Msc project: Hybrid simulations for heat transfer in chemically reacting flows

The prediction and control of heat transfer on micro/nano-scale in chemically reacting flows has become one major issue within many application fields. Thermodynamic and chemical non-equilibrium near phase boundaries have a strong impact on the macroscopic heat fluxes in the systems. Continuum models coupled with different catalytic and thermal boundary conditions give large deviations of heat flux predictions registered in realistic systems. The majority of the present kinetic models overlook the role of the surface and phase-boundary by introducing empirical coefficients for the boundary conditions. To relate these macroscopic coefficients to material properties and to include the surface effects on the hat flux predictions, multi-scale simulation techniques are required in order to bridge the gap from molecular material properties to the macroscopic ones.

A breakthrough will be possible by using the combination of continuum, Monte Carlo and Molecular Dynamics methods. A hybrid Monte Carlo-Molecular Dynamics method to treat the boundary regions already exists and it was implemented in [1]. The purpose of this project is to couple continuum approach with either Monte Carlo or Molecular Dynamics in the region of their validity in order to predict the thermal behavior of the system and to determine the impact of system characteristic parameters (size, density, temperature, geometry, flow profiles) and phase boundaries on the heat transfer when coupling the surface catalytic reactions and chemically reactive flows.

Approach

A hybrid MC-MD simulation method able to combine the advantages of the two methods by simulating particles near the wall using MD for accurate interactions near the boundaries and particles in the bulk using MC was already developed and validated[1]. This method was used to study systems in stationary and flow regime by keeping the atomistic description of matter near wall and inter-phase boundaries while simulating the bulk by less costly stochastic methods.

This hybrid method will be extended to study the coupling between surface properties (e.g. catalytic reactions) on small scale and flows on a larger scale.
Using the continuum Navier Stokes models, a coupling interphase will be built from continuum to the hybrid MC-MD based on investigation of molecular fluxes in the domain boundaries. This coupling can be done directly by explicitly including the walls in the simulations, but also by using more accurate boundary conditions computed from the molecular properties. For instance, macroscopic values of diffusion, thermal and catalytic coefficients can be computed using hybrid Molecular Dynamics - Monte Carlo techniques and can be then integrated in the three dimensional Navier Stokes equation solver. In Fig.1 is the example of a molecular reactive system, consisting of three particle types (blue-Pt surface, red-1st type(CO) gas and white-2nd type(O) gas). The mixture of two gases is impinging on a surface and the simulation domain can include the surface reactions explicitly (Fig1.a), where all the molecular transport properties and surface reactions are accurately simulated (Fig.2b), or these effects can be incorporated via boundary conditions on the given simulation domain (Fig1.c).
Philips Applied Technologies will provide experimental, data and numerical tests for the validation of the model regarding the application: on micro-channel cooling and/or fuel cells.

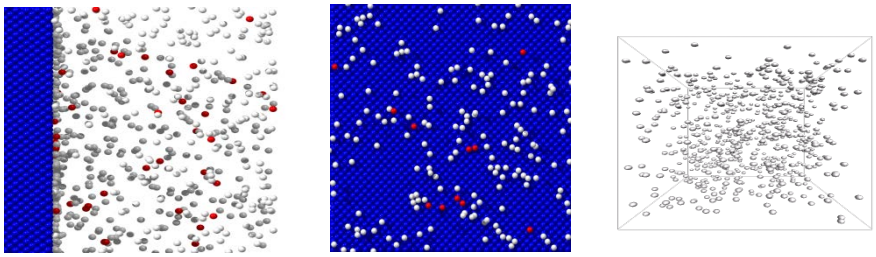

Fig.1. The *gas-surface interface of a mixture of two gases impinging on a surface can be modelled explicitly a) by incorporating all the surface reactions b) or by using boundary condition c).*

This project is going to be realized under the supervision coming from two departments (Mechanical Engineering and Mathematics -Computer Science), with short stay in Philips Applied Technologies at High Tech Campus for model validation.

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