Membranes with a 3D architecture designed at nanoscale: what are the transfer opportunities?

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Membranes are often merely reduced to their 2D properties (surface area, surface porosity, pore size). However, when trying to biomimic the transport efficiency of biological channels (such as aquaporin), the importance of the interaction across the third dimension (i.e. along the pore) becomes obvious. In addition, the elaboration of membranes having a well-defined pore design becomes possible through self-assembly, nanofluidic or thin film composite techniques. In the future, a higher resolution of 3D-printers will also favor the production of membranes with a 3D design controlled at pore scale. It is therefore important to know how the transfer through the pore can be modified by the shape of the pores (like the hourglass shape) or by specific pore-solute interaction (the wall of the biological pore exhibits a mosaic of interactions) in order to optimize 3D pore architecture with respect to targeted separation.

The main objective of the presentation will be to investigate the new opportunities opened by membranes with an architecture designed at nanoscale. The discussion will be based on a theoretical analysis of the transport in pores driven by interfacial (i.e. pore-colloids) interactions. This analysis is based on new simulation tools for the transport of solute or colloids through channels combining the Navier-Stokes equation and a mass transport equation integrating colloid/colloid and colloid/wall interactions [1].

The main results show that the pore geometry plays an important role in transfer efficiencies: i) the mass transport efficiency leading to the transmission of colloid through the channels and ii) the mixture (colloids and liquid) transport efficiency determining the energy required to flow the liquid through the channel. To highlight this point, different aspects will be presented and discussed:

1) It will be shown, how the colloid (or solute)-wall interactions lead to an interfacially driven transport phenomena (diffusio-osmosis) inside the pore [2] which describes the dynamics of the osmosis and the reverse-osmosis mechanisms [3]. When considering the mechanism at the pore scale, the simulations put in evidence the existence of secondary flow which controls the mass accumulation and the counter pressure (Fig. 1a). It will be presented how the hourglass pore shape changes the flow configuration and minimizes the energy cost of separation [4].
2) It will be presented how the coupling between these flows and the mass accumulation can lead to different pattern in mass accumulation: homogeneous film accumulation, clog at the pore entrance or accumulation on the channel pillar (Fig. 2b). The consequences on the transmission of colloids trough the pore will also be presented. Filtration conditions leading to the transition between these different patterns will be discussed.
3) It will be shown that for specific filtration conditions, the interplay between the interfacial interaction and the viscous flow leads to instabilities that, in turn, leads to a rapid expulsion of accumulated layers through the pore. A pore hourglass shape changes the appearance of these instabilities. These instabilities will be discussed and compared to the ones experimentally observed in microfluidic channels [5].

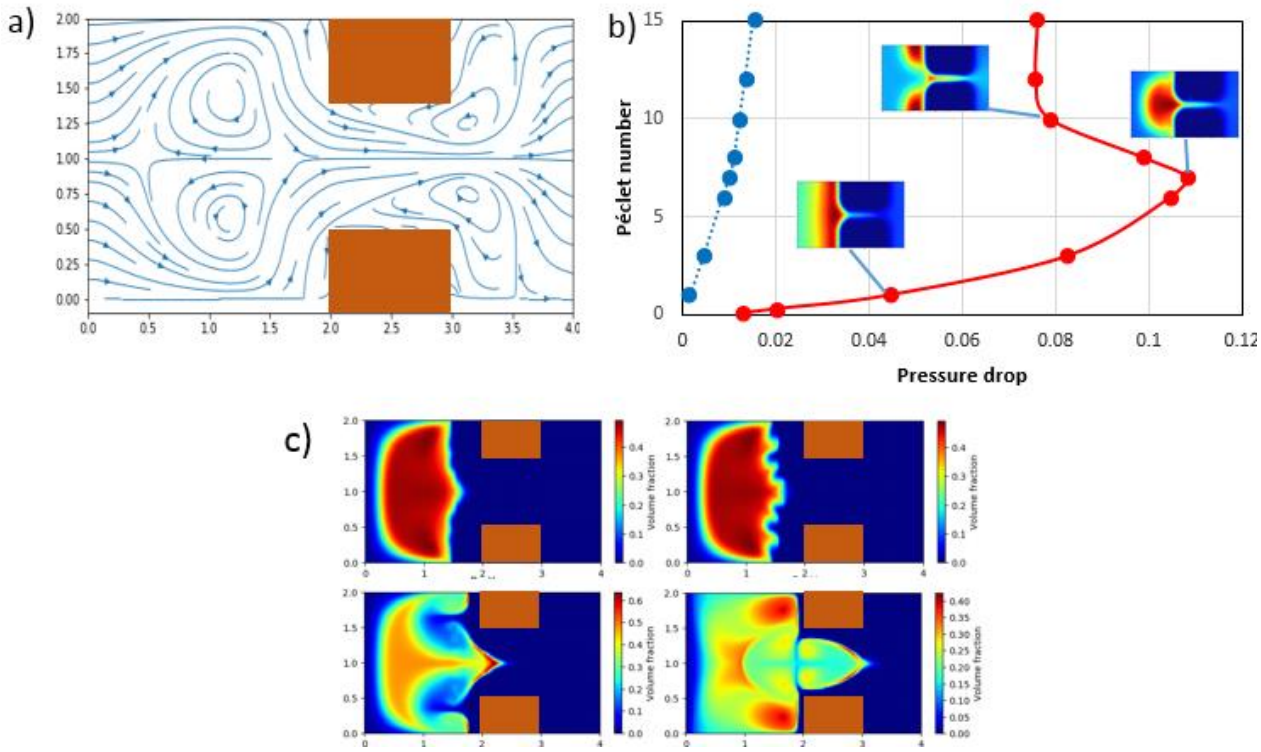


Fig. 1a) Secondary flows inside a pore due to the coupling between diffusio-osmosis and forced convection during reverse-osmosis 1b) Different accumulation patterns at pore entrance for different couple of applied pressure-permeate flux (from [2]) 1c) Temporal instabilities leading to the ejection of accumulated layers through the pore

All these studies change the traditional representation of the transport inside the membrane: the fluid velocity close to the membrane is not homogeneous but exhibit secondary flows (Fig. 1a), the accumulation does not always have the form of a homogeneous layer (Fig. 1b) and temporal instabilities can occur during the filtration process (Fig. 1c). Due to these fluctuations, the pore geometry but also the mosaic of interaction at the pore surface and along the pathway within the pore can be optimized. Simulations show that the stiffness of solute-wall interactions has an impact on the process efficiency: a gradual increase in interactions (as with hourglass pore shape) can reduce the separation energetic cost. Asymmetric interactions thus lead to direction-dependent transfer properties and the membrane exhibits diode behavior. All these new transfer opportunities will be discussed.

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