A steric pore-flow model to predict the transport of small and uncharged solutes through a reverse osmosis membrane

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SUPPLEMENTARY INFORMATION

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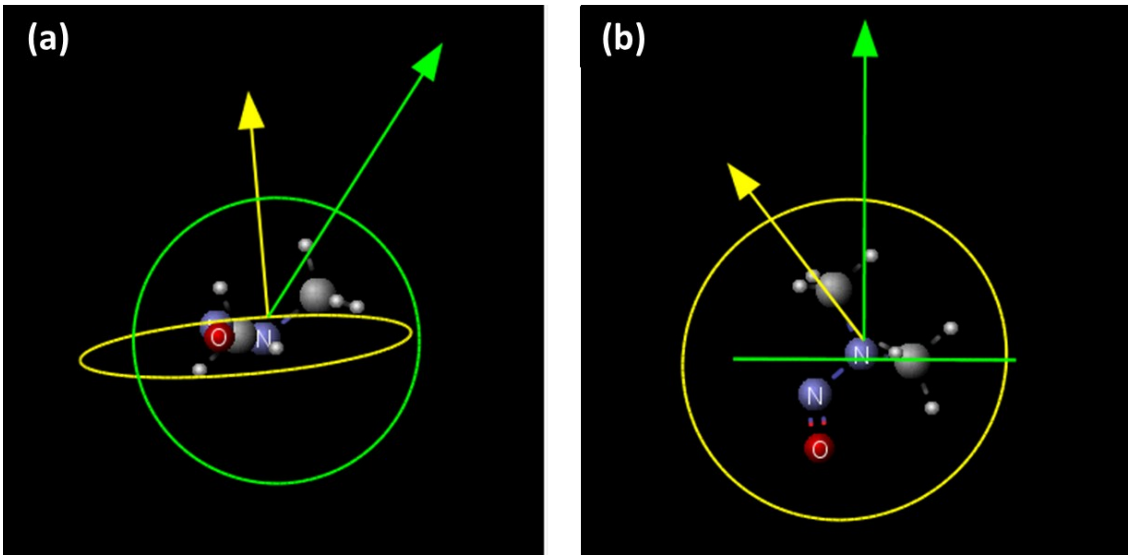

Fig. S1. (a) Minimally projected graphic of NDMA (green circle) and (b) the side view. These figures were illustrated with a software Marvin Sketch (ChemAxon, Budapest, Hungary). Molecular radius (r_c) is defined as a radius of the minimally projected graphic.

Table. S2. Experimentally obtained observed and real rejections.

Compound	Diffusion coefficient at 20 °C [nm²/s]	Mass transfer coefficient at 20 °C [m/s]	2.6 L/m²h		5 L/m²h		10 L/m²h		20 L/m²h	
			R_{obs} [%]	R_{real} [%]	R_{obs} [%]	R_{real} [%]	R_{obs} [%]	R_{real} [%]	R_{obs} [%]	R_{real} [%]
NDMA	8.88×10^{8}	1.16×10^{-4}	14	14	31	31	35	36	54	56
NMEA	7.84×10^{8}	1.07×10^{-4}	45	45	66	66	76	77	83	84
NPYR	6.96×10^{8}	9.96×10^{-5}	64	64	81	81	86	87	88	89
NDEA	7.17×10^{8}	1.02×10^{-4}	85	86	91	91	93	93	96	96
NPIP	6.18×10^{8}	9.25×10^{-5}	95	95	96	96	98	98	98	99
NMOR	6.53×10^{8}	9.75×10^{-5}	89	90	93	93	96	96	98	98
NDPA	6.43×10^{8}	9.48×10^{-5}	96	96	97	97	98	98	99	99
NDBA	6.19×10^{8}	9.25×10^{-5}	99	99	99	99	99	99	99	99
1,1,2-trichloroethane	6.86×10^{8}	1.06×10^{-4}	80	80	89	89	86	87	84	85
1,2-Dichloropropane	7.72×10^{8}	1.06×10^{-4}	91	91	94	94	92	92	89	90
Bromodichloromethane	8.27×10^{8}	1.11×10^{-4}	75	75	82	83	76	77	67	69
Bromoform	7.64×10^{8}	1.06×10^{-4}	84	84	93	93	92	92	91	91
Chloroform	8.63×10^{8}	1.14×10^{-4}	57	57	68	68	61	62	53	54
Dibromochloromethane	9.22×10^{8}	1.09×10^{-4}	80	80	89	89	86	87	82	83
Dichloroacetonitrile	8.27×10^{8}	1.10×10^{-4}	52	53	72	74	74	77	78	84

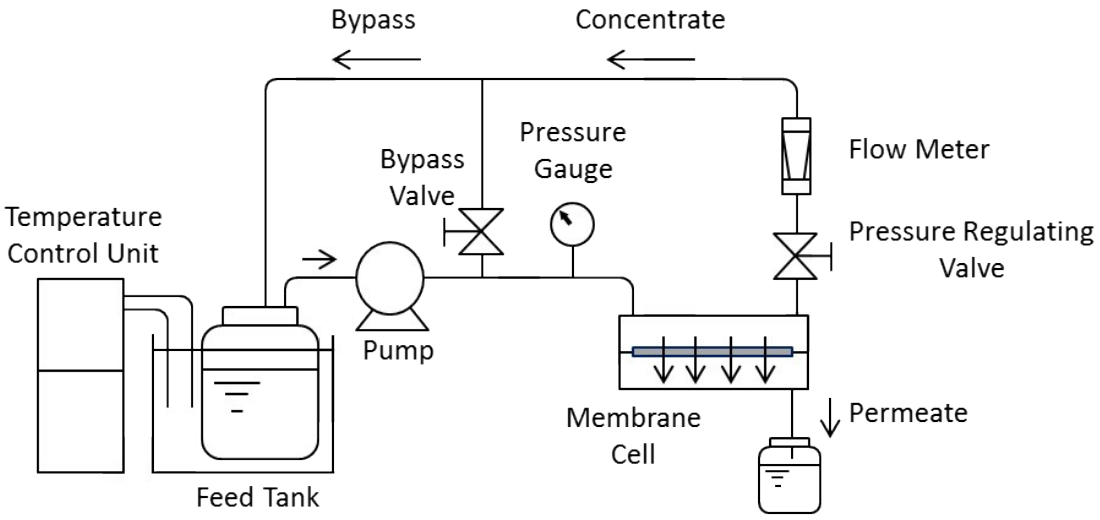

Fig. S3. Schematic diagram of the bench-scale cross-flow filtration system.

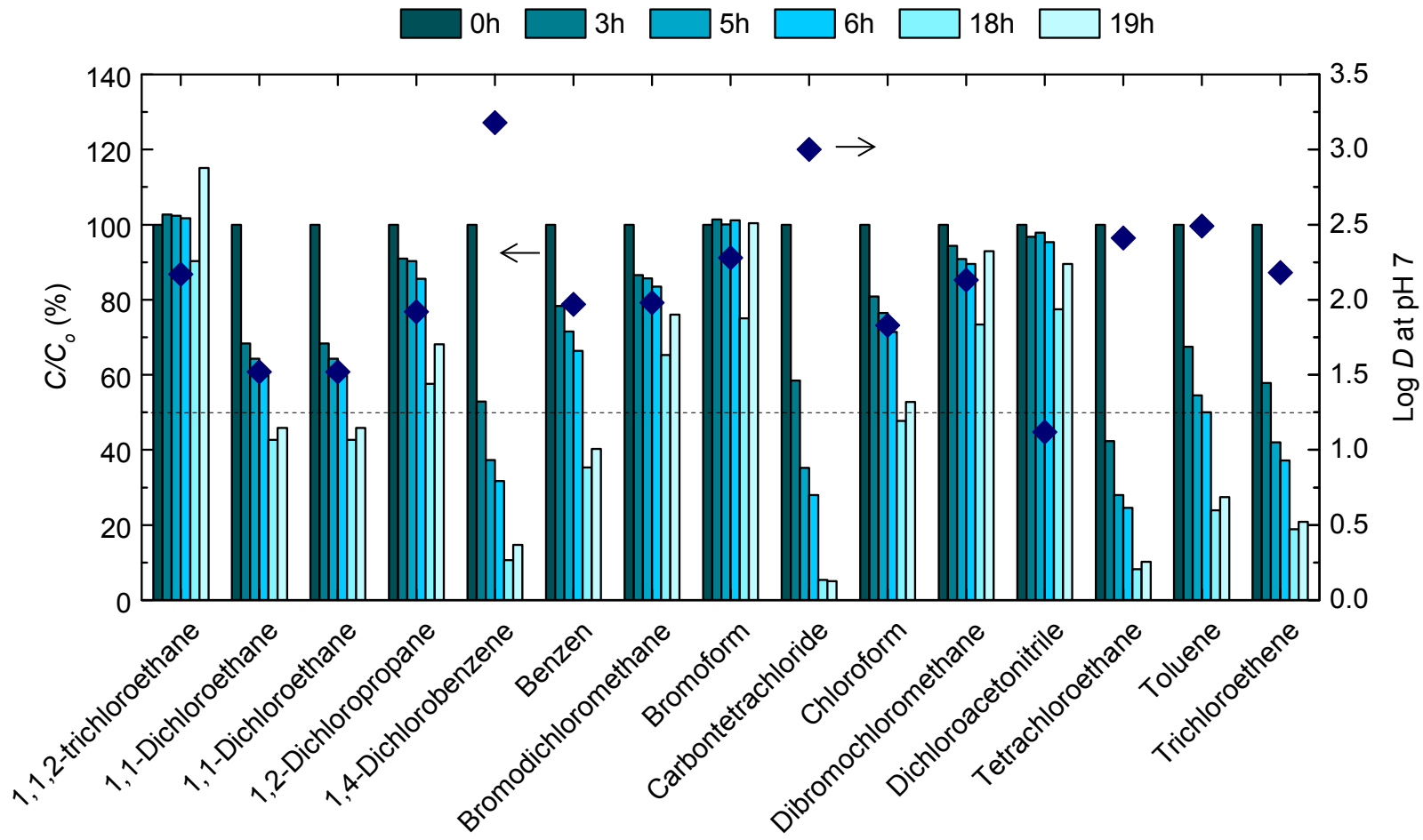

Fig. S4. Normalized VOC concentrations in the RO feed during 19 h of membrane system operation.

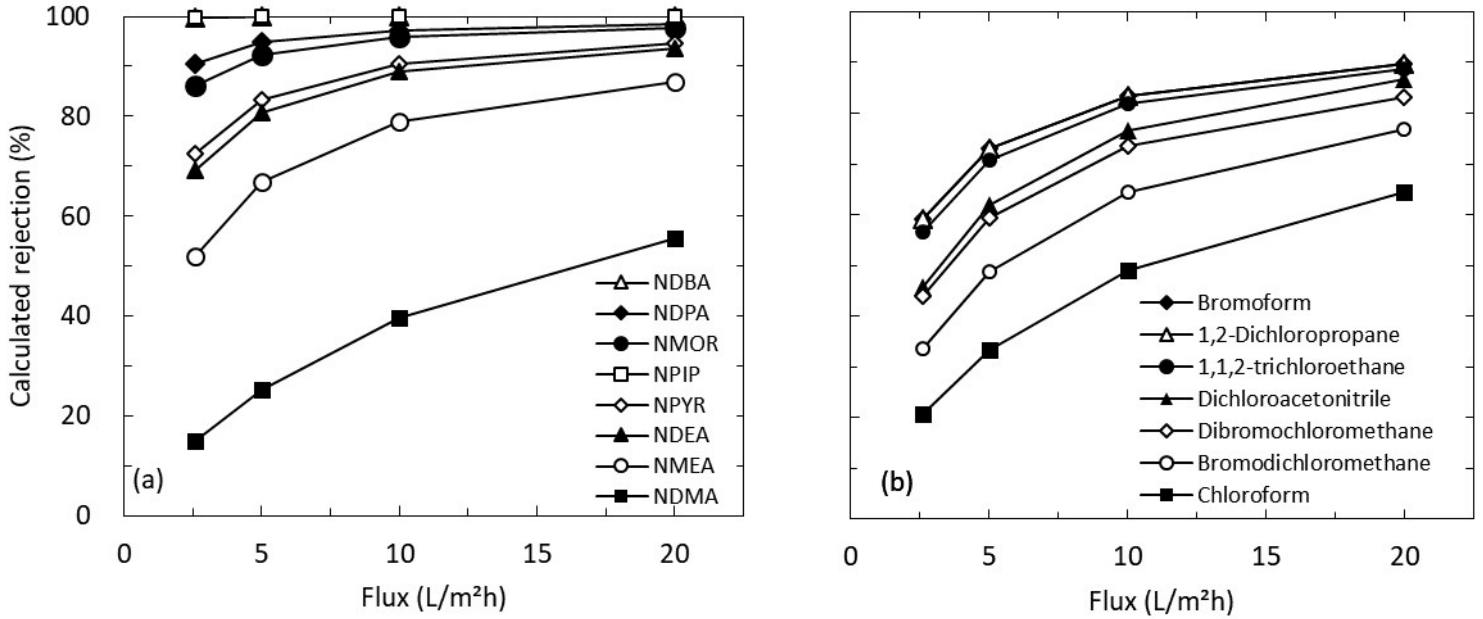

Fig. S5. Calculated rejection of (a) *N*-nitrosamines and (b) VOCs by the ESPA2 membrane as a function of permeate flux (feed solution temperature = 20 °C and permeate flux = 2.6–30 L/m^{2}h). The rejections were predicted by incorporating the estimated free-volume hole-radius (0.348 nm).

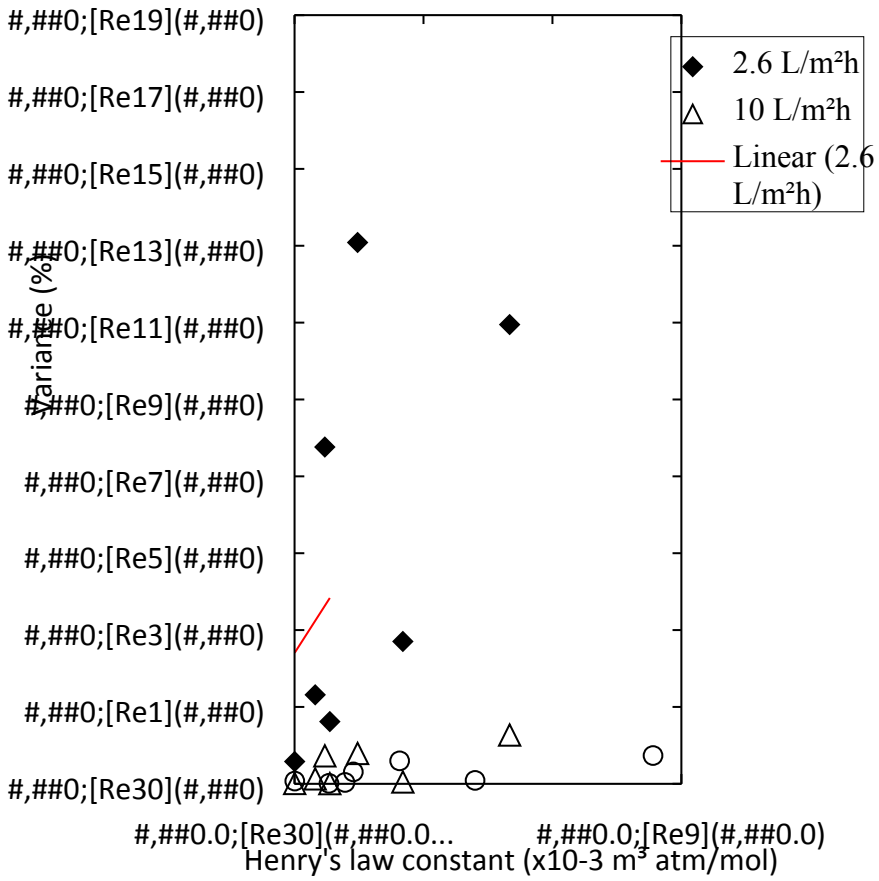

Fig. S6. Variance between calculated and experimentally obtained rejections of seven VOCs under the permeate flux of 2.6–20 L/m^{2}h as a function of their Henry's law constant. The solid line represents the linear regression line for data obtained under 2.6 L/m^{2}h.