Membrane technology for water reuse in decentralised non-sewered sanitation systems: Comparison of pressure driven (Reverse Osmosis) and thermally driven processes (Membrane Distillation and Pervaporation)

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Supplementary information

Functional group	Alcohols	Aldehydes	Est	ers	Ketones	Aromatic he	eterocycles	Phenol	Sulphur
Compound	1-Butanol	Benzaldehyde	Ethyl butyrate	Ethyl propionate	2-Butanone	Indole	Skatole	<i>p</i> -Cresol	Dimethyl disulfide
Chemical structure	H ₃ C CH ₂ OH CH ₂ CH ₂	ОН	о H ₃ COCH ₃	0 H ₃ CO ^CH ₃	H ₃ C CH ₃		CH ₃	H ₃ C OH	$^{\rm H_3C}s^{\rm S}CH_3$
Molecular weight ^a	74.12	106.12	116.16	102.13	72.11	117.15	131.17	108.14	94.19
(g mol ⁻¹)									
Acid dissociation constant	16.1ª	14.9ª	-7 ^b	-7 ^b	14.7ª	-2.4°	-3.4°	10.26ª	NA
(pKa)									
Hydrophobicity ^a	0.88	1.48	1.85	1.21	0.29	2.14	2.6	1.94	1.77
(logK _{ow} at 20 °C)									
Water solubility	63.2ª	6.95 ^a	2.7 ^b	19.2ª	223ª	3.56 ^a	0.498ª	21.5	3
(g L ⁻¹ at 25 °C)									
Henry's volatility constant ^d	1.2	0.38	0.029	0.041	8.1	19.1	4.7	10 ^c	0.0065ª
(mol m ⁻³ Pa ⁻¹ at 25°C)									
Boiling point ^a	111.7	179	121	99.2	79.59	254	265	201.9	110
(°C)									
Vapour pressure ^a	7	1.27	14	35.8	90.6	0.0122	0.0055	0.11	28.7
(mm Hg at 25 °C)									
Molar volume ^e	92.1	101.1	131.1	114.6	91.7	101.9	118.1	104.1	89.5
(cm ³)									
Hansen solubility δ	23.1	21.5	17.4	17.9	19	22.14	22.1	22.7	20.4
$(MPa m^{-1/2})$									
Polar surface area ^e	20	17	26	26	17	16	16	20	51
$(Å^2)$								~	-
Odour descriptor ^a	Alcohol like	Bitter almond	Pineapple	Fruity, rum	Acetone like	Faecal	Faecal, nauseating	Sweet, tar like	Rotten cabbage

Table S1. VOC chemical parameters

^a Pubchem (2017), ^b YMDB (2017), ^c Gu and Berry (1991), ^d Sander (2015), ^e ChemSpider (2017), ^f Hansen (2007). NA, not available.

VOC	Reverse Osmosis (Poly	yamide-urea)	Pervaporation (Polyvinyl alcohol)			
	Average (%)	±	Average (%)	±		
2-Butanone	110.20	4.96	98.04	4.29		
1-Butanol	105.62	4.61	102.87	5.54		
Ethyl propionate	105.06	6.07	98.67	4.99		
Dimethyl disulfide	110.98	5.65	98.20	13.81		
Ethyl butyrate	103.95	0.65	102.88	11.02		
Benzaldehyde	103.23	4.23	98.64	9.53		
p-Cresol	98.27	10.34	93.12	8.97		
Indole	92.76	12.30	95.05	7.55		
Skatole	96.67	12.48	92.80	7.99		

Table S2. Average volatile organic compound (VOC) mass balance recoveries from the hydrophilic membrane trials.

 \pm represents the standard deviation of a triplicated experiment.

Parameter	COD (Urine)	COD (CB)	TSS (CB)	TP (Urine)	TP (CB)	NH4 ⁺ -N (Urine)	NH4 ⁺ -N (CB)	C (Urine)	C (CB)	E-coli (CB)	Other coliforms	Total coliforms	pH (Urine)	pH (CB)
Unit	g L-1	g L-1	g L-1	mg L ⁻¹	mg L ⁻¹	mg L ⁻¹	mg L ⁻¹	mS cm ⁻¹	mS cm ⁻¹	CFU mL ⁻¹	CFU mL ⁻¹	CFU mL ⁻¹	pН	pН
RO (PA-UREA)	4.01 ± 0.16	13.63 ± 1.06	6.12 ± 2.33	$165.00 \\ \pm \\ 49.50$	$156.80 \\ \pm \\ 20.8$	195.50 ± 30.40	1788.50 ± 163.90	10.37 ± 2.50	13.80 ± 2.55	6.36 x 10 ⁶ ± 6.93 x 10 ⁶	ND	$6.36 \ge 10^{6} \\ \pm \\ 6.93 \ge 10^{6}$	6.94 ± 0.32	9.00 \pm 0.30
PV (PVA)	2.93 ± 1.82	$15.43 \\ \pm \\ 0.45$	$5.44 \\ \pm \\ 0.50$	90.67 \pm 123.40	237.35 ± 187	88.67 ± 83.76	290.03 ± 10.00	5.92 ± 3.89	7.77 ± 3.41	$1.81 \ge 10^7$ \pm $3.82 \ge 10^6$	2.18 x 10 ⁶ ± 2.10 x 10 ⁶	$2.01 \times 10^{7} \\ \pm \\ 2.1 \times 10^{6}$	$6.86 \\ \pm \\ 0.21$	9.08 ± 0.14
PV (PDMS)	$4.70 \\ \pm \\ 1.81$	19.50 ± 1.97	7.15 ± 1.22	$104.33 \\ \pm \\ 55.30$	380.00 ± 265.14	$142.67 \\ \pm \\ 25.70$	$343.33 \\ \pm 106.93$	$10.38 \\ \pm \\ 2.88$	13.52 ± 6.22	$7.62 \times 10^{6} \pm 1.22 \times 10^{7}$	2.25 x 10 ⁵ ± 3.66 x 10 ⁵	$7.84 \ge 10^{6} \\ \pm \\ 1.26 \ge 10^{7}$	$6.92 \\ \pm \\ 0.73$	$7.97 \\ \pm \\ 0.81$
MD (PP)	4.54 ± 1.82	16.37 ± 3.89	5.45 ± 2.44	230.00 ± 154.85	370.00 ± 160.93	149.67 ± 49.52	300.00 ± 100.00	10.36 ± 2.91	12.20 ± 3.38	1.51 x 10 ⁷ ± 9.96 x 10 ⁶	9.50 x 10 ⁵ ± 1.48 x 10 ⁶	$1.60 \ge 10^7$ \pm $8.74 \ge 10^6$	$6.72 \\ \pm \\ 0.45$	7.84 ± 0.47
All trials	4.05 ± 1.46	15.36 ± 2.97	5.99 ± 1.49	$140.38 \\ \pm \\ 153.01$	$203.39 \\ \pm \\ 142.57$	139.15 ± 54.54	998.24 ± 739.62	9.54 ± 3.21	13.07 ± 3.81	7.63 x 10 ⁶ ± 8.99 x 10 ⁶	$2.63 \times 10^{6} \\ \pm \\ 6.18 \times 10^{6}$	8.11 x 10 ⁶ ± 9.43 x 10 ⁶	6.79 ± 0.43	$\begin{array}{c} 8.64 \\ \pm \\ 0.61 \end{array}$

Table S3. Feed water characterisation for urine and concentrated blackwater (9:1, urine: faeces by mass) from this study.

COD (Chemical oxygen demand); TSS (Total suspended solids); TP (Total phosphorus); C (Conductivity); RO (Reverse Osmosis); PA-UREA (Polyamide-urea); PV (Pervaporation); PVA (Polyvinyl alcohol); PDMS (Polydimethylsiloxane); MD (Membrane distillation); PP (Polypropylene).

Table S4. Initial water flux	
Membrane process	Deionised water flux (J ₀ , L m ⁻² h ⁻¹)
RO (PA-UREA)	50.9
PV (PVA)	0.34
PV (PDMS)	0.06
MD (PP)	0.08

RO (Reverse Osmosis); PA-UREA (Polyamide-urea); PV (Pervaporation); PVA (Polyvinyl alcohol); PDMS (Polydimethylsiloxane); MD (Membrane distillation); PP (Polypropylene).



Figure S1. Feed odour development during storage, expressed as the ratio of the final feed concentration (C_f) to the initial feed (C_i) for pervaporation (polyvinyl alcohol) during concentrated blackwater trials and synthetic trials. Operated at 50 °C. Error bars represent standard deviation of a triplicated experiment. Mean filtration time 4.77 hours.



Figure S2. Transition of pH as a function of time for triplicated concentrated blackwater at 50 °C (CB 50 °C 1, CB 50 °C 2 and CB 50 °C 3). The equilibrium between NH_3 and NH_4^+ at 50 °C is overlaid.



Figure S3. A visual comparison of the treatment of concentrated blackwater using membrane processes. (a) reverse osmosis feed and permeate (b) pervaporation (polyvinyl alcohol) feed, permeate and retentate (c) pervaporation (polydimethylsiloxane) feed permeate and retentate (d) membrane distillation feed, permeate and retentate.

Volatile organic compound detection and quantification (Mercer et al., 2019)

Solid phase extraction (SPE) Oasis® HLB cartridges (1 g), sourced from Waters (Milford, USA), were attached to an Agilent VacElut20 manifold (Agilent Technologies, Stockport, UK). The cartridges were first conditioned by subsequently passing 10 mL of diethyl ether, methanol and deionised water, facilitated by a vacuum pump (N 022 AN.18, KNF Neuberger, Whitney, UK). Samples (20 mL) were then loaded onto the cartridges. The VOCs were eluted with 1 mL of methyl octanoate (IS) in diethyl ether (0.057 µg mL⁻¹) followed by 5 mL of pure diethyl ether. The residual sample water which collected at the bottom of the beaker was removed carefully using a glass Pasteur pipette (Fisher Scientific, Loughborough, UK). Diethyl ether extracts were concentrated to 0.5 mL under nitrogen gas and then analysed by GC-MS.

Compound identification and quantification were performed by a Shimazdu-TQ8040 GC-MS (Shimadzu, Milton Keynes, UK), equipped with a semi polar ZB-624 fused silica GC column 60 m \times 0.25 mm, 1.4 µm (Phenomenex, Macclesfield, UK). The initial oven temperature was held at 35 °C for 5 min then increased to 170 °C at a rate of 10 °C min⁻¹ to elute 1-propanol, 2-butanone, 1-butanol, ethyl propionate, dimethyl disulfide, and ethyl butyrate. This temperature was sustained for 2 min to provide separation between dimethyl trisulfide, benzaldehyde and limonene. Then the temperature was ramped at 30 °C min⁻¹ up to 240 °C for the detection of the internal standard (methyl octanoate) and p-cresol and further increased to 250 °C at 5 °C min⁻¹, which was maintained for 5 min, allowing for the separation of indole and skatole. The total runtime was 29.83 min. Helium was used as the carrier gas (236.1 kPa) at a linear column flow rate of 2.47 mL min⁻¹ to maintain a velocity of 40 cm s⁻¹. The mass spectrometer was operated in single quad mode with a detector voltage relative to the tuning result (0.2 kV), ionisation energy of -70 eV at an ion source temperature of 200 °C and interface temperature of 250 °C. A solvent cut time was applied until 8.95 min.

References

E. Mercer, C. J. Davey, P. Campo, D. Fowler, L. Williams, A. Kolios, A. Parker, S. Tyrrel, C. Walton, E. Cartmell, M. Pidou and E. J. McAdam, Quantification of liquid phase faecal odourants to evaluate membrane technology for wastewater reuse from decentralised sanitation facilities, *Environ. Sci. Water Res. Technol.*, , DOI:10.1039/C8EW00693H.