

MODELLING ENHANCED HEAT TRANSFER AND SURFACE REACTIONS ON THE MICRO-SCALE

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Heat transfer on micro/hano-scale has become one of the major issues within many application fields, like micro-channel cooling for microelectronics and surface catalysis in micro reactors. In such miniaturized systems, the surface-volume ratio is large. This property can be used for example to increase the heat transfer considerably. The small-scale wall interactions affect the material properties up to the micro- and mini-scale level. Therefore, understanding the gas-wall or fluid-wall interactions thoroughly is indispensable for the temperature control and has to be studied on a molecular-scale. We developed a multi-scale hybrid method that combines the advantages of molecular dynamics (MD) and the stochastic direct simulation Monte Carlo method (DSMC): the accuracy of the interactions at the interfaces by MD, and DSMC in the bulk for low computational costs. The hybrid MD-DSMC method [1] is coupling the MD and MC simulation domains using a buffer layer at the interface of these domains (see Figure 1). For instance, for the heat transfer between a cold and a warm wall, high peaks and density oscillations appear near the wall boundary, and they are more pronounced near the cold wall. This wetting effect is studied with the hybrid method where the MD domain covers the entire oscillation region for accurate simulation of the interaction with the wall and MC in the bulk (see Figure 1). The results show that hybrid simulations give very accurate results compared to pure MD simulations, while MC simulations give higher deviations. The hybrid method is also five times faster than pure MD simulations and therefore also the simulation domains can be increased making the step towards real applications possible.

In a two-phase flow, the phase transition between liquid phase and gas phase is important, since evaporation can dissipate a large amount of heat. It is important that in the MD simulations and in the hybrid MD-DSMC simulations, this phase transition is modeled thermodynamically correct. We simulated an equilibrium situation and compared the temperature profile, density profile, pressure profile and enthalpy with literature values (Fig. 2). The thermodynamic properties agreed with experimental results from literature. Now we are describing the liquid-vapour phase transition at a heated solid wall.

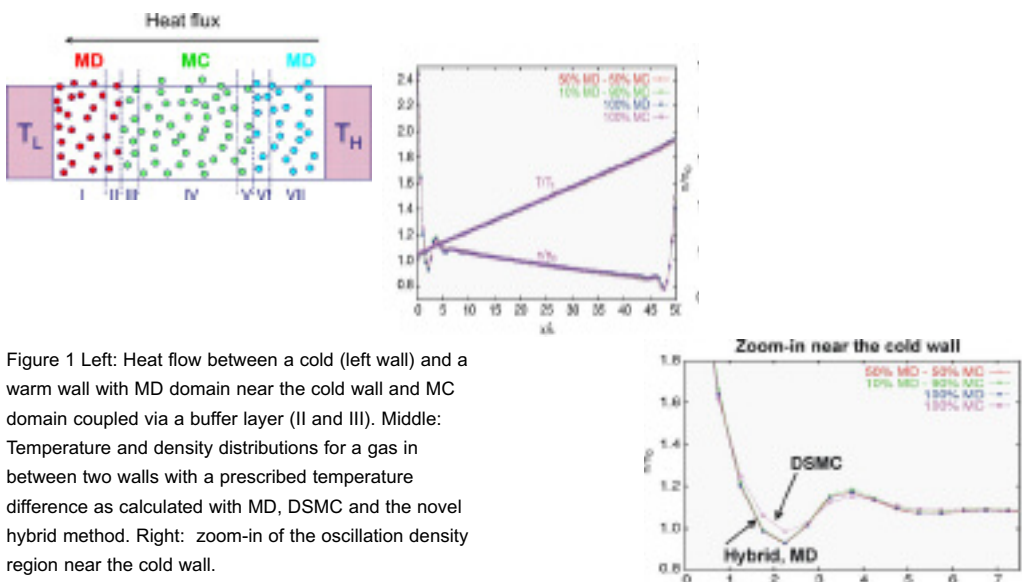


Figure 1 Left: Heat flow between a cold (left wall) and a warm wall with MD domain near the cold wall and MC domain coupled via a buffer layer (II and III). Middle: Temperature and density distributions for a gas in between two walls with a prescribed temperature difference as calculated with MD, DSMC and the novel hybrid method. Right: zoom-in of the oscillation density region near the cold wall.

A similar approach can also be used to study surface reactions where accurate boundary effects are computed from the molecular properties. From these boundary conditions for a continuum model can be derived. For instance, macroscopic values of diffusion, thermal and catalytic coefficients can be computed using hybrid MD - DSMC techniques and can be then integrated in the three dimensional Navier-Stokes equation solver. A direct coupling of the hybrid MD-DSMC method with the continuum model and also new kinetic models and scattering kernels describing the gas-wall interactions are investigated.

REFERENCES

1. S.V. Nedeia, A.J. Markvoort, A.J.H. Frijns, A.A. van Steenhoven, P.A.J. Hilbers, Hybrid method coupling molecular dynamics and Monte Carlo simulations to study the properties of gases in micro and nanochannels. Phys. Rev. E, 72, 016705, 2005

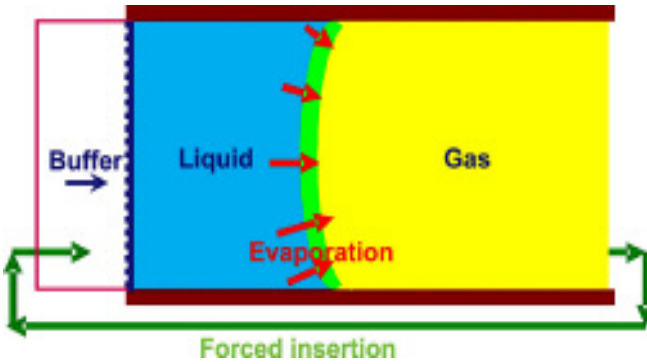


Figure 2 Above: Schematic view of the MD simulation box with boundary conditions. Right: Enthalpy jump over the liquid-vapor interface ($x=5 - 8\text{nm}$) for Argon molecules.

