# Optimizing nanochannel spacing and pore morphology in graphene oxide multilayers for pressure-driven filtration: MD simulations

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The interplay between interlayer spacing (H) and pore width (A) strongly governs the desalination performance of graphene oxide (GO) membranes [1,2]. Here, atomistic molecular dynamics simulations (OPLS-AA force field, TIP3P water) are used to study pressure-driven water and ion transport through multilayer porous GO membranes [3]. To isolate geometric confinement from tortuosity, H and A are systematically decoupled by keeping a constant pore offset (Fig. 1). We find that spacings near H ≈ 11.0 Å improve mechanical stability at high pressure by promoting robust hydration layering, preventing the channel collapse observed in more confined geometries. Transport analysis (Fig. 2) reveals a high-flux plateau where changes in hydraulic permeability become statistically marginal across multiple designs. Within this regime, restricted pore entrances combined with moderately expanded interlayer spacing provide a favorable balance between water throughput and structural robustness. While no ion permeation events occur within the simulated time window, internal ion behavior depends strongly on pore architecture: wider pores favor intra-membrane ion accumulation, whereas restricted pores limit ion retention via steric exclusion at the feed interface. Overall, the results suggest shifting optimization from maximizing flux alone toward controlling intra-channel ion accumulation for improved long-term stability.

## References

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[3] A. Gogoi, K. A. Reddy, P. K. Mondal, Nanoscale, 12 (2020) 7273
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## Figures

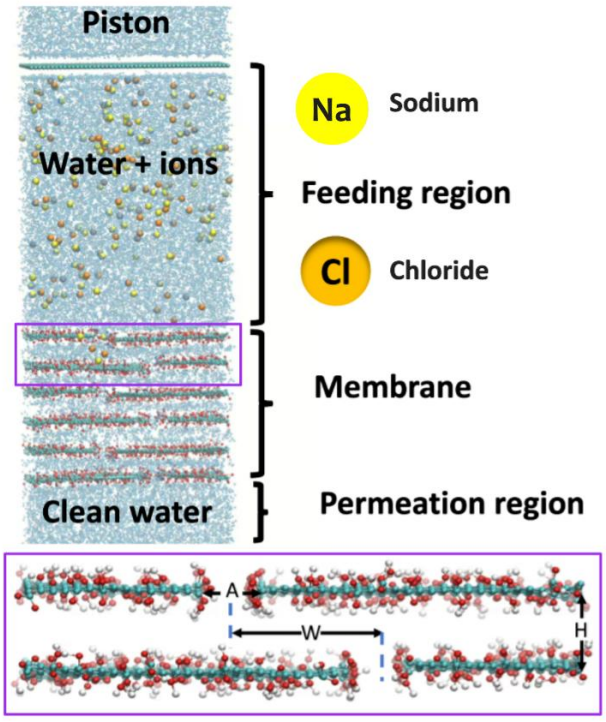


**Figure 1:** Simulation setup featuring a graphene piston applying 300 atm to the feed solution. The membrane separates the saline feed (top) from the pure permeate (bottom).

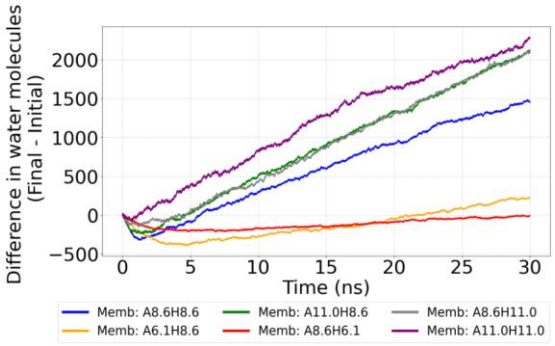


**Figure 2:** Cumulative water transport into the permeation region. The initial negative dip ($t < 5$ ns) corresponds to the system's compressive relaxation phase prior to establishing steady-state hydraulic flow