Modeling the Concentration of Volatile and Semi-Volatile Contaminants in Direct Contact Membrane Distillation (DCMD) Product Water:

Supplementary Information

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Supplementary information consisting of one table describing a list of compounds used to model overall mass transfer coefficients and equilibrium ratio values for treatment by the large-scale DCMD system. This table extends across two pages.

SI Table 1. List of compounds used to model overall mass transfer coefficients and equilibrium ratio values for treatment by the large-scale DCMD system. Henry's constants calculated using the method described in the manuscript.

Compound	Chemical Formula	Molecular Weight (g/mol)	Activity at Infinite Dilution[1]	Henry's constant at 25°C [PaL/mol] $Log_{10}(H)$
Ammonia	NH3	17.03	1.00E+00	4.26
Ethanol	C2H6O	46.07	4.09E+00	2.81
Acetone	C3H6O	58.08	1.01E+01	3.74
Butane	C4H10	58.12	4.60E+04	8.31
Propanol	C3H8O	60.10	1.73E+01	3.01
Methyl ethyl ketone	C4H8O	72.11	2.93E+01	3.79
Butanol	C4H10O	74.12	5.42E+01	2.93
Benzene	C6H6	78.11	2.47E+03	5.68
Pyridine	C5H5N	79.10	2.10E+01	3.02
Dichloromethane	CH2Cl2	84.93	3.57E+02	5.57
Diethyl ketone	C5H10O	86.13	9.36E+01	3.89
Methyl propyl ketone	C5H10O	86.13	8.30E+01	3.92
Methyl tert-butyl ether	C5H12O	88.15	1.47E+02	4.95
Pentanol	C5H12O	88.15	2.26E+02	3.10
Toluene	C7H8	92.14	8.92E+03	5.79
Epichlorohydrin	C3H5ClO	92.53	8.64E+01	3.58
Aniline	C6H7N	93.13	1.21E+02	2.13
Phenol	C6H6O	94.11	5.69E+01	1.61
1,1-Dichloroethylene	C2H2Cl2	96.94	2.30E+03	6.51
cis-1,2-Dichloroethylene	C2H2Cl2	96.94	8.40E+02	5.60
trans-1,2-Dichloroethylene	C2H2Cl2	96.94	1.19E+03	5.96
Cyclohexanone	C6H10O	98.15	7.99E+01	2.86
1,2-Dichloroethane	C2H4Cl2	98.96	6.36E+02	5.07
Methyl butyl ketone	C6H12O	100.16	3.50E+02	3.80
Hexanol	C6H14O	102.18	9.52E+02	3.51
Styrene	C8H8	104.15	1.85E+04	5.45
1,4 Xylene	C8H10	106.17	3.18E+04	5.83
Ethylbenzene	C8H10	106.17	3.33E+04	5.91
Xylenes (total)	C8H10	106.17	5.55E+04	5.95
2-Methylphenol	C7H8O	108.14	9.49E+01	0.49
3-Methylphenol	C7H8O	108.14	9.49E+01	1.68
4-Methylphenol	C7H8O	108.14	9.49E+01	1.38
Phenoxymethanol	C7H8O	108.14	3.10E+03	1.03
Phenylmethanol	C7H8O	108.14	5.48E+01	4.45
Chlorobenzene	C6H5Cl	112.56	1.15E+04	5.55

1,2-Dichloropropane	C3H6Cl2	112.99	2.20E+03	5.44
Octane	C8H18	114.23	1.47E+07	8.72
Heptanol	C7H16O	116.20	3.94E+03	3.47
Acetophenone	C6H8O	120.15	1.28E+03	3.08
1,2,4-Trimethylbenzene	C9H12	120.19	1.17E+05	6.06
Propylbenzene	C9H12	120.19	1.28E+05	5.58
2-Phenylethanol	C8H10O	122.17	2.77E+02	1.76
2,4-Dimethylphenol	C8H10O	122.17	8.56E+02	2.29
Octanol	C8H18O	130.23	1.57E+04	3.60
Trichloroethylene	C2HCl3	131.39	6.62E+03	5.99
1,1,1-Trichloroethane	C2H3Cl3	133.40	5.72E+03	6.22
1,1,2-Trichloroethane	C2H3Cl3	133.40	1.61E+03	4.97
1,3-Dimethoxybenzene	C8H10O2	138.17	6.31E+03	0.85
2-Phenoxyethanol	C8H10O2	138.17	2.59E+02	2.46
Di-tertbutyl ketone	C9H18O	142.24	2.39E+03	4.24
Decane	C10H22	142.29	3.99E+08	9.18
o-Dichlorobenzene	C6H4Cl2	147.00	5.88E+04	5.32
p-Dichlorobenzene	C6H4Cl2	147.00	1.06E+05	5.80
Carbon tetrachloride	CCl4	153.82	1.05E+04	6.45
Tetrachloroethylene	C2Cl4	165.83	4.35E+04	6.30
Dodecane	C12H26	170.34	2.50E+09	8.95
1,2,4-Trichlorobenzene	C6H3Cl3	181.45	7.42E+05	5.89
Ethylene dibromide	C2H4Br2	187.86	2.65E+03	4.93
Nonylphenol	C15H24O	220.36	1.75E+06	2.59
Hexachlorocyclopentadiene	C5Cl6	272.77	1.88E+07	6.45

(1) Yaws, C. L. *Yaws' Handbook of Properties for Aqueous Systems*; Knovel, 2012.