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Towards realistic multiscale molecular-continuum modelling of water flow through nanotube membranes KONSTANTINOS RITOS, MATTHEW BORG, Mechanical & Aerospace Engineering, University of Strathclyde, Glasgow G1 1XJ, UK, DUNCAN LOCKERBY, School of Engineering, University of Warwick, Coventry CV4 7AL, UK, SPELA IVEKOVIC, YONGHAO ZHANG, JASON REESE, Mechanical & Aerospace Engineering, University of Strathclyde, Glasgow G1 1XJ, UK — We present a new hybrid molecular-continuum method for modelling the nano flows inside micrometer-thick membranes. Our aim is to obtain results for practical filtration membranes that are as accurate as molecular dynamics (MD) and at the same time significantly more computationally efficient. Computational savings are obtained by replacing long nanotube sections - that are highly scale-separated - by much smaller but representative MD simulations, without any substantial loss of accuracy. These individual MD simulations are coupled together via standard continuum fluid-dynamics equations that dictate the overall macroscopic flow in the membrane. For this specific problem we use the conservative continuity and momentum equations as we consider the flow isothermal, incompressible and low-speed. Our iterative algorithm computes at each iteration the new constraints on the pressure differences applied to individual micro elements, and enforces overall continuity within the membrane. Validation tests are through direct comparison with full MD simulations of 50 and 150 nm thick membranes. We show results for micrometer-thick membranes and compare our predictions with previously-published experimental data.

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