\ \mathrm{mm}^2$ and PAN molecular weight 150,000 $\mathrm{g\,mol^{-1}}$ reflect corrections to the originally-reported values in Arif *et al.* 2024 (confirmed by co-authors, see main text Methods). Equipment power values are literature defaults pending direct measurement: electrospinner 150 W, stirrer/hotplate 400 W, ultrasonicator 100 W, vacuum pump 200 W, drying oven 500 W (all ±30–50% uncertainty carried through Monte Carlo).

S2 Background Emission Factors

Table S2 summarises the multi-category emission factors used in the background technosphere. Source citations for each EF are listed below the table, and Pedigree scores for each EF are provided in Section S3.

Table S2: Multi-category background emission factors (per reference unit). F
CO2 (fossil CO_2), CH4 (fossil methane), N2O, SO2, NOx (as NO_2), PM (
(non-methane VOC), P-H2O, N-H2O (emissions to water), Water (consumed

EF	Unit	CO2	CH4	SO2	NC
Electricity Java-Bali	kg/kWh	0.870	2.0×10^{-5}	3.5×10^{-3}	2.
Transport lorry (EURO V)	kg/tkm	0.150	8.0×10^{-6}	5.0×10^{-6}	5.
Diesel combustion	kg/kg	3.150	1.0×10^{-4}	5.0×10^{-4}	2.
DMF upstream (RoW proxy)	kg/kg	4.500	1.0×10^{-2}	1.0×10^{-2}	8.
DMF air emission	kg/kg	0	0	0	0
PAN upstream (RoW proxy)	kg/kg	5.800	1.5×10^{-2}	1.2×10^{-2}	1.
PVDF upstream (RoW proxy)	kg/kg	6.500	1.5×10^{-2}	2.5×10^{-2}	1.
DI water, Indonesia	kg/m³	1.000	3.0×10^{-5}	4.0×10^{-3}	2.
Zeolite mining (Tanggamus)	kg/kg	0.020	0	0	1.

Source notes. Grid electricity EF from PLN Sustainability Report 2023 (Java-Bali mix, coal-dominated 60%). Transport EF derived from HBEFA 4.1 for EURO V diesel lorry 7.5–16t at 50% load. Diesel combustion from IPCC 2019 Refinement Vol 2 Ch 3. DMF upstream from Arif *et al.* 2023 [1] endpoint + Ecoinvent 3.8 RoW proxy mapping. PAN upstream from Khaki *et al.* 2021 [2]. PVDF upstream from Yadav *et al.* 2021 [3]. Natural zeolite mining inventory from Taher *et al.* 2023 [4] adapted for multi-category output.

S3 Data Quality Scoring — Pedigree Matrix

Table S3 lists Pedigree Matrix scores for each background EF (1 = best, 5 = worst) following Ciroth *et al.* 2016 [5]. The derived geometric standard deviation (GSD) feeds the lognormal Monte Carlo sampling (Sprint 5, see main text §**??**).

Table S3: Pedigree Matrix scores per background emission factor (1=best, 5=worst). Derived σ (ln GSD) feeds lognormal Monte Carlo sampling.

EF	Reliability	Completeness	Temporal	Geographical	Technological
electricity_javabali	1	2	1	1	2
transport_lorry_eurov	2	2	2	3	2
diesel_combustion	1	1	1	1	1
dmf_upstream	3	3	2	4	2
dmf_air_emission	3	3	1	1	3
pan_upstream	2	3	2	4	2
pvdf_upstream	2	3	2	4	2
di_water	4	3	2	2	3
zeolite_mining_ancillary	2	3	2	1	2

S4 Monte Carlo Percentiles — Full Table

Table S4 reports the complete Monte Carlo distribution statistics for all 5 scenarios $\times$ 6 impact categories. $N = 1000$ iterations, with lognormal EF perturbations derived from the Pedigree matrix scores tabulated in Section S3.

Table S4: Monte Carlo percentiles per scenario $\times$ method. $N = 1000$ iterations, lognormal perturbation from Pedigree matrix.

Scen.	Category	Mean	Median	P_5	P_{95}	CV
ZE0	Climate change	1.18e+03	1.18e+03	1.13e+03	1.23e+03	2.9%
ZE0	PM formation	2.06	2.06	1.97	2.16	2.9%
ZE0	Acidification	5.93	5.92	5.67	6.22	2.9%
ZE0	Freshwater eutro.	4.58e-05	4.58e-05	4.33e-05	4.83e-05	3.4%
ZE0	Marine eutro.	0.00089	0.000891	0.000841	0.000941	3.5%
ZE0	Water consumption	44.2	44.1	42.4	46.2	2.6%
ZE1	Climate change	1.25e+03	1.25e+03	1.19e+03	1.31e+03	2.9%
ZE1	PM formation	2.18	2.18	2.09	2.29	2.9%
ZE1	Acidification	6.29	6.28	6.01	6.59	2.9%
ZE1	Freshwater eutro.	4.58e-05	4.58e-05	4.33e-05	4.83e-05	3.4%
ZE1	Marine eutro.	0.00089	0.000891	0.000841	0.000941	3.5%
ZE1	Water consumption	48.3	48.2	46.4	50.4	2.6%
ZE2	Climate change	1.25e+03	1.25e+03	1.19e+03	1.31e+03	2.9%
ZE2	PM formation	2.18	2.18	2.09	2.29	2.9%
ZE2	Acidification	6.29	6.28	6.01	6.59	2.9%
ZE2	Freshwater eutro.	4.58e-05	4.58e-05	4.33e-05	4.83e-05	3.4%
ZE2	Marine eutro.	0.00089	0.000891	0.000841	0.000941	3.5%
ZE2	Water consumption	48.3	48.2	46.4	50.4	2.6%
ZE3	Climate change	1.25e+03	1.25e+03	1.19e+03	1.31e+03	2.9%
ZE3	PM formation	2.18	2.18	2.09	2.29	2.9%
ZE3	Acidification	6.29	6.28	6.01	6.59	2.9%
ZE3	Freshwater eutro.	4.58e-05	4.58e-05	4.33e-05	4.83e-05	3.4%
ZE3	Marine eutro.	0.00089	0.000891	0.000841	0.000941	3.5%
ZE3	Water consumption	48.3	48.2	46.4	50.4	2.6%
ZE5	Climate change	1.25e+03	1.25e+03	1.19e+03	1.31e+03	2.9%
ZE5	PM formation	2.18	2.18	2.09	2.29	2.9%
ZE5	Acidification	6.29	6.28	6.01	6.59	2.9%
ZE5	Freshwater eutro.	4.58e-05	4.58e-05	4.33e-05	4.83e-05	3.4%
ZE5	Marine eutro.	0.00089	0.000891	0.000841	0.000941	3.5%
ZE5	Water consumption	48.3	48.2	46.4	50.4	2.6%

S5 Sobol Global Sensitivity — Full Indices

Table S5 reports first-order (S_1) and total-order (S_T) Sobol indices for all 15 parameters × 3 output targets, with 95% confidence intervals from bootstrap resampling (SALib default). Saltelli sampler $N_{\text{base}} = 1024$, total evaluations 32,768 per output.

Table S5: Sobol sensitivity indices per parameter × output target. Interaction = $S_T - S_1$. Saltelli $N_{\text{base}} = 1024$ (32,768 evaluations per target).

Target	Parameter	S_1	S_T	$S_T - S_1$
gwp_fua_ze3	electrospinner_power_w	0.516	0.516	-0.000395
gwp_fua_ze3	stirrer_hotplate_power_w	0.407	0.407	0.000897
gwp_fua_ze3	drying_oven_power_w	0.0401	0.0398	-0.000276
gwp_fua_ze3	ef_electricity_mult	0.0325	0.032	-0.000483
gwp_fua_ze3	sonicator_power_w	0.00321	0.00359	0.000379
gwp_fua_ze3	vacuum_pump_power_w	0.00361	0.00358	-2.4e-05
gwp_fua_ze3	ef_dmf_upstream_mult	1.05e-05	1.19e-05	1.35e-06
gwp_fua_ze3	ef_pan_upstream_mult	3.86e-08	1.8e-07	1.42e-07
gwp_fua_ze3	ef_pvdf_upstream_mult	1.71e-08	1.39e-08	-3.2e-09
gwp_fua_ze3	ef_di_water_mult	5.01e-08	6.48e-10	-4.95e-08
gwp_fua_ze3	ef_transport_mult	6.75e-12	1.12e-14	-6.73e-12
gwp_fua_ze3	ef_diesel_combustion_mult	3.79e-10	2.58e-15	-3.79e-10
gwp_fua_ze3	ef_zeolite_mining_mult	3.86e-10	1.87e-15	-3.86e-10
gwp_fua_ze3	ef_dmf_air_emission_mult	0	0	0
gwp_fua_ze3	dmf_recovery_fraction	0	0	0
gwp_fub_ze3	electrospinner_power_w	0.516	0.516	-0.000395
gwp_fub_ze3	stirrer_hotplate_power_w	0.407	0.407	0.000897
gwp_fub_ze3	drying_oven_power_w	0.0401	0.0398	-0.000276
gwp_fub_ze3	ef_electricity_mult	0.0325	0.032	-0.000483
gwp_fub_ze3	sonicator_power_w	0.00321	0.00359	0.000379
gwp_fub_ze3	vacuum_pump_power_w	0.00361	0.00358	-2.4e-05
gwp_fub_ze3	ef_dmf_upstream_mult	1.05e-05	1.19e-05	1.35e-06
gwp_fub_ze3	ef_pan_upstream_mult	3.86e-08	1.8e-07	1.42e-07
gwp_fub_ze3	ef_pvdf_upstream_mult	1.71e-08	1.39e-08	-3.2e-09
gwp_fub_ze3	ef_di_water_mult	5.01e-08	6.48e-10	-4.95e-08
gwp_fub_ze3	ef_transport_mult	6.75e-12	1.12e-14	-6.73e-12
gwp_fub_ze3	ef_diesel_combustion_mult	3.79e-10	2.58e-15	-3.79e-10
gwp_fub_ze3	ef_zeolite_mining_mult	3.86e-10	1.87e-15	-3.86e-10
gwp_fub_ze3	ef_dmf_air_emission_mult	0	0	0
gwp_fub_ze3	dmf_recovery_fraction	0	0	0
ratio_ze5_over_ze3	electrospinner_power_w	0.516	0.516	-0.000395
ratio_ze5_over_ze3	stirrer_hotplate_power_w	0.407	0.407	0.000897
ratio_ze5_over_ze3	drying_oven_power_w	0.0401	0.0398	-0.000276
ratio_ze5_over_ze3	ef_electricity_mult	0.0325	0.032	-0.000483
ratio_ze5_over_ze3	sonicator_power_w	0.00321	0.00359	0.000379
ratio_ze5_over_ze3	vacuum_pump_power_w	0.00361	0.00358	-2.4e-05
ratio_ze5_over_ze3	ef_dmf_upstream_mult	1.05e-05	1.19e-05	1.35e-06
ratio_ze5_over_ze3	ef_pan_upstream_mult	3.86e-08	1.8e-07	1.42e-07
ratio_ze5_over_ze3	ef_pvdf_upstream_mult	1.71e-08	1.39e-08	-3.2e-09
ratio_ze5_over_ze3	ef_di_water_mult	5.01e-08	6.48e-10	-4.95e-08
ratio_ze5_over_ze3	ef_transport_mult	6.75e-12	1.12e-14	-6.73e-12
ratio_ze5_over_ze3	ef_diesel_combustion_mult	3.79e-10	2.58e-15	-3.79e-10
ratio_ze5_over_ze3	ef_zeolite_mining_mult	3.86e-10	1.87e-15	-3.86e-10
ratio_ze5_over_ze3	ef_dmf_air_emission_mult	0	0	0
ratio_ze5_over_ze3	dmf_recovery_fraction	0	0	0

Interaction analysis. Where $S_T - S_1$ exceeds 0.1 for any parameter, this indicates significant interaction effects. Our analysis identifies [TBD: interacting parameter] as the primary interacting term, coupling with other factors through the DMF mass balance (main text §**??**).

S6 Breakeven Grid — Impact per kg MB

Table S6 presents the optimum scenario (lowest GWP100 per kg MB) for each combination of membrane lifetime (1, 2, 5, 10, 15, 20, 30 cycles) and DMF recovery fraction (0%, 50%, 80%, 95%). The full 840-row grid of impacts per kg MB for each scenario $\times$ lifetime $\times$ recovery combination underpins this summary.

Table S6: Optimum scenario (lowest GWP100 per kg MB) per (lifetime $\times$ DMF recovery) combination. Rows: membrane lifetime (cycles). Columns: DMF recovery fraction.

Lifetime	0%	50%	80%	95%
1	ZE3	ZE3	ZE3	ZE3
2	ZE3	ZE3	ZE3	ZE3
5	ZE3	ZE3	ZE3	ZE3
10	ZE3	ZE3	ZE3	ZE3
15	ZE3	ZE3	ZE3	ZE3
20	ZE3	ZE3	ZE3	ZE3
30	ZE3	ZE3	ZE3	ZE3

S7 Dye Physicochemical Properties

Table S7 collects the physicochemical properties of the four dyes characterised by Arif *et al.* 2024 [6] on Ze5-PAN/PVDF membranes. This context supports the selectivity discussion (main text §3.2).

Table S7: Physicochemical properties of the four test dyes from Arif 2024 [6], cycle 5 rejection on Ze5-PAN/PVDF.

Dye	Charge	Formula	pK_a	Molecular dim. (nm)	Rejection (%)
Methylene blue (MB)	cationic	$C_{16}H_{18}ClN_3S$	3.80	$1.43 \times 0.56 \times 0.21$	100
Crystal violet (CV)	cationic	$C_{25}H_{30}ClN_3$	5.31	$1.35 \times 1.34 \times 0.36$	100
Congo red (CR)	anionic	$C_{32}H_{22}N_6Na_2O_6S_2$	7.73	$2.62 \times 0.71 \times 0.35$	78
Methyl orange (MO)	anionic	$C_{14}H_{14}N_3NaO_3S$	6.75	$1.49 \times 0.48 \times 0.26$	1

The high rejection of MB and CV (both cationic) is governed by electrostatic attraction to the negatively-charged zeolite surface (pH_{pzc} of clinoptilolite $= 6.9$). The lower rejection of anionic CR (78%) and MO (1%) reflects weaker electrostatic interaction; CR's larger molecular size partially compensates via size-exclusion, explaining its higher rejection than the smaller MO.

S8 Reproducibility

The complete computational architecture used to produce the results in this study is documented below. All inventory data, characterisation factors, and analysis logic are reported in this Supporting Information; the source code is structured for transparent re-implementation by independent researchers.

Inventory and characterisation data The foreground inventory per scenario is given in Section S1. Background emission factors with sources are tabulated in Section S2. Pedigree-matrix data quality scores are reported in Section S3. Monte Carlo and Sobol output statistics are tabulated in Sections S4 and S5, and the breakeven grid optimum mapping appears in Section S6.

Code architecture (Python + R) The analysis pipeline used to compute the reported LCIA scores is organised as a two-language workflow. The computational side runs on Python 3.11 with the Brightway 2.5 LCA framework and the SALib sensitivity-analysis library, with a conda environment specification distributed alongside the manuscript. Five sequential Jupyter notebooks execute the pipeline in order: foreground inventory construction, background linking of emission factors and biosphere flows, six-category LCIA computation, Monte Carlo uncertainty and one-at-a-time tornado analysis, and Sobol global sensitivity analysis together with the breakeven grid. Six reusable Python modules provide the building blocks: an Elsevier-compliant matplotlib style configuration, per-scenario foreground inventory builders, the multi-category emission-factor table, the six characterisation-factor tables, a Python-native LCIA engine that enables fast Monte Carlo evaluation, and a Saltelli-sampler evaluator that feeds the Sobol analysis and the breakeven grid. Publication figures are generated by a separate R script using the ggplot2 library and a custom Elsevier theme, consuming the CSV outputs of the Python pipeline.

Reproduction workflow

```
# 1. Environment setup
conda env create -f environment.yml
conda activate lca

# 2. Run Python notebooks in order (01 -> 02 -> 03 -> 04 -> 05)
jupyter lab

# 3. Auto-populate manuscript numerical values
python scripts/populate_values_tex.py
python scripts/csv_to_latex_si.py

# 4. Generate publication figures
Rscript R/06_figures.R

# 5. Compile manuscript and SI
cd manuscript
latexmk -pdf main.tex
cd supporting-information
latexmk -pdf SI.tex
```

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