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Supplementary Material: Atomistic and continuum scale modeling of functionalized graphyne membranes for water desalination

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The flow parallel to the membrane surface is closely coupled to the flux of permeate water across it. The system performance depends on the membrane geometric and mass-transfer properties. An eddy-promoting feed spacer is used in the current setting, for greater mixing, but it also means that the mass transfer kinetics deviate from traditional results for laminar flow in empty channels. These parameters also evolve as a function of distance down the RO vessel, and thus the functional dependence must be known to fully simulate the RO system. This supplementary material is thus divided into three main parts based on the requirement for the upscaling description, namely, membrane parameters, description of the RO vessel and the mass-transfer relations.

Membrane Parameters

Various membranes have been used to compare the performance of RO systems based on them in this study. Two key quantities required from the MD simulation for the upscaling analysis are water permeability A_m and the salt rejection rate R_0. The results for the various membranes are summarized in Table 1.

Membrane	**Water Permeability** $A_m(L\,m^{-2}hr^{-1}bar^{-1})$	**Salt Rejection Rate** R_0 **(%)**
α-graphyne	1059.18	100
γ-2-graphyne	613.29	100
γ-3-graphyne	1419.31	96.6
γ-4-graphyne	3570.01	83.3
H α-graphyne	323.47	100
H γ-2-graphyne	37.45	100
H γ-3-graphyne	503.12	100
H γ-4-graphyne	1914.21	86.6
TFC RO	5.81	86.6
Graphene	337.32	100

Table 1 Membrane parameters obtained from MD simulations used in the upscaling analysis

This information is used in Eq. (4) in the paper to obtain the permeate flux for various membranes, and dictates the permeate recovery from the RO vessel and in turn, the energy consumption.

RO Vessel Parameters

The geometrical parameters for the RO vessel have been used from Cohen-Tanugi *et al.*[1] These parameters are summarized in Table 2.

Reference Parameter	SWRO
RO Vessel Length L_c [m]	8
RO Vessel Radius r_c [m]	6.5
Effective Membrane Span W_c [m]	41
Wall-Membrane Gap H_c [mm]	7

Table 2 Geometrical parameters for seawater RO system used in this work

Mass Transfer Relations

The mass transfer coefficient k governs the extent of concentration polarization. For laminar flow, it depends on the solute diffusivity $\mathcal{D}$ as well as on the Reynolds number. However, the presence of feed spacers promote mixing by creating eddies in the feed channel and require further modifications. Given the gap between the wall and membrane H_c, the feed velocity u, the solution density ρ and viscosity μ, to estimate mass transfer coefficient for a given flow condition, data from Li *et al.*[2] on Sherwood ($Sh = kH_c/D$) and Reynolds numbers ($Re = uH_c\rho/\mu$) for RO channels in the presence of feed spacers is used. By fitting the data using power laws, the following equations are obtained

$$Sh = 2.53Pn^{0.262}$$

where the power number Pn is given by

$$Pn = 16Re^2 + 0.4892Re^{0.2964}$$

The coefficients used here correspond to the traditional case in which the mesh filaments are spaced $H_c/4$ apart from each other and a flow attack angle of 30°. In summary, the mass transfer coefficient can be written in terms of the fluid properties and geometric parameters as

$$k = 2.53\frac{D}{H_c}\left(16\frac{H_c^2u^2\rho^2}{\mu^2} + 0.4892\left(\frac{H_cu\rho}{\mu}\right)^{2.964}\right)^{0.2362}$$

References

[1] Cohen-Tanugi, D., McGovern, R. K., Dave, S. H., Lienhard, J. H., & Grossman, J. C. (2014). Quantifying the potential of ultra-permeable membranes for water desalination. *Energy & Environmental Science*, *7*(3), 1134-1141.

[2] F. Li, W. Meindersma, A. B. De Haan, and T. Reith, *Journal of Membrane Science*, 2002, 208, 289–302.