Optimizing water permeability through the hourglass shape of aquaporins: From hydrodynamics to single file transport

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In fluid transport across nanopores, there is a fundamental dissipation that arises from the connection between the pore and the macroscopic reservoirs. This entrance effect can hinder the whole transport in certain situations, for highly slipping channels such as carbon nanotubes and/or for short pores such as Aquaporins. Aquaporin channels are able to conduct water across cell membranes, combining the seemingly antagonist functions of a very high selectivity with a remarkable permeability. Inspired by he shape of aquaporins, we explored the hydrodynamic permeability of hourglass shape nanopores using both finite element (FE) calculations and molecular dynamics (MD) simulations. An optimum of permeability is found for an opening angle around 5°, yielding a permeability five times larger than for a straight nanotube. Surprisingly, the agreement between MD results and continuum hydrodynamic predictions is really good, even for the smallest systems undergoing single file transport of water. Moreover, the optimal opening angles that maximize the permeability are found to compare well with the angles measured in a large variety of aquaporins. This suggests that the hourglass shape of aquaporins could be the result of a natural selection process toward optimal hydrodynamic transport. Finally, in a biomimetic perspective, these results provide guidelines to design artificial nanopores with optimal performances.