Supplementary Information

Wood-Supported Cationic Polyelectrolyte Membranes from A Reactive Ionic Liquid for Water Detoxification

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Additional Description

Additional Figures

Additional Tables

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AD SI-1. Spectral characterisation data for ECH and TEA

ECH: ^{1}H NMR (400 MHz, $CDCl_3$): 3.52 (1H, dd, C**H**-Cl, *J* = 4.6 and 11.8 Hz), 3.41 (1H, dd, C**H**-Cl, *J* = 6.1 and 11.8 Hz), 3.11 (1H, dddd, C**H,** *J* = 6.3, 4.5, 3.9 and 2.5 Hz), 2.76 (1H, dd, C**H**$_2$, *J* = 3.9 and 4.9 Hz), 2.56 (1H, dd, C**H**$_2$, *J* = 3.9 and 4.9 Hz) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): 51.4 (**C**H_2), 46.9 (**C**H), 45.4 (**C**H_2Cl) ppm. FTIR (ATR): 3040-2988 (st, CH_2), 1428 (b, CH_2), 1381 (b, *gem*-CH_2), 1248 (st, C-O), 1101 (st, C-O-C), 924 (b, CH-CH_2 (glycidyl)), 816-718 (st, C-Cl) cm^{-1}.

TEA: ^{1}H NMR (400 MHz, $CDCl_3$): 2.37 (6H, q, C**H**$_2$-N, *J* = 7.1 Hz), 0.88 (9H, t, C**H**$_3$. *J* = 7.2 Hz) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): 11.9 (**C**H_3), 11.7 (**C**H_2-N) ppm. FTIR (ATR): 2973-2934 (st, CH_3), 2889-2807 (st, CH_2), 1473-1385 (st, CH_2), 1202-1064 (b, C-NR_3) cm^{-1}.

Additional Figures

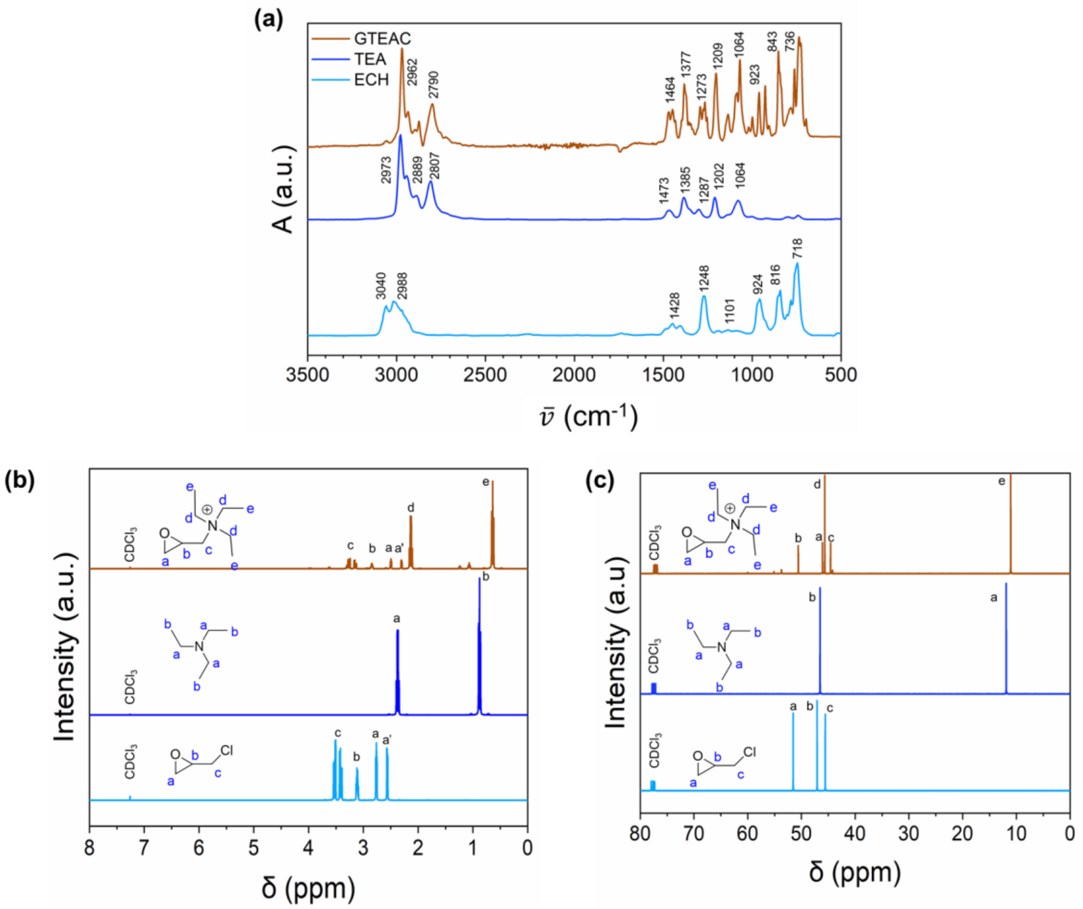

Fig. SI-1 (a) FTIR-ATR, (b) ^{1}H NMR, and (c) ^{13}C NMR spectra for GTEAC, TEA and ECH.

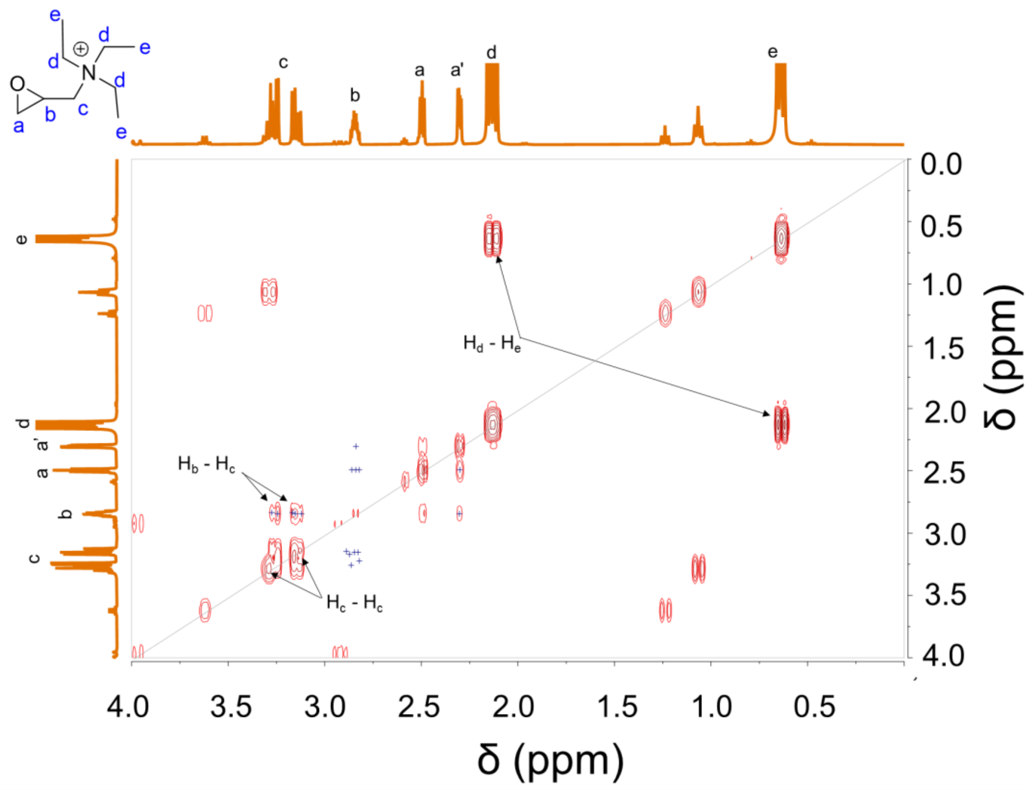

Fig. SI-2 ^{1}H-^{1}H Correlation Spectroscopy (COSY) spectrum of GTEAC.

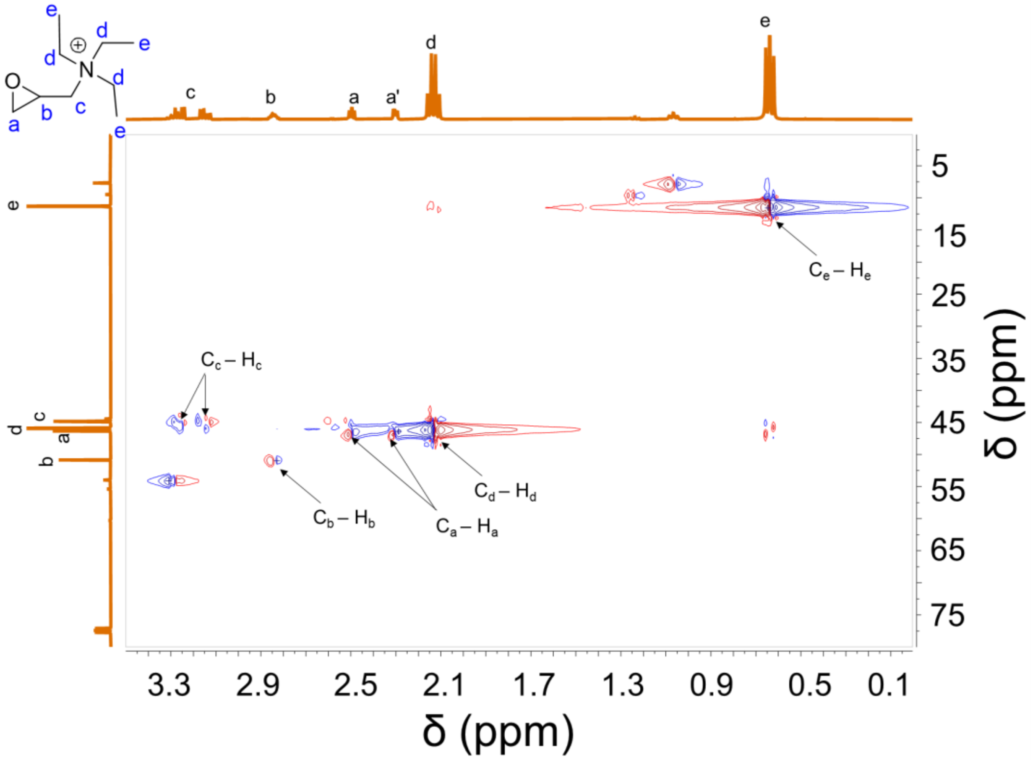

Fig. SI-3 ^{1}H-^{13}C Heteronuclear Single-Quantum Correlation (HSQC) spectrum of GTEAC.

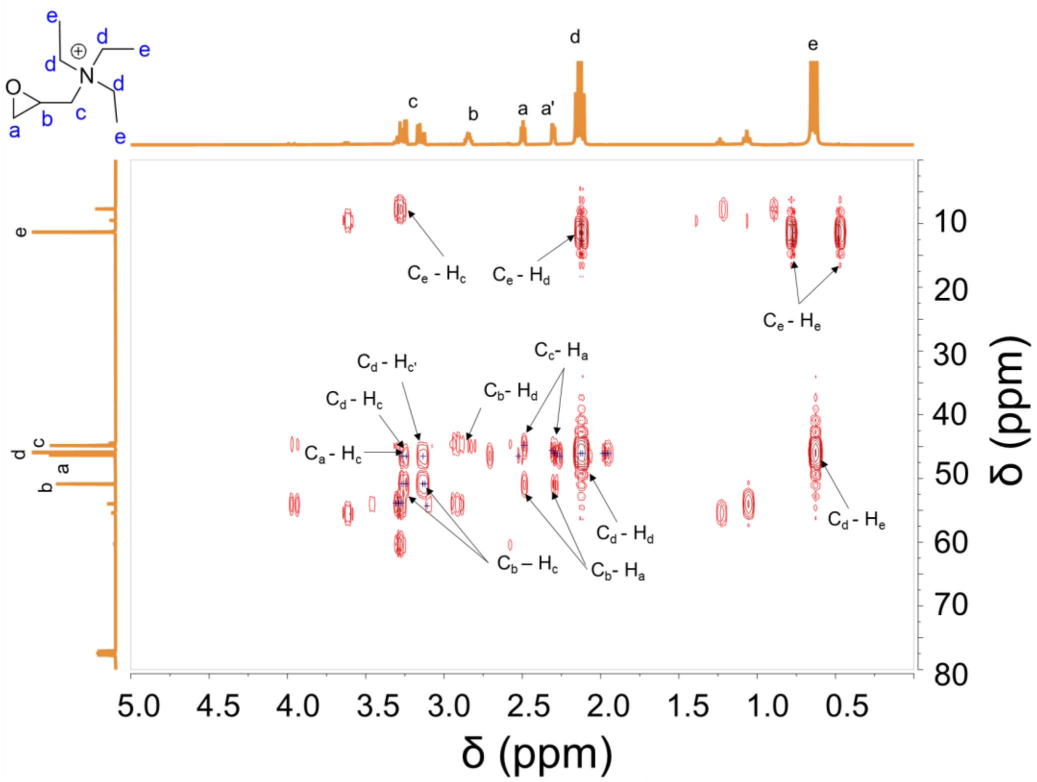

Fig. SI-4 ^{1}H-^{13}C Heteronuclear Multiple-Quantum Correlation (HMBC) spectrum of GTEAC.

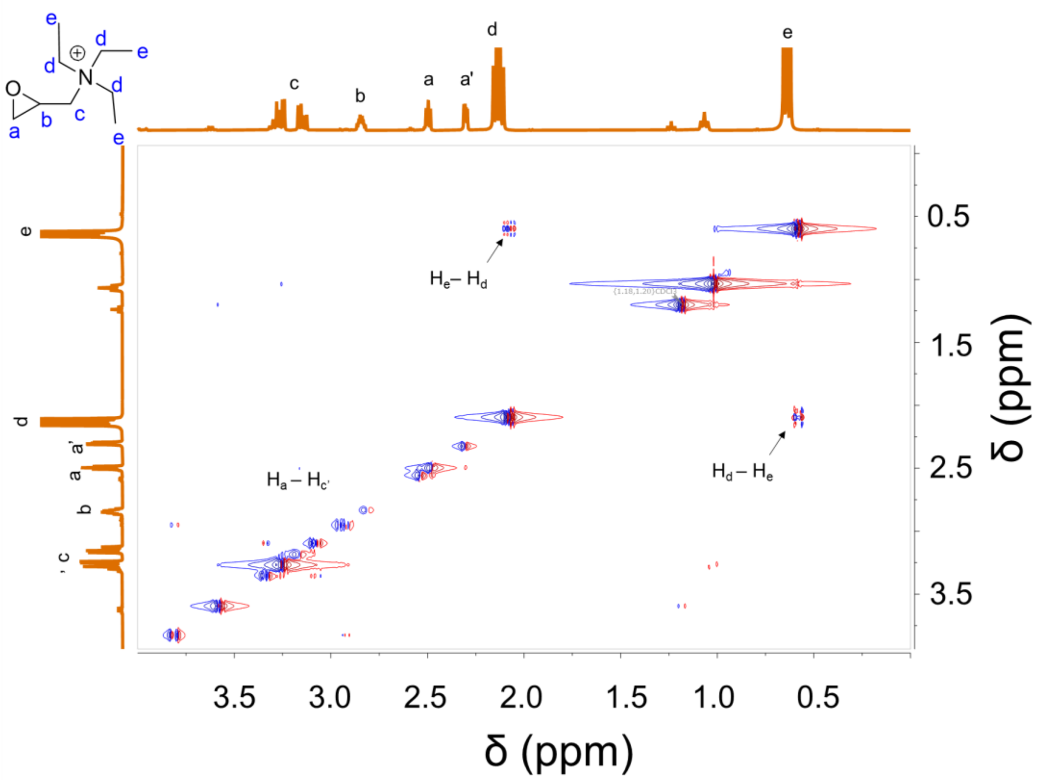

Fig. SI-5 ^{1}H-^{1}H Nuclear Overhauser Effect Spectroscopy (NOESY) spectrum of GTEAC.

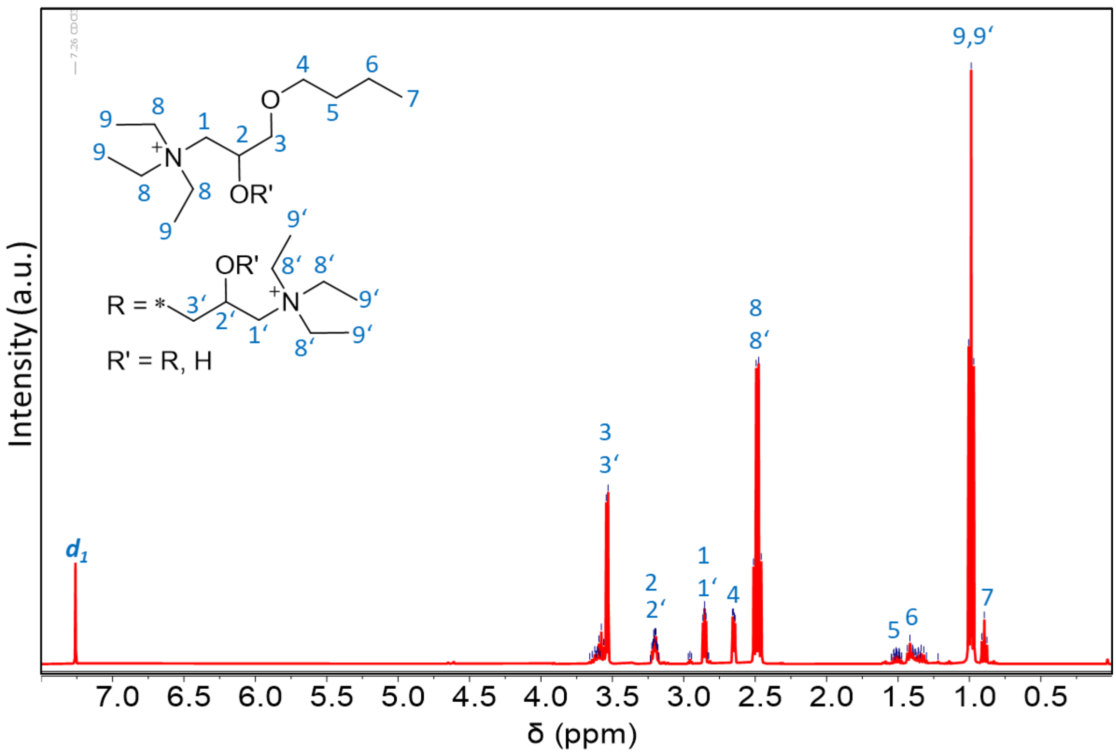

Fig. SI-6 ^{1}H NMR spectrum of poly-GTEAC.

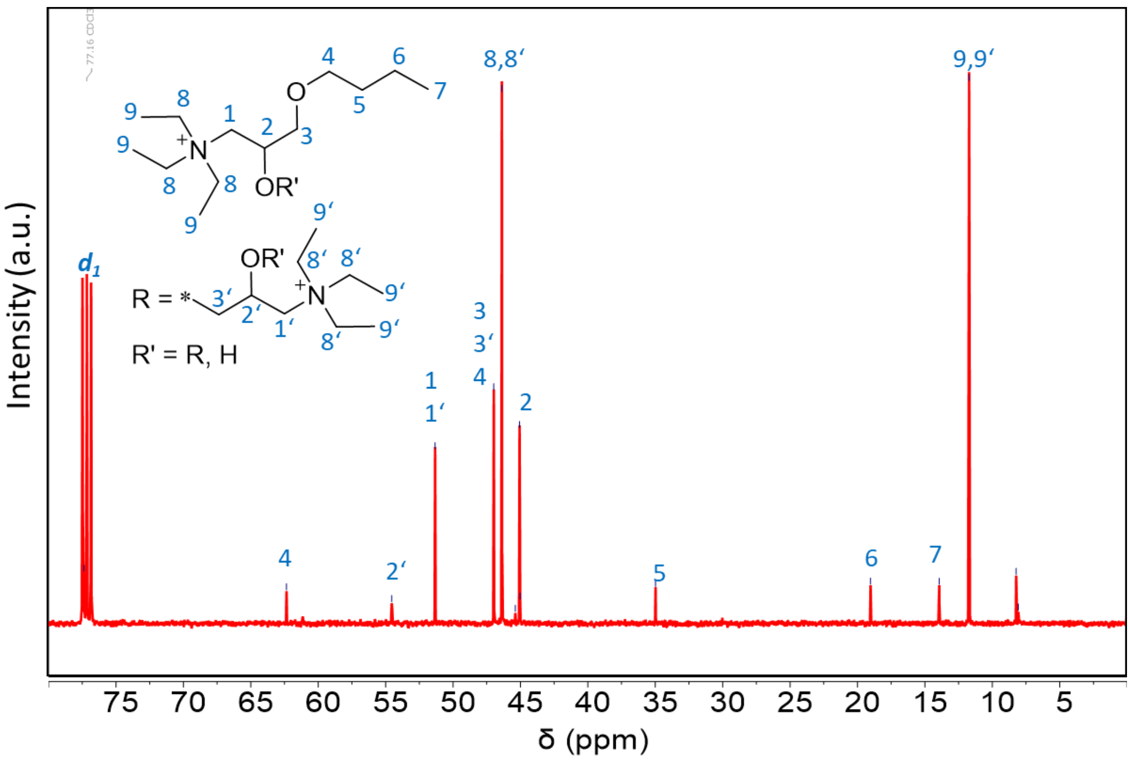

Fig. SI-7 ^{13}C NMR spectrum of poly-GTEAC.

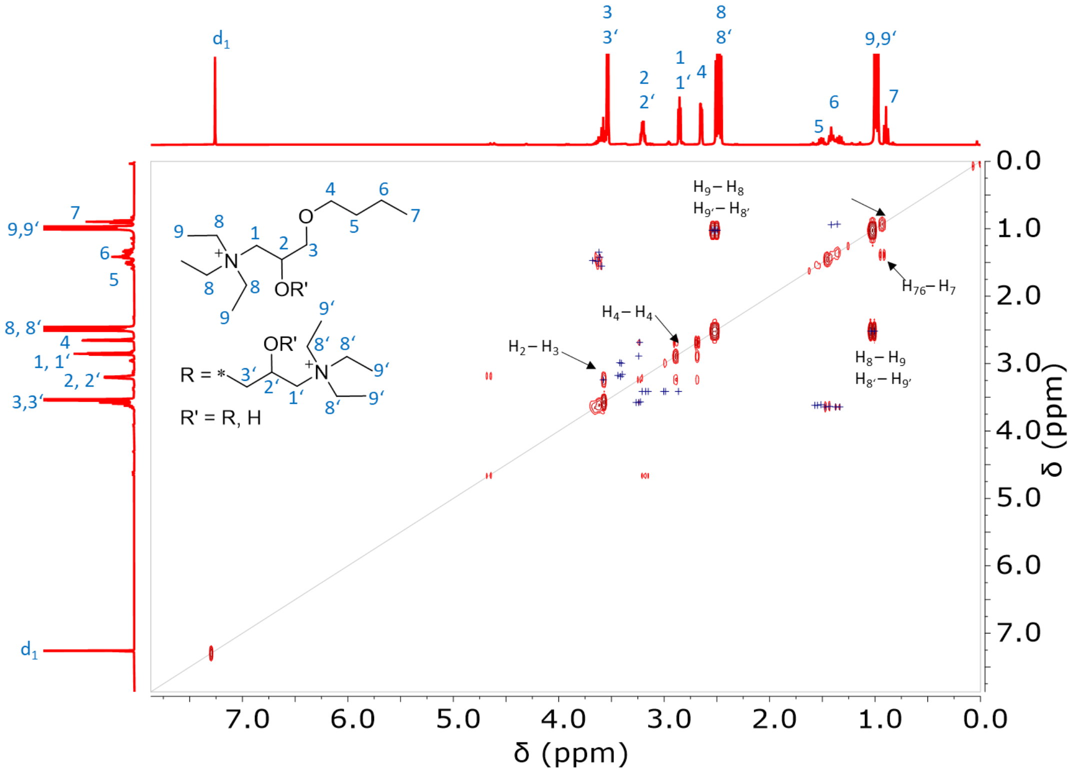

Fig. SI-8 ^{1}H-^{1}H Correlation Spectroscopy (COSY) spectrum of poly-GTEAC.

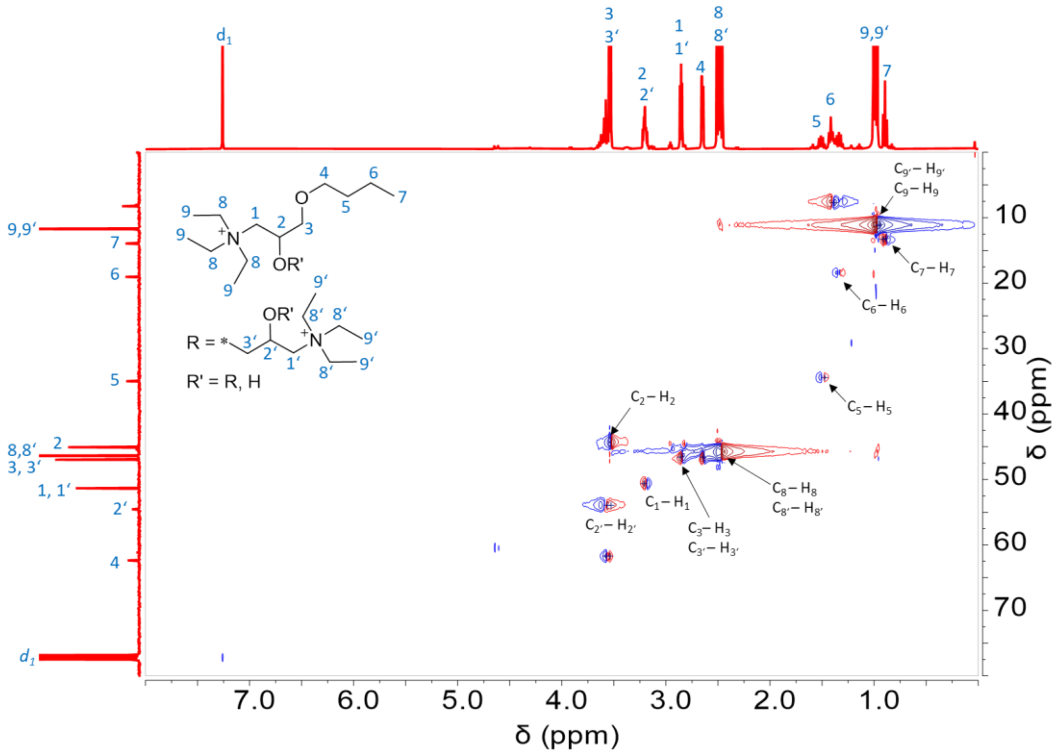

Fig. SI-9 ^{1}H-^{13}C Heteronuclear Single-Quantum Correlation (HSQC) spectrum of poly-GTEAC.

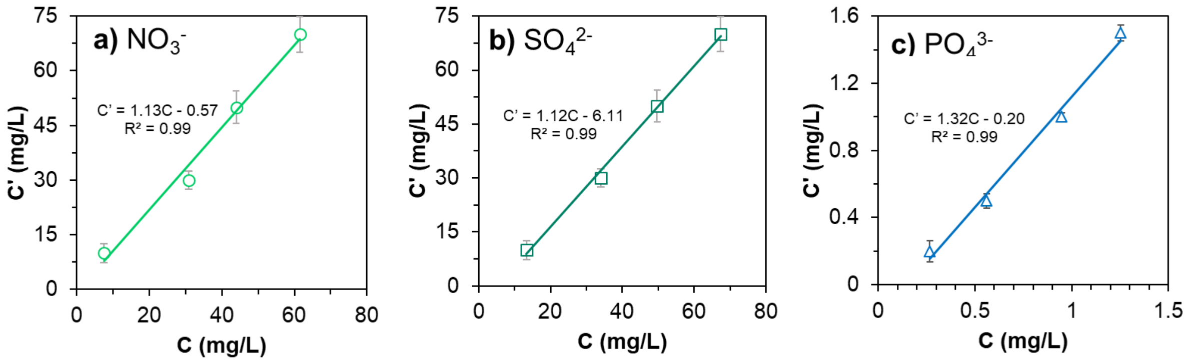

Fig. SI-10 Calibration curves for the spectrophotometric determination of (a) NO_3^-, (b) SO_4^{2-} and (c) PO_4^{3-} oxoanions. Note: C' and C are the measured concentration and the standard concentration, respectively.

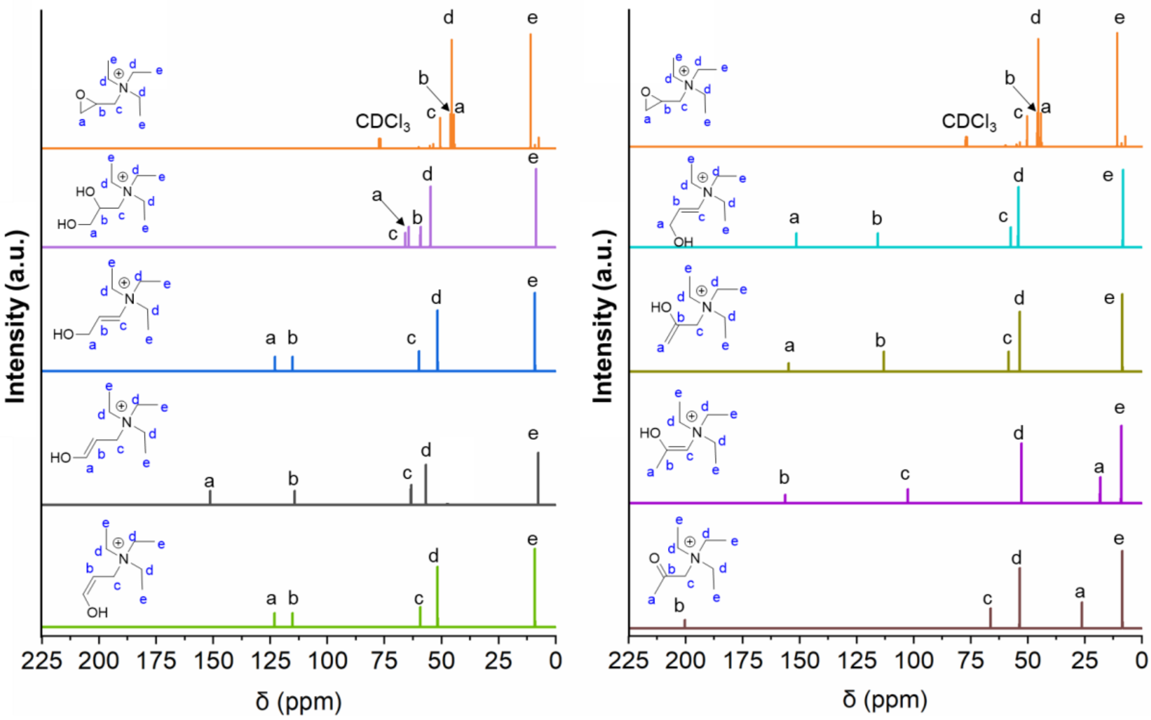

Fig. SI-11 Experimental (orange signal) and predicted ^{13}C NMR spectra of GTEAC and potential decomposates, respectively, in the oil component of the synthesised reactive ionic liquid (RIL) - GTEAC.

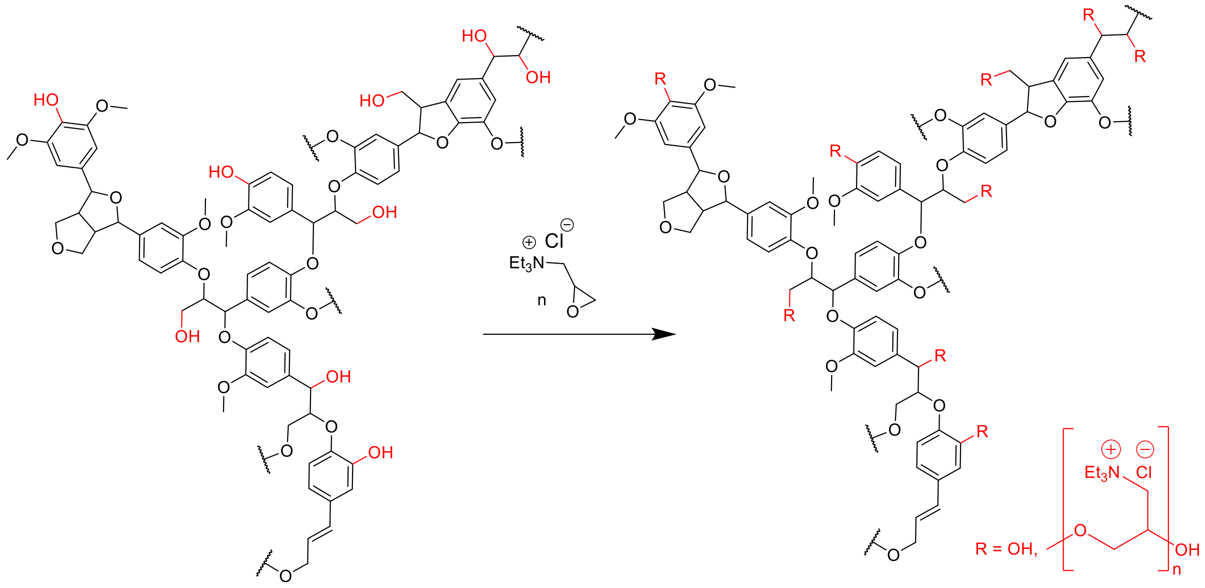

Fig. SI-12 Quaternisation of lignin moieties in wood.

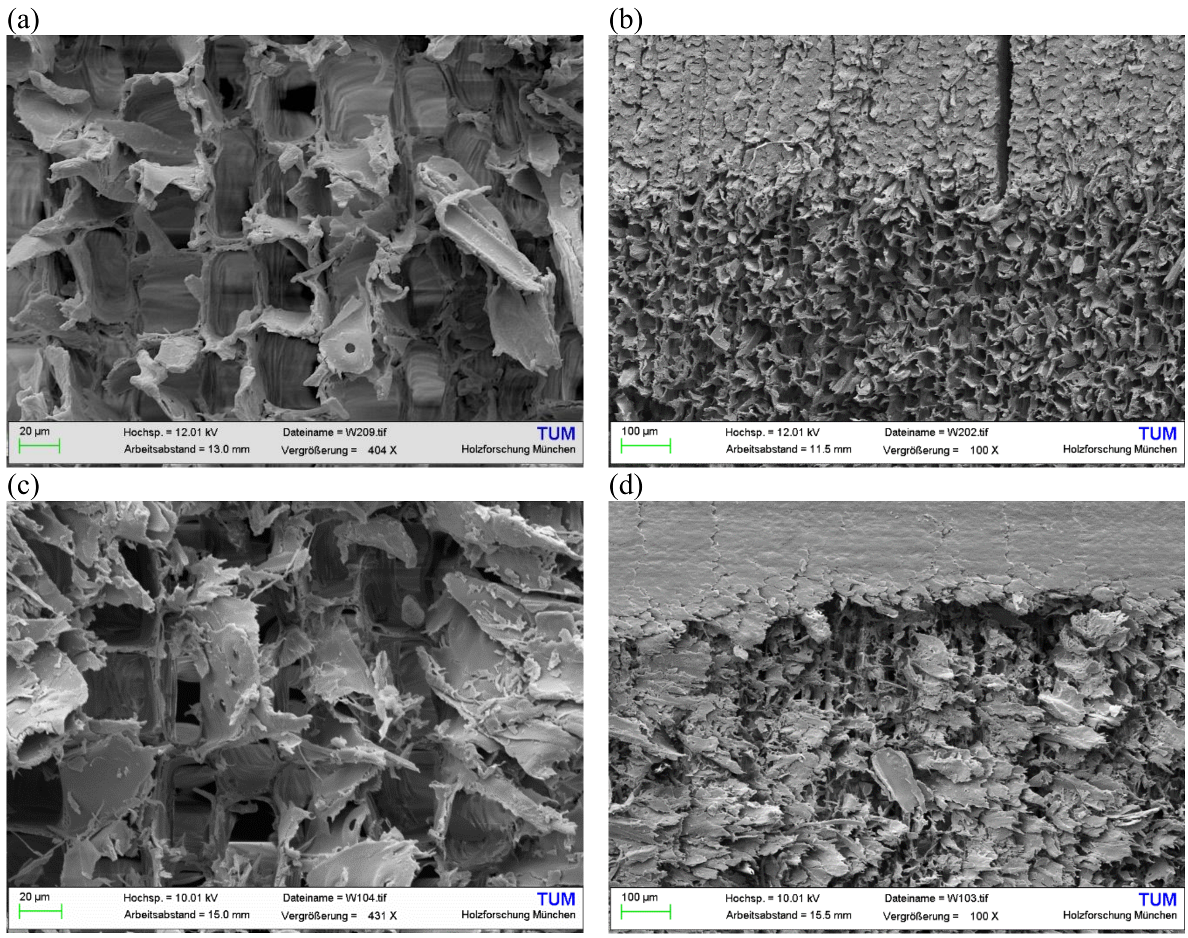

Fig. SI-13 SEM micrographs (cross-section) of Pinewood (a: 20 µm scale bar; and b: 100 µm scale bar) and QWM L22 (c: 20 µm scale bar; and d: 100 µm scale bar).

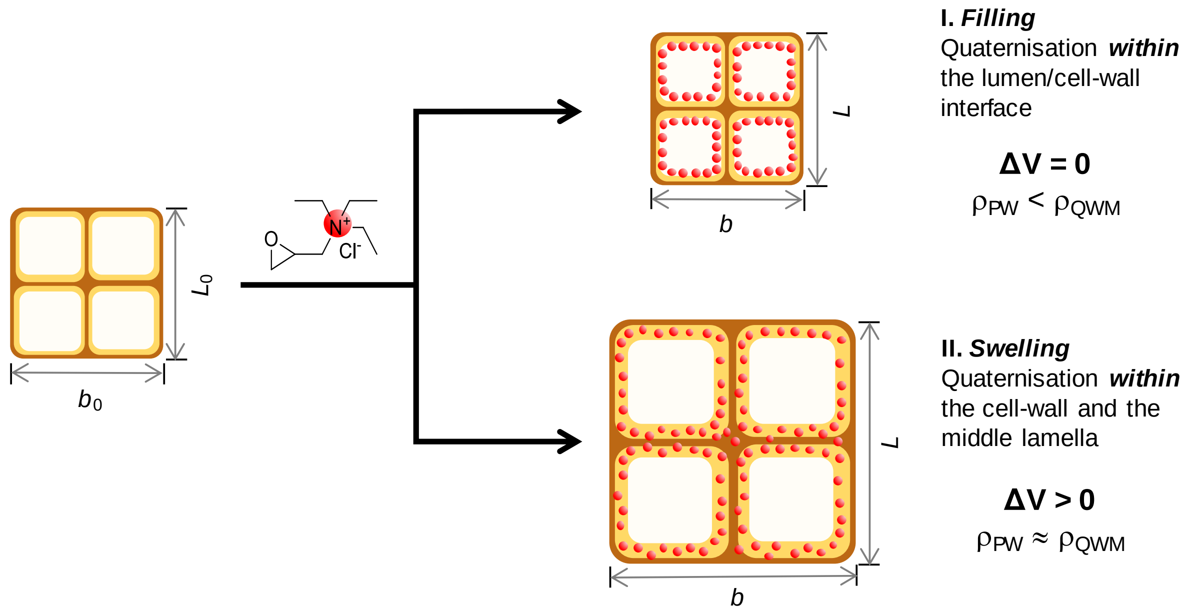

Fig. SI-14 Impact of GTEAC modification at the wood microscale.

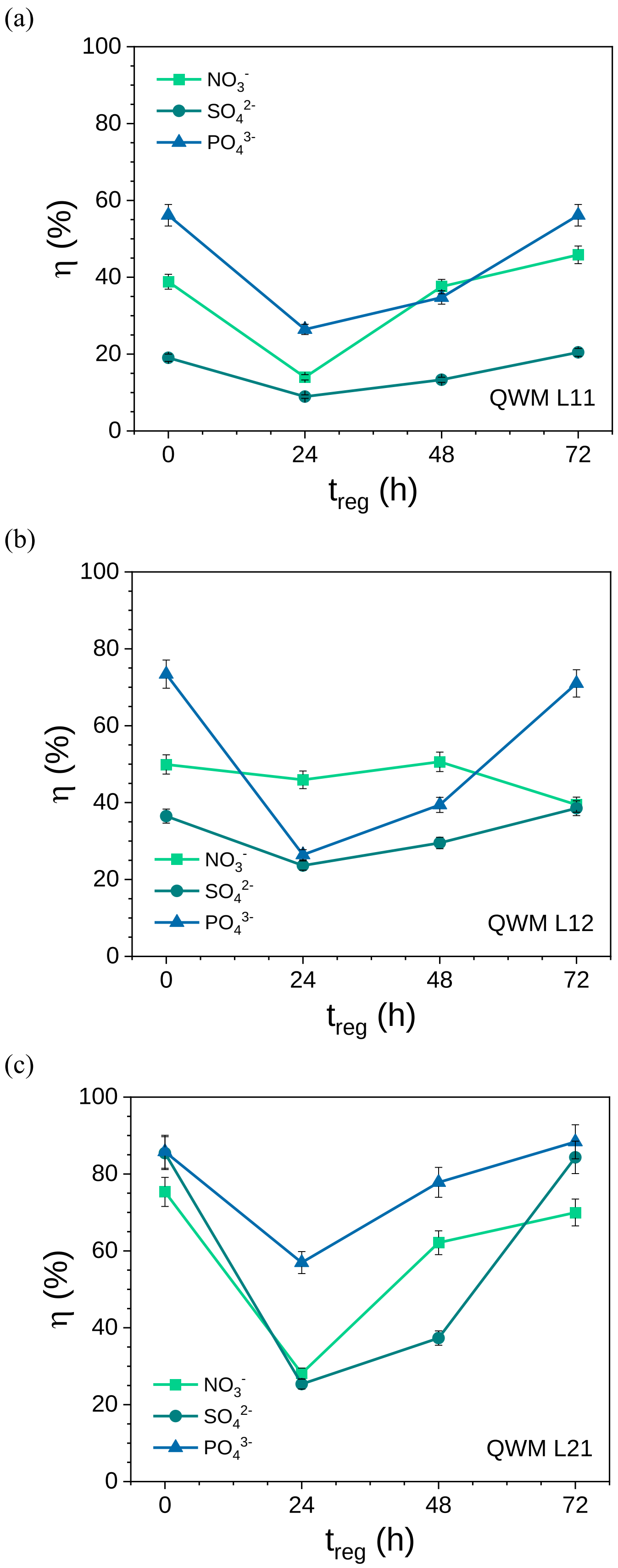

Fig. SI-15 The removal efficiency η_i after the first filtration cycles for QWM filter discs: (a) QWM L11, (b) QWM L12 and (c) QWM L21 across different regeneration times t_{reg}.

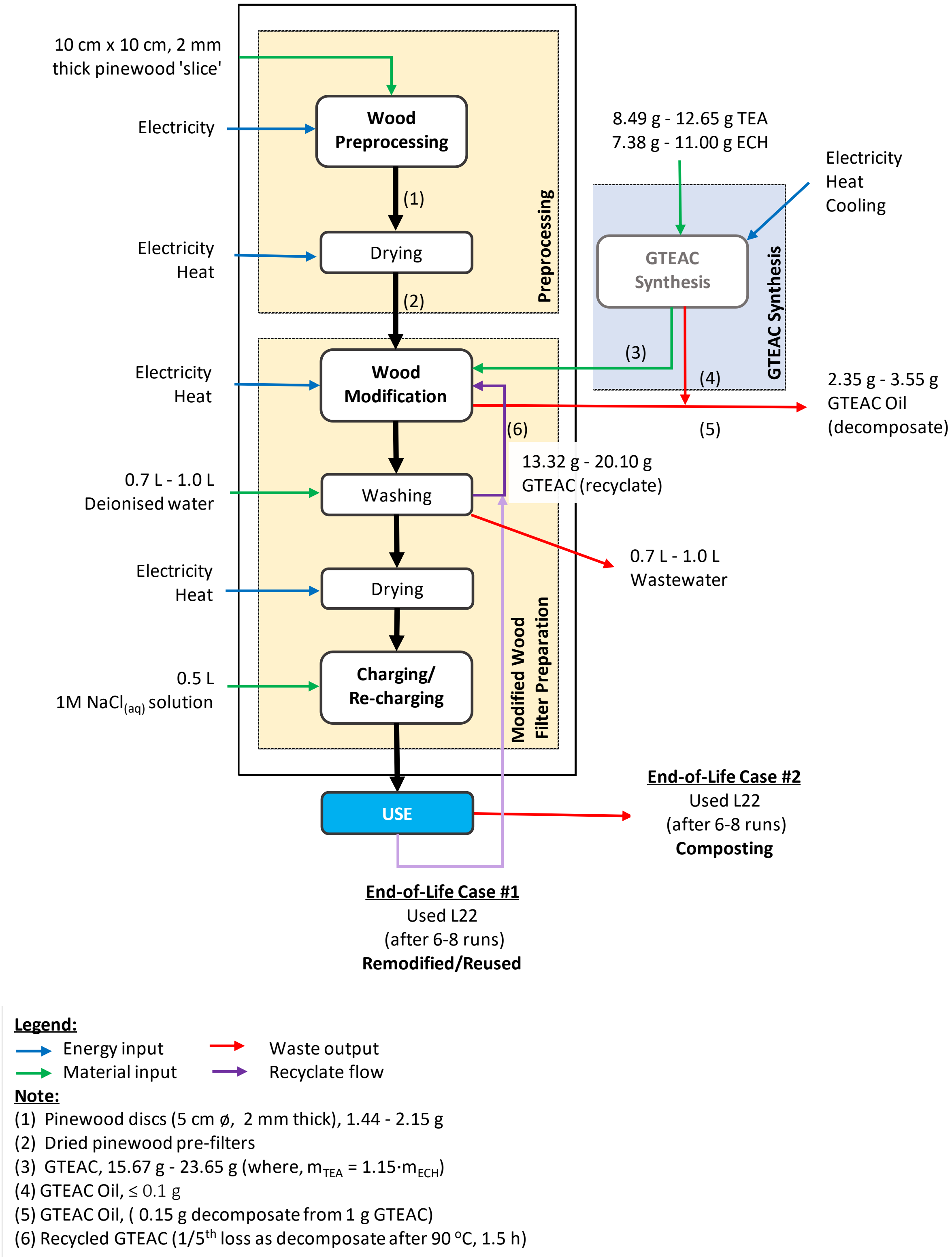

Fig. SI-16 Process Flow (Material and Energy flows) for the preparation of QWM filter discs. The end-of-life outcomes for the product are indicated.

Additional Tables

Table SI-1 Effect of quaternisation on additional physicochemical and performance-related properties, *e.g.*, mass swelling parameter q_m, volume swelling parameter q_v, density ratios ρ/ρ_0, SFQ and BSQ ratios, oxoanion removal efficiency η_i (i = NO_3^-, SO_4^{2-} and PO_4^{3-}) and flux J_i (L/(m²·h)) for the four QWM filters.

Sample	L11	L12	L21	L22
T (°C)	60	60	90	90
t (h)	1	1.5	1	1.5
q_m	1.74	1.89	1.72	1.85
q_V	1.10	1.28	1.10	1.31
ρ/ρ_0 [a]	1.13	1.13	1.27	1.33
$(\rho/\rho_0)_{swelling}$ [b]	1.09	1.10	1.19	1.21
$(\rho/\rho_0)_{filling}$ [c]	1.15	1.16	1.32	1.40
SFQ	0.67	0.50	0.62	0.63
BSQ	0.33	0.50	0.38	0.37
$\eta_{NO_3^-}$ (%)	38.8	49.9	75.3	83.9
$\eta_{SO_4^{2-}}$ (%)	19.1	36.5	85.4	98.3
$\eta_{PO_4^{3-}}$ (%)	56.1	73.4	85.8	88.9
$Loss_{\eta_i}$ (%) [d]	2.5	8.4	6.0	11
$J_{NO_3^-}$ (L/(m²·h))	348	348	385	440
$J_{SO_4^{2-}}$ (L/(m²·h))	293	348	385	403
$J_{PO_4^{3-}}$ (L/(m²·h))	257	275	348	385

Note: [a] post-modification density ratio for dry QWM filters at 55-60 ˚C after 1 h; [b] upper limit (maximum bulk swelling, BSQ); [c] lower limit (maximum surface filling, SFQ); [d] max η_i loss after > 8 runs.

Table SI-2 Effect of V_f/V_{QWM} on the oxoanion removal efficiency for QWM L22.

V_f/V_{QWM}	63.7 [a]	12.7 [b]
$\eta_{NO_3^-}$ (%)	51.5	84.9
$\eta_{SO_4^{2-}}$ (%)	89.1	98.6
$\eta_{PO_4^{3-}}$ (%)	76.0	88.5

Note: V_f: [a] 250 mL; [b] 50 mL. V_{QWM}: 3.93 cm³

Table SI-3 Costing analysis for the QWM L22 filter disc (50 mm ∅, 2 mm, ~540 kg/m^3).

	Inputs	Unit	Amount Min	Amount Max	Unit Cost (€/unit)	Cost (€/ut) Min	Cost (€/ut) Max	Comment
1	Pinewood discs [a]	kg	0.001	0.002	4.585	0.007	0.010	Technical Supplier 25.4 mm (4/4) thickness, €5.41 per 2360 cm^3 (1 FBM [b]), avg. density 500 kg/m^3
2	Epichlorohydrin (ECH), ThermoSci, 99% pure	kg	0.007	0.011	41.200	0.304	0.453	Technical Supplier
3	Triethylamine (TEA), Sigma-Aldrich, 99.7% pure, water-free	kg	0.008	0.013	64.279	0.546	0.813	Technical Supplier
4	Deionised Water	kg	1.296	1.496	1.798	2.330	2.688	Technical Supplier
5	Sodium Chloride, VWR	kg	0.029		0.034	0.001		Technical Supplier
6	Electricity [c]	kWh	2.931	3.183	0.048	0.141 [d]	0.153 [d]	SWM Versorgungs GmbH; 57.66 €/kW/mo
			Cost per piece		€/kg	3.33	4.12	
					€/m^2	4.16	5.15	As dry weight, 2.54 g avg., and area: 19.63 cm^3
					€/m^3	1797.10	2223.63	As density: 540 kg/m^3

Note: [a] 5 cm ∅, 2 mm thickness, 510-540 kg/m^3 and V_{mem} = 3.91 cm^3; [b] Board Foot (FBM); [c] München, Bayern, Germany; [d] 0.03 kWh for GTEAC synthesis (for general mixing and synthesis apparatus).

Table SI-4 Penalty calculation for the GTEAC synthesis and PW quaternisation using the Eco-Scale approach.

	Method Parameters	P_i
1.	Yield (83.2%) [a]	8.4
2.	Price of Reaction Components [b]	
	Inexpensive (<10 €/kg)	0
3.	Safety [c,d]	
	ECH (F, T, T^+, C) (99%, 0.01 kg)	10
	TEA (F, T, C) (99.7%, 0.01 kg)	5
	PW (Nil.) (0.001 – 0.002 kg)	0
4.	Technical Setup	
	Common setup	0
	Inert Gas setup	1
5.	Temperature/time	
	Heating, < 1 h	2
6.	Workup and Purification	
	None	0
	Cooling to room temperature	0
	Total Penalty Score, TPS $= \sum_{I=1}^{N} P_i$	26.4
	Eco-Scale Score [e]:	**73.6**

Note: [a] (100 - Yield)/2; [b] *cf.* Table SI-3, and Methods: Glycidyltriethylammonium Chloride (GTEAC) Synthesis; [c] Based on the hazard warning symbols - Highest penalty reported; [d] Detailed scoring system provided elsewhere (Van Aken *et al.*, 2006); [e] 100 – TPS.

References

Van Aken, K., Strekowski, L., Patiny, L. (2006). EcoScale, a Semi-Quantitative Tool to Select an Organic Preparation Based on Economical and Ecological Parameters. *Beilstein J. Org. Chem.*, *2*. https://doi.org/10.1186/1860-5397-2-3