Active Sieving :
from flapping nano-doors to vibrating nanotubes

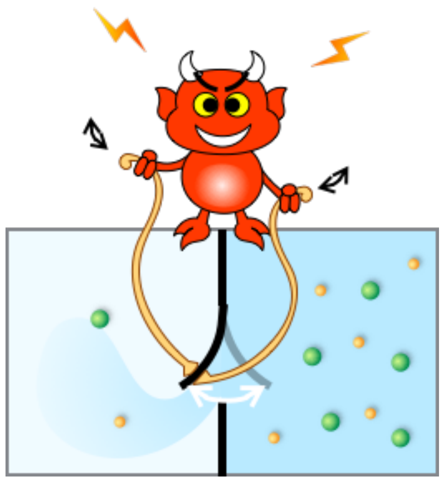
S. Marbach[a], A. Niguès[a], A. Siria[a], D. Dean[b], L. Bocquet[ac]
[a]laboratoire de physique statistique, Ecole Normale Supérieure, 75005 Paris, France
[b]laboratoire onde et matière d'aquitaine, Université de Bordeaux, 33400 Talence, France
[c]Institut Pierre-Gilles de Gennes, 75005 Paris, France

Key words: out of equilibrium sieving, filtration, Maxwell demon

1. Abstract

Filtering specific molecules is a challenge faced for several vital needs: from biomedical applications like dialysis to the intensive production of clean water. The domain has been boosted over the last decades by the possibilities offered by nanoscale materials [1]. Filtration is however always designed according to a passive sieving perspective: a membrane with small and properly decorated pores allows for the selection of the targeted molecules. This inevitably impedes the flux and transport, making separation processes costly in terms of energy.

Here we investigate alternative approaches to separation and filtration. We explore the possibility of non-equilibrium sieving, harnessing the difference in the molecular dynamics of particles to separate them across nanopores. We investigate a simplified model for an "active pore" where gating is dynamically controlled, and mimic to some extent a minimal Maxwell demon process. This model points to a rich variety of behaviors in terms of dynamical selectivity, and unravels the basic principles of active sieving [2]. We give preliminary results of a nanoscale experiment counterpart. We also solve completely a model for an "active channel" where the channel boundaries are dynamically controlled, and find yet broader perspectives on dynamical sieving. These results are corroborated by molecular dynamics simulations of water confined between flexible graphene sheets. All these principles could be readily mimicked using existing technologies to build alternatives for advanced water recycling.



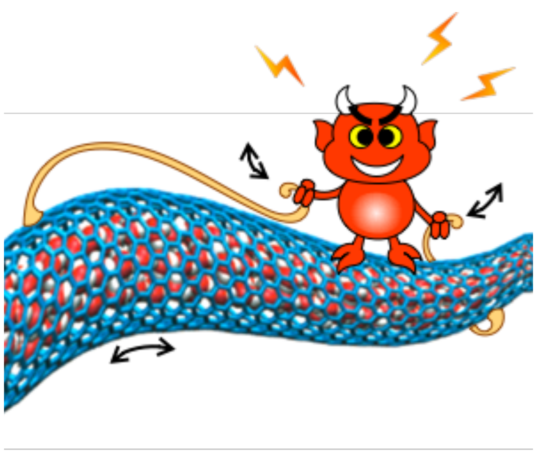


Figure 1: (left) Active sieving can be thought of in terms of a door that is mechanically opened and closed by some "crazy" Maxwell Demon and impacts the transport of particles through the door according to their dynamical properties. (right) Active sieving can also be thought of in the longitudinal direction, for instance in actively vibrating nanotubes (the vibrations being excited vibrations of the nanotube itself).

References

[1] "Materials for next-generation desalination and water purification membranes" Werber, J, Osuji, C. and Elimelech M., *Nature Rev. Mater.* (2016)

[2] "Active sieving across forced nanopores for tunable selectivity ", Marbach, S and Bocquet, L., *J. Chem. Phys.* (2017).