Modélisation et Simulation Multi Echelle **MSME UMR 8208**

Post-doctoral position: Development of a multiscale modeling coupling continuum and molecular approaches in order to simulate the heat and mass transfers of gas in nano-/microtubes

1 year full-time position starting approximately Mai 2016

Funding: CNRS, Net salary: about 2100€/month (gross salary: 2600€/month)

Location: Université Paris-Est Marne-la-Vallée, Laboratoire MSME (http://msme.u-pem.fr/)

Key words: Molecular Dynamics, nano-/microfluidics, heat and mass transfer

Supervisors: Dr. Benoît TROUETTE, Dr. Quy Dong TO, Pr. Céline LEONARD

A 12-month post-doctoral fellowship in the area of computational heat and mass transfer science is available in our laboratory at Marne-la-Vallée.

The Micro-Electro-Mechanical Systems (MEMS) used in industry, allow miniaturizing processes and improving time responses. In the case of fluidic systems, this reduction is also a way to increase the exchange surfaces in order to improve the heat transfer or to facilitate the migration of species through selective membranes. Reducing the characteristic dimensions compared to molecular mean free path gives rise to many new physical phenomena related to the fluid/solid interface, i.e. velocity slip, temperature jump and thermal creep which are typically negligible at large-scale. Using continuum mechanics, those effects can be modeled by rewriting classical boundary conditions at the interface. However, such an approach depends on many unknown parameters, e.g. slip length or thermal resistance and cannot capture all the complexity of the fluid/wall interactions determined at the atomic scale.

To enhance the description of fluid flows in extended nano-/microtubes, a hybrid numerical model, coupling Molecular Dynamics and Finite Volumes, has been developed in the MSME laboratory taking into account the multiscale characteristics of transport phenomena for incompressible flows. An atomistic approach is used in molecular blocks located along the fluid/solid interface in order to accurately describe the complex interactions at small-scales while a description based on the continuum mechanics is adopted in the bulk to model, at the large-scales, the transfer phenomena in the flow direction. The aim of the project is to extend this hybrid numerical model to compressible flows to simulate and optimize micro heat exchangers accounting for the fluid phase changing. The expected results could help to develop a unified methodology describing this kind of flows.

This work is a part of the interdisciplinary research project (MIG) of MSME involving the Heat and Mass Transfer and the Theoretical Chemistry groups.

Qualifications:
Candidate must have a PhD in Physical-Chemistry or Physics of Fluids. Applicant should be highly motivated and have a strong experience in programming (C and/or Fortran) and in Molecular Dynamics simulations. Basic knowledge in fluid dynamics, and heat and mass transfer are mandatory. Good communication skills are required for the collaborative work, in particular written and spoken English.

To apply:
Applicants must send including publication list, prior research experience and contact information of two references to benoit.trouette@u-pem.fr, and/or quy-dong.to@u-pem.fr and/or celine.leonard@u-pem.fr before 03.31.2016 (March 31, 2016).