

Supporting information

Environmental assessment of metal-organic framework DUT-4 synthesis and its application for siloxane removal

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S1. Synthesis stage

The energy balance in the autoclave was evaluated through Equation S1, which was proposed considering the scheme of Figure S1. The description of the parameters in Eq. (S1) is presented in Table S1. The first term represents the sensible heat, the second and third terms corresponded to Teflon and stainless steel (autoclave) heating, respectively.

$$E = m_1 \int_{T_e}^{T_w} C_{p_{mix}} dT + m_2 \int_{T_e}^{T_w} C_{p_{tf}} dT + m_3 \int_{T_e}^{T_w} C_{p_{ss}} dT \quad \text{Eq. (S1)}$$

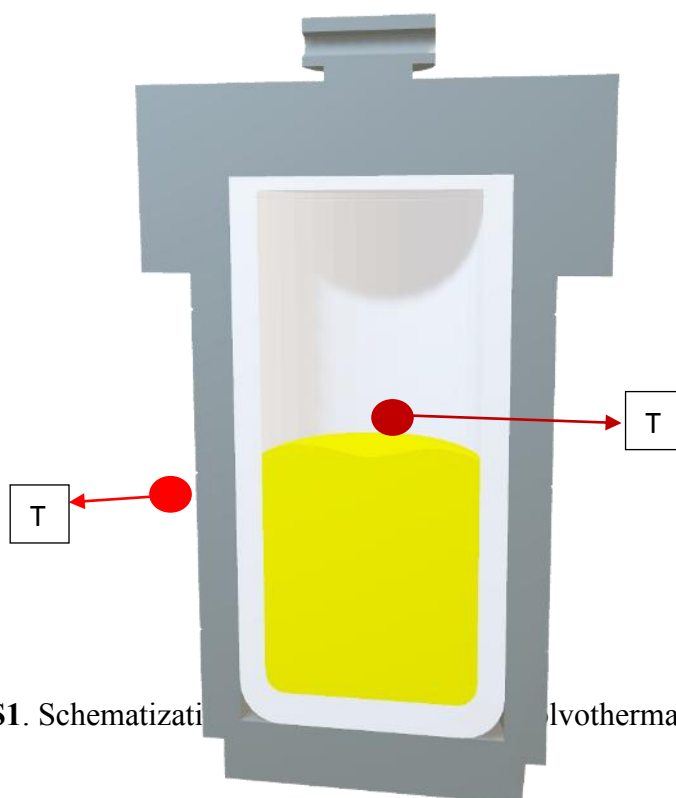


Figure S1. Schematization of the solvothermal reactor.

Table S1. Value of each variable and parameters used for the energy balance into the solvothermal reactor.

Variable	Description/unit	Value
m_1	Fluid mass (g)	60.0
m_2	Stainless steel mass of autoclave (g)	4600.0
m_3	Teflon liner mass of autoclave (g)	403.0
T_w	Work temperature (°C)	120.0
T_e	Environmental temperature (°C)	25.0
$C_{p_{mix}}$	Fluid specific heat (J/g K)	4.1
$C_{p_{ss}}$	Stainless steel specific heat (J/g K)	0.5
$C_{p_{tf}}$	Teflon liner specific heat (J/g K)	1.0

S2. Cleaning and solvent exchange stages

The energy consumption in the cleaning and solvent stages was evaluated using Eq. (S2):

$$E_{cr} = \frac{1}{2} * m * r^2 * (2\pi f)^2 * f_r \quad \text{Eq. (S2)}$$

where r is the rotor radius (0.068 m, Refrigerated Microcentrifuge Prism R, LabNet), f is the frequency (166.67 s^{-1}), m is the mass to centrifuge (0.069, 0.087, 0.082, and 0.161 kg for DUT-4 (DMF), DUT-4 (DCM), DUT-4 (H), and DUT-4 (W) scenarios respectively), and f_r is the friction factor (1.45).

S3. Drying stage

The energy required for the drying of solid DUT-4 was estimated using Eq. (S3). The parameters used in the drying stage for each study scenario are given in Table S2.

$$\frac{q_T}{m_s} = C_{ps}(T_{sb} - T_{sa}) + X_a C_{pL}(T_v - T_{sa}) + (X_a - X_b)\lambda + X_b C_{pL}(T_{sb} - T_v) + (X_a - X_b)C_{pV}(T_{va} - T_v) \quad \text{Eq. (S3)}$$

Where:

- q_T/m_s is the amount of heat transferred per unit mass of solids (J/g);
- C_{ps} , C_{pL} , and C_{pV} are the solid specific heat, the liquid specific heat, and the steam specific heat, respectively (J/g·K);
- T_{sb} and T_{sa} are the final temperature of the solids and the feed temperature, respectively (K);
- X_a and X_b are the initial and final mass per unit mass of dry solids, respectively;
- T_v and T_{va} is the vaporization temperature and the final vapour temperature (K), respectively.
- λ is the latent vaporization heat (J/g).

Table S2. Parameters and variables for determining the energy consumption in the drying stage of DUT-4(DMF), DUT-4(DCM), DUT-4(H), and DUT-4 (W) scenarios.

Parameter	DUT-4(DMF)	DUT-4(DCM)	DUT-4(H)	DUT-4(W)
T_{sa} (K)	298.150	298.150	298.150	298.150
T_v (K)	426.150	312.750	341.150	373.150
T_{sb} (K)	393.150	393.150	393.150	393.150
T_{va} (K)	393.150	393.150	393.150	393.150
l (J/g)	639.476	329.517	335.000	2260.872

C_{p_s} (J/g·K)	4.105	1.003	2.167	4.105
C_{p_l} (J/g·K)	4.181	1.000	2.206	4.181
C_{p_v} (J/g·K)	1.610	1.804	1.419	1.825
X_a	2.691	9.768	4.501	4.029
X_b	0.000	0.000	0.000	0.000

S4. Eco-inventories

The eco-inventories used in the Life Cycle Inventory (LCI) to produce DUT-4, through four scenarios, are shown in Table S3.

Table S3. Eco-inventories used in LCI for DUT-4 production.

Input	Eco-inventory from Ecoinvent v3.3 database
Electricity	Electricity, medium voltage {MX} market for Alloc Def, U
N, N-Dimethylformamide	N,N-dimethylformamide {GLO} market for Alloc Def, U
2,6-Naphthalene dicarboxylic acid	Purified terephthalic acid {GLO} market for Alloc Def, U
Nonahydrate aluminum nitrate	Aluminium sulfate, without water, in 4.33% aluminium solution state {GLO} market for Alloc Def, U
Deionized water	Water, deionised, from tap water, at user {RoW} production Alloc Def, U
Dichloromethane	Dichloromethane {GLO} market for Alloc Def, U
Hexane	Hexane {GLO} market for Alloc Def, U

S5. Life Cycle Impact Assessment midpoint indicators

The characterization of the environmental impact indicators for the DUT-4(DMF), DUT-4(DCM), DUT-4(H) and DUT-4(W) scenarios, using the ReCiPe point of view, is shown in Figure S2 and Table S4.

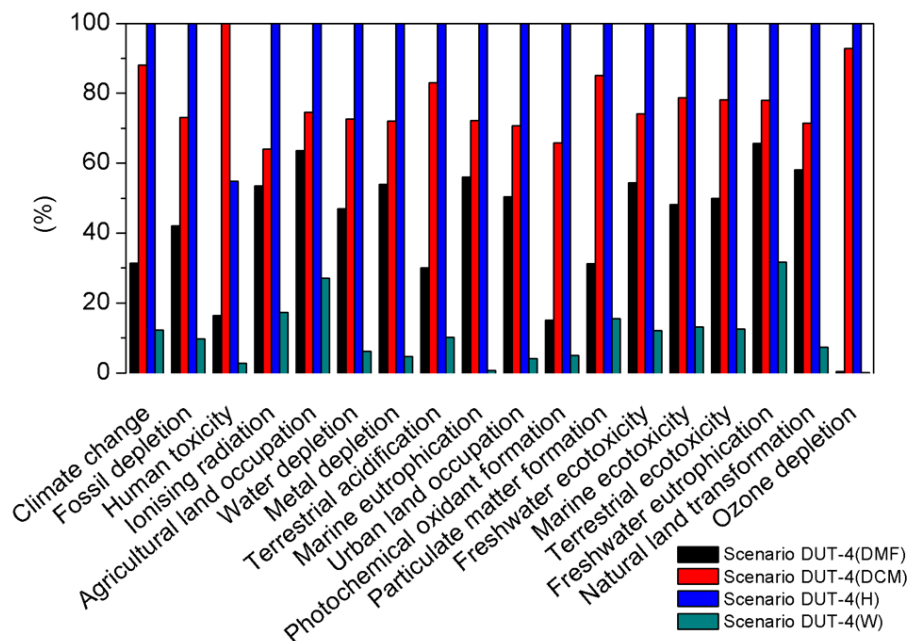


Figure S2. Indicators of environmental impact for DUT-4(DMF), DUT-4(DCM), DUT-4(H), and DUT-4(W) scenarios.

Table S4. Units of the midpoint indicators for the DUT-4 production scenarios.

Indicator	Unit	Scenario DUT-4(DMF)	Scenario DUT-4(DCM)	Scenario DUT-4(H)	Scenario DUT-4(W)
Climate change	kg CO ₂ eq	0.6317	1.7752	2.0164	0.2483
Fossil depletion	kg oil eq	0.3400	0.5912	0.8092	0.0794
Human toxicity	kg 1,4-DB eq	0.0689	0.4209	0.2306	0.0116
Ionising radiation	kBq U235 eq	0.0394	0.0471	0.0736	0.0127
Agricultural land occupation	m ² a	0.0217	0.0255	0.0342	0.0093
Water depletion	m ³	0.0085	0.0132	0.0182	0.0011
Metal depletion	kg Fe eq	0.0052	0.0070	0.0097	0.0005
Terrestrial acidification	kg SO ₂ eq	0.0037	0.0101	0.0122	0.0012
Marine eutrophication	kg N eq	0.0019	0.0025	0.0035	0.0000
Urban land occupation	m ² a	0.0019	0.0026	0.0037	0.0002
Photochemical oxidant formation	kg NMVOC	0.0018	0.0080	0.0121	0.0006
Particulate matter formation	kg PM10 eq	0.0016	0.0044	0.0052	0.0008
Freshwater ecotoxicity	kg 1,4-DB eq	0.0016	0.0022	0.0030	0.0004
Marine ecotoxicity	kg 1,4-DB eq	0.0008	0.0013	0.0017	0.0002
Terrestrial ecotoxicity	kg 1,4-DB eq	6.12×10 ⁻⁵	9.56×10 ⁻⁵	1.22×10 ⁻⁴	1.53×10 ⁻⁵
Freshwater eutrophication	kg P eq	2.87×10 ⁻⁵	3.41×10 ⁻⁵	4.37×10 ⁻⁵	1.39×10 ⁻⁵
Natural land transformation	m ²	9.01×10 ⁻⁶	1.11×10 ⁻⁵	1.55×10 ⁻⁵	1.14×10 ⁻⁶
Ozone depletion	kg CFC-11 eq	1.07×10 ⁻⁷	2.42×10 ⁻⁵	2.61×10 ⁻⁵	1.98×10 ⁻⁸

The contribution of solvents and electricity used in the production of DUT-4 for fossil depletion and climate change indicators (ReCiPe midpoint) is shown in Table S5.

Table S5. Contribution of solvents and electricity in the production of DUT-4.

Input	Scenario DUT-4(DMF)	Scenario DUT-4(DCM)	Scenario DUT-4(H)	Scenario DUT-4(W)
<i>Fossil depletion (kg oil eq)</i>				
DMF	0.28	0.34	0.48	-
Dichloromethane	-	0.19	0.20	-
Hexane	-	-	0.07	-
Water	-	-	-	-
Electricity	0.06	0.06	0.06	0.08
<i>Climate change (kg CO₂ eq)</i>				
DMF	0.45	0.55	0.77	-
Dichloromethane	-	0.95	1.02	-
Hexane	-	-	0.04	-
Water	-	-	-	7.23×10 ⁻⁴
Electricity	0.18	0.19	0.19	0.24