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Does the hourglass shape of aquaporins optimize water permeability?[1] SIMON GRAVELLE, LAURENT JOLY, FRANÇOIS DETCHEVERRY, CHRISTOPHE YBERT, CECILE COTTIN-BIZONNE, LYDERIC BOCQUET, Institut Lumiere Matiere, LIQUIDE ET INTERFACES TEAM — The ubiquitous aquaporin channels are able to conduct water across cell membranes, combining the seemingly antagonist functions of a very high selectivity with a remarkable permeability. While molecular details are obvious keys to perform these tasks, the overall efficiency of transport in such nanopores is also strongly limited by viscous dissipation arising at the connection between the nanoconstriction and the nearby bulk reservoirs. In this contribution, we focus on these so-called entrance effects and specifically examine whether the characteristic hourglass shape of aquaporins may arise from a geometrical optimum for such hydrodynamic dissipation. Using a combination of finite element calculations and analytical modeling, we show that conical entrances with suitable opening angle can indeed provide a large increase of the overall channel permeability. 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.

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