Electronic Supplementary Information for

Concentration gradient driven molecular dynamics: A new method for simulations of membrane permeation and separation

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Table S1. The deviation of ICR concentration from the target value as a function of inlet force constant, k_i^I. Obtained over 40ns production run after 10ns initial run. The outlet force constant, k_i^O, was kept fixed at 500,000 kJ.nm^3/mol. Other parameters were as follows; w =0.25 nm, Z_F^I=4.875, Z_F^O= 23.625, and width of the control regions, $V^{CR}/(L_x \, x \, L_y)$=2.5.

	k_i^I (kJ.nm^3/mol)	1000	3000	5000	7000	8000
Deviation from ICR target concentration (molecule/nm^3)	Target ICR concentration = 0.2454 molecule/nm^3, corresponding to 10 bar.	0.0581	0.0296	0.0218	0.0163	0.0144
	Target ICR concentration = 0.1217 molecule/nm^3, corresponding to 5 bar.	0.0265	0.0163	0.0123	0.0116	0.0056
	Target ICR concentration = 0.0972 molecule/nm^3, corresponding to 4 bar.	0.0144	0.0005	0.0020	-0.0038	-0.0018

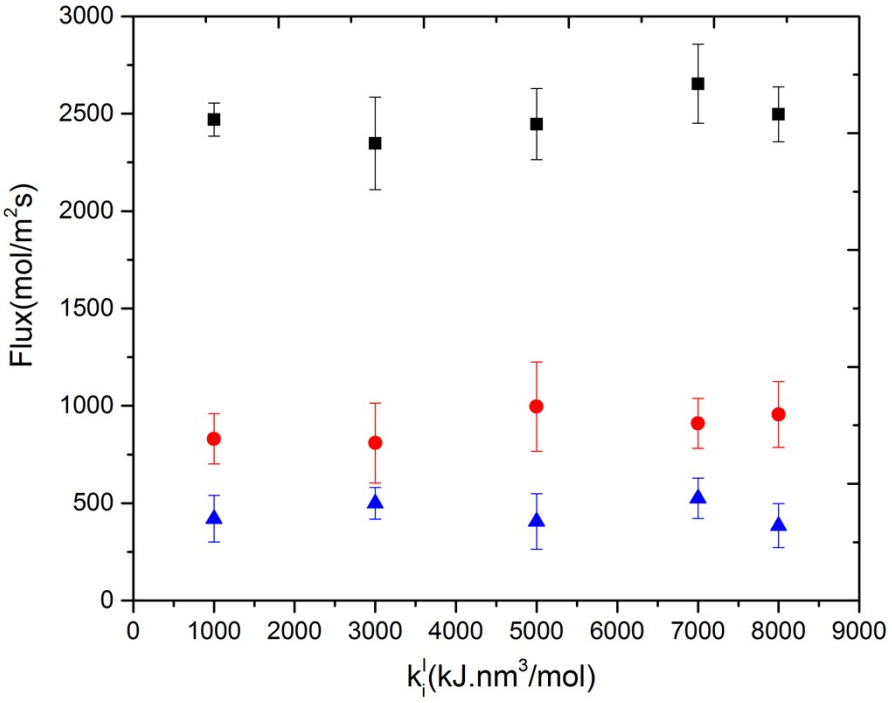
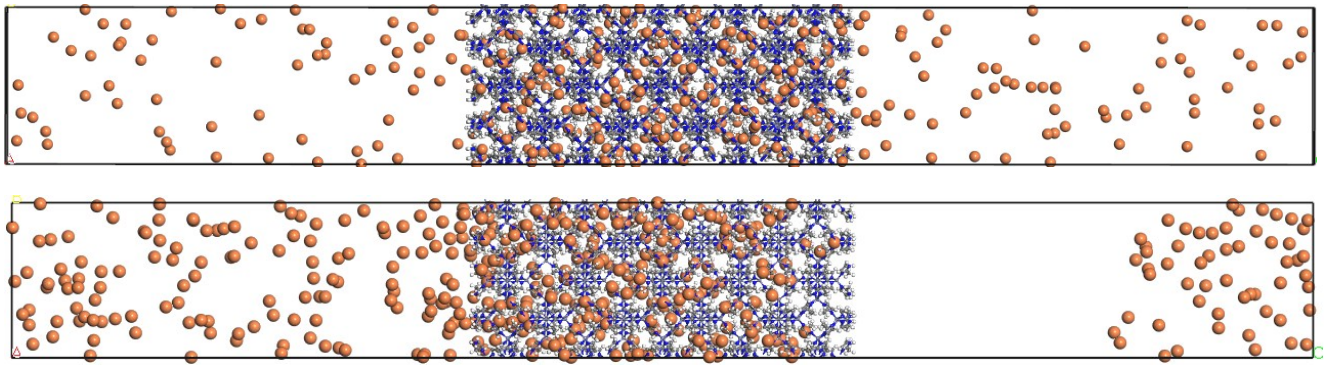


Figure S1. The variation of flux with respect to inlet force constant, k_i^I. The outlet force constant, k_i^O, was kept fixed at 500,000 kJ.nm^3/mol. The flux remains same within the margin of statistical error. Black squares 10 bar feed pressure, red circles 5 bar feed pressure and blue triangles 4bar feed pressure.

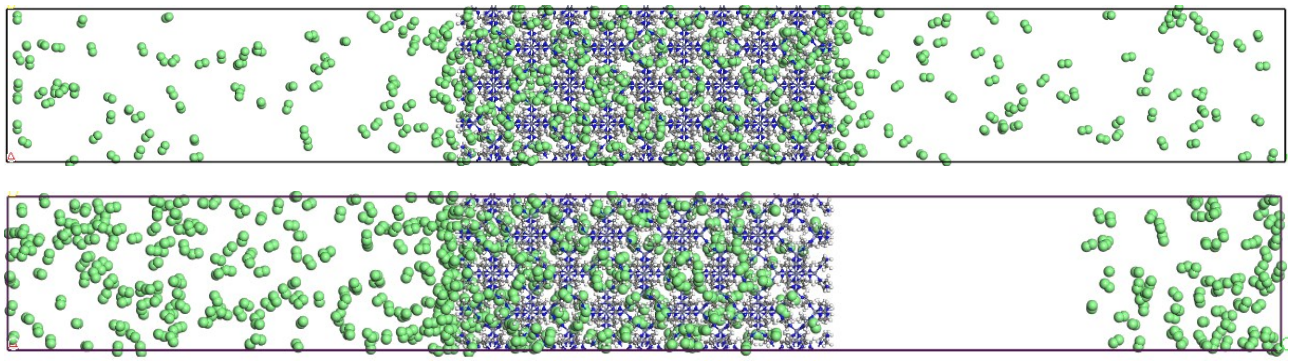
Table S2. Parameters used in Eq. 1 and 2 and the width of the control regions, $V^{CR}/(L_x \times L_y)$.

Relevant simulation results in the main text	Side	w (nm)	k_i (kJ nm^3/mol)	Z_F (nm)	$V^{CR}/(L_x \times L_y)$ (nm)
Figure 3 and Table 1	Inlet	0.25	$k_{methane}$ =8,000 $k_{ethylene}$ =8,000 k_{ethane} =3,000	4.875	2.5
	Outlet	0.25	500,000	23.625	2.5
Table 2	Inlet	0.25	$k_{methane}$ =8,000 $k_{ethylene}$ =25,000 k_{ethane} =25,000	4.875	2.5
	Outlet	0.25	500,000	23.625	2.5
Figure 6 and Table 3	Inlet	0.25	$k_{ethylene}$ =25,000 k_{ethane} =50,000	4.875	2.5
	Outlet	0.25	500,000	23.625	2.5

a)



b)



c)

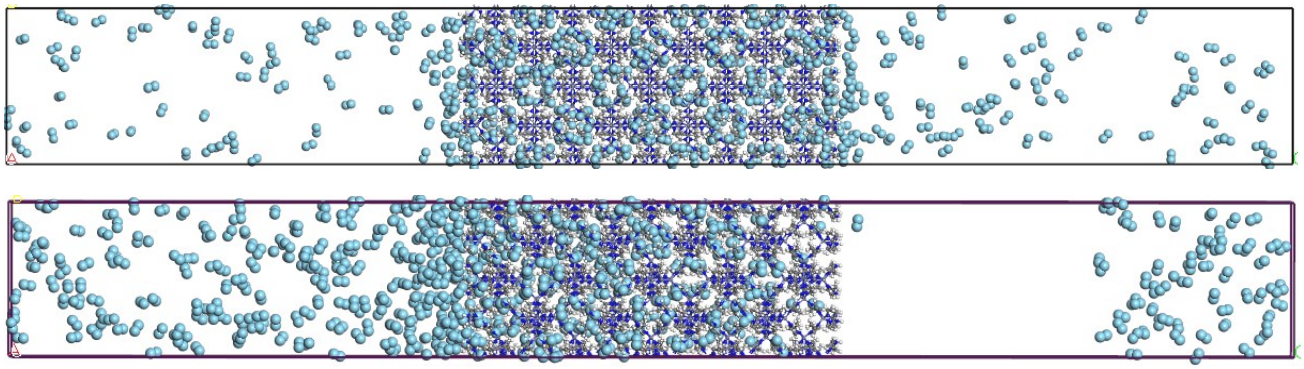
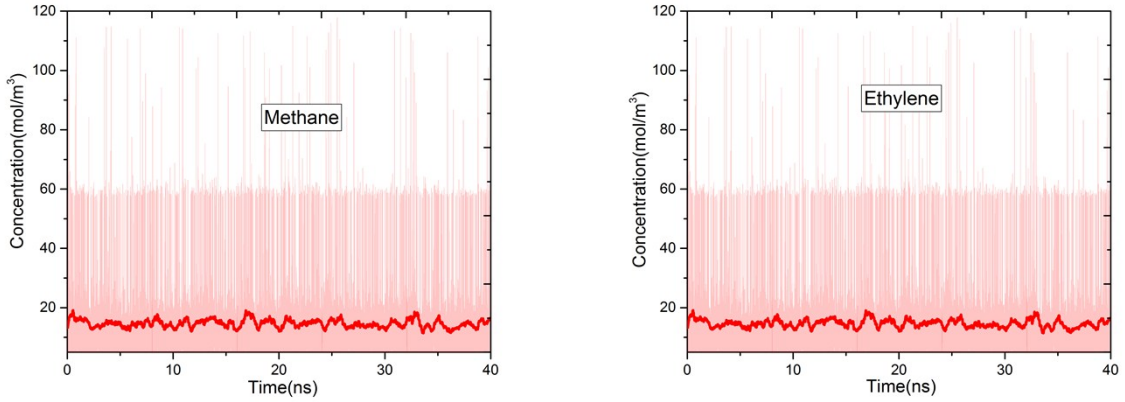


Figure S2. Starting (top) and after 10ns (bottom) configurations for pure (a) methane, (b) ethylene and (c) ethane.

a) b)



c)

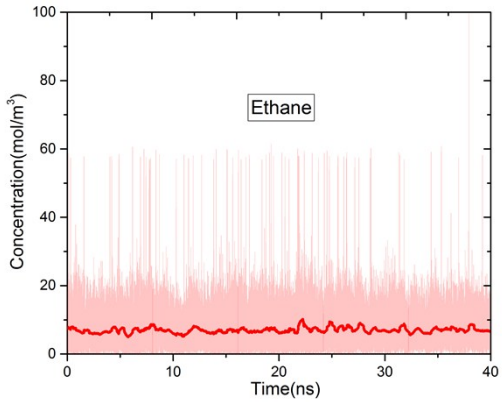


Figure S3. The variation of outlet concentrations for (a) methane, (b) ethylene and (c) ethane as a function of simulation time in production runs. The instantaneous values are represented with faded colour, while the full-colour curves are moving averages obtained with a characteristic smoothing time of 0.5 ns.

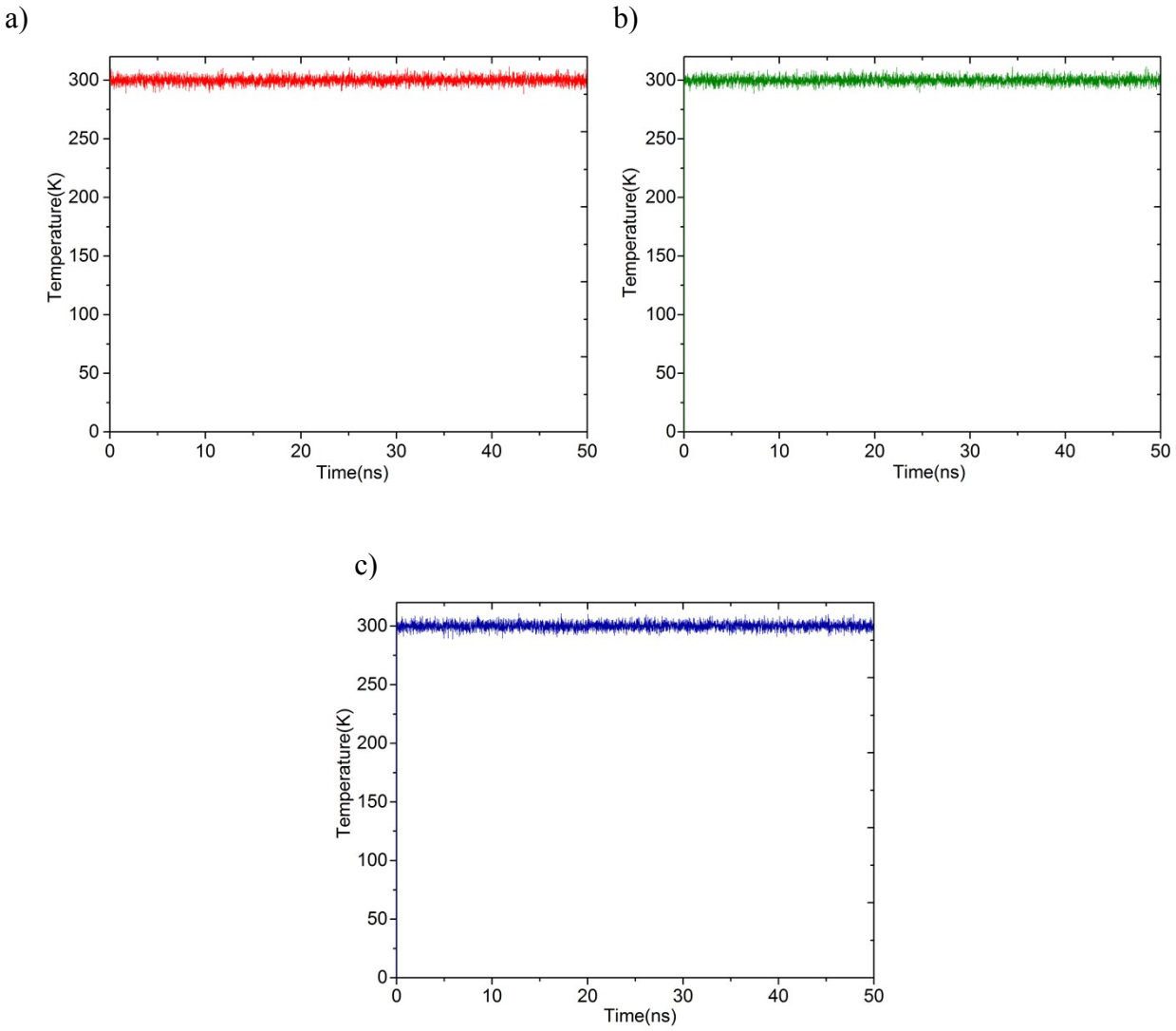


Figure S4. Temperature variation during pure a) methane, b) ethylene and c) ethane permeation simulations shown in Figure 3.

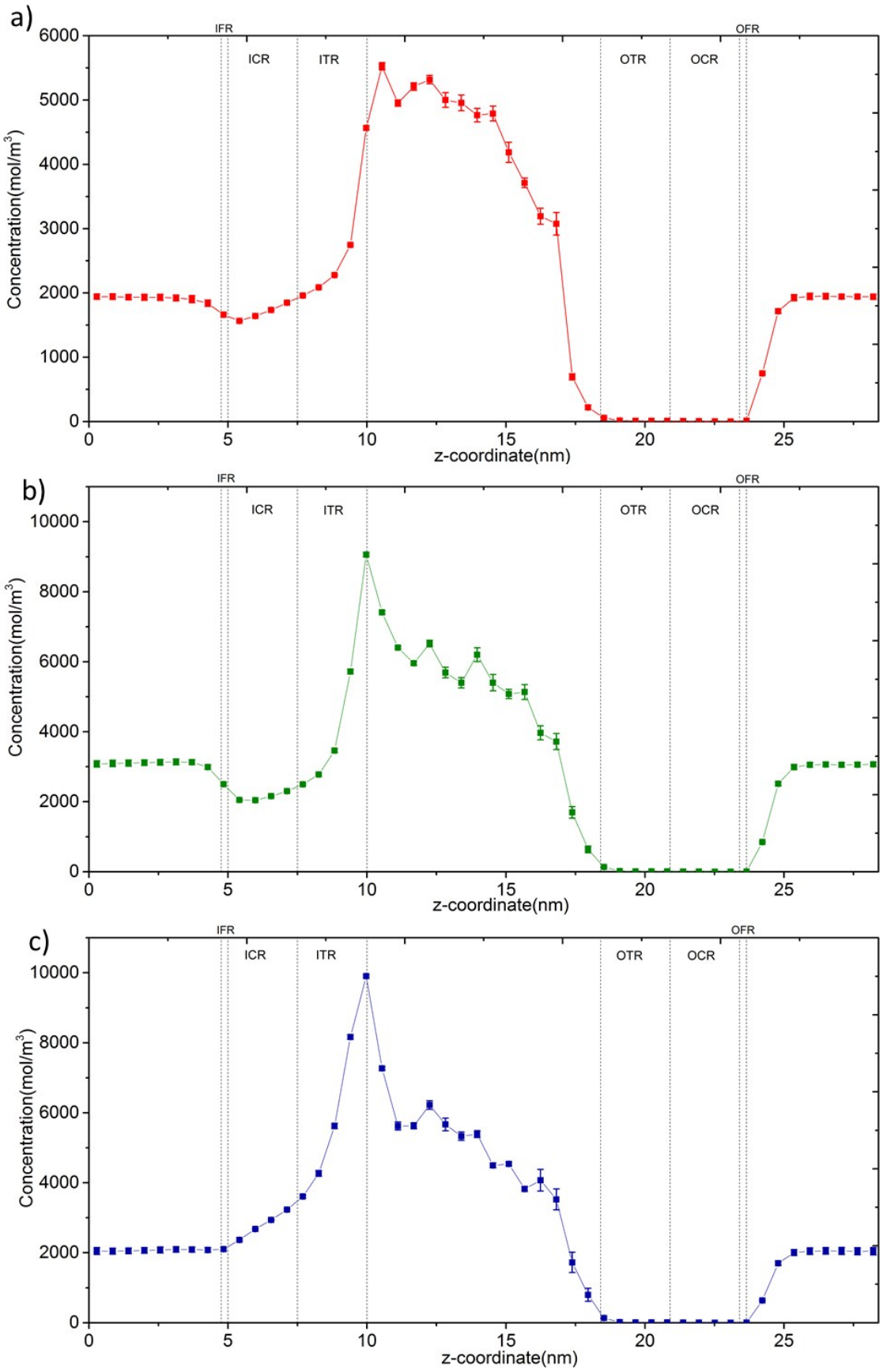


Figure S5. Concentration profiles of (a) methane, (b) ethylene and (c) ethane molecules along the z coordinate of the simulation box and the location of the FRs, CRs and TRs.

Table S3. Computed fluxes (mol/m^{2}s) used for the calculation of simulated permeabilities in Table 2.

Methane	Ethylene	Ethane
384 ± 112	625 ± 89	280 ± 109

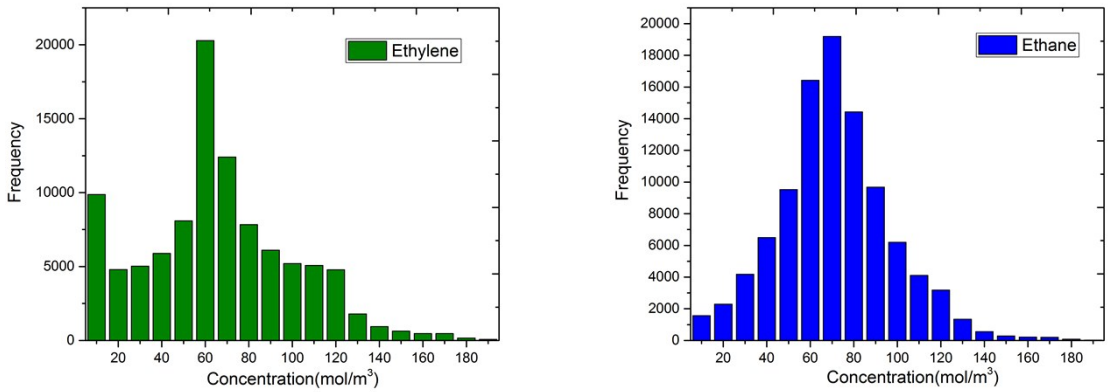


Figure S6. Concentration histograms of ethylene (left) and ethane (right) in ICR during the equimolar mixture simulation.

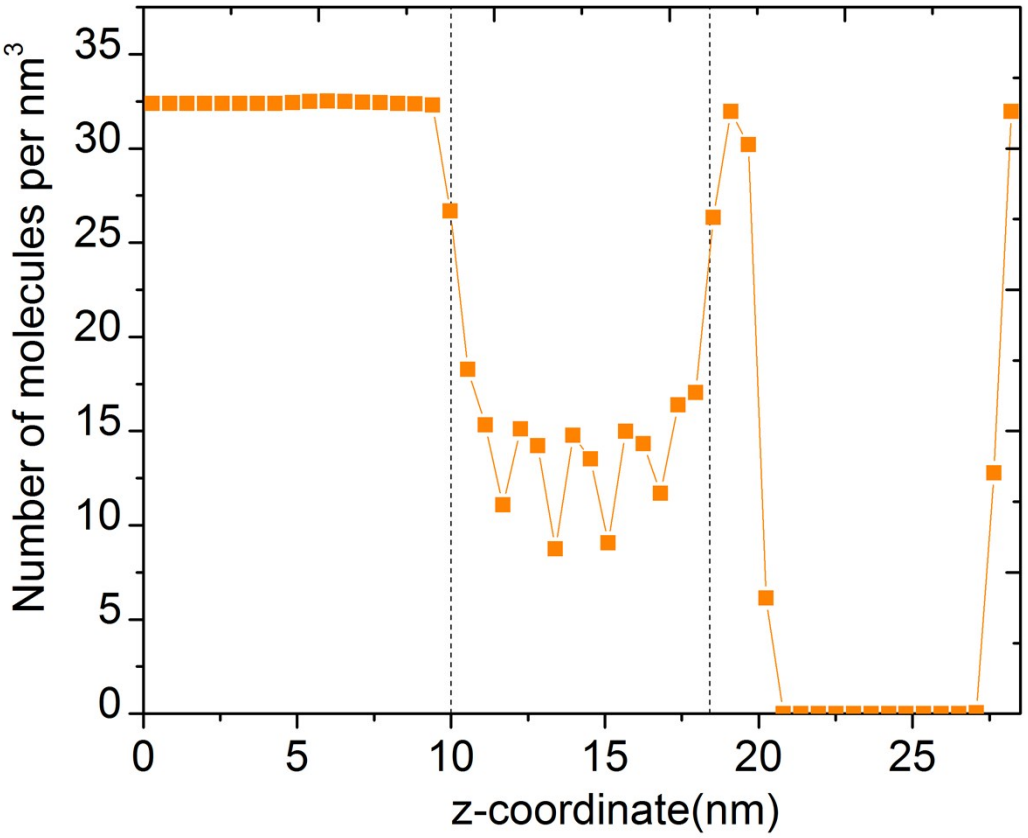


Figure S7. Number distribution of water[i] molecules along the z coordinate of the simulation box. Averaged over 20ns simulation time after 30ns of equilibration. Dashed lines show entrance and exit points of the membrane. The increase in the density of water towards the exit of the membrane is due to the presence of hydroxyl groups. Otherwise, ZIF-8 is known to be a hydrophobic material; hence the much less density within the membrane; i.e. between the two dashed lines.

Table S4. The average density of SPC water in ICR and OCR, and the water flux due to the presence of concentration gradient created across the ZIF-8 membrane.

ICR (kg/L)	OCR (kg/L)	Flux (mol/m^{2}s)
0.962* ± 0.011	0.0066 ± 0.0004	114

*Density of SPC water at 1bar and 300K is 0.971 kg/L (van der Spoel et al., J. Chem. Phys., Vol. 108, No. 24, 22 June 1998).

[i] For the water simulations SPC model was used (H. J. C. Berendsen, J. P. M. Postma, W. F. van Gunsteren,and J. Hermans, In Intermolecular Forces,B.Pullman, Ed.,Reidel, Dordrecht, 1981, p. 331).