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GAS-WALL INTERACTIONS UNDER RAREFIED CONDITIONS

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Rarefied gas flows, heat transfer, gas-wall interactions, potential walls

ABSTRACT

The past decade has seen a considerable growth in portable devices with mobile connectivity. This growth has been enabled by the development of high capacity telecommunication networks globally. Individuals require high data transfer capabilities to remotely stream large information sets (i.e. HD video) and this is leading to greater demands for next generation networks (i.e. 5G). To ensure this growth continues, hardware devices must be smaller, more energy-efficient and provide greater functionality. This requirement poses a thermal management challenge, increasing heat transfer density significantly. Novel materials and cooling methods, which are engineered at the micro- and nanoscale, are necessary to address this. In this paper the focus is on the numerical modelling of the gas-wall interactions that determine the heat transfer.

Rarefaction phenomena on micro- and nanoscales cause the Navier-Stokes equation to break down, making the CFD solution invalid. For such conditions, particle based methods, such as Molecular Dynamics (MD) are preferred. For modelling heat and mass transfer correctly, the interactions between the gas and the solid device surfaces are essential. However, gas-wall interactions for poly-atomic gases are often not sufficiently well modeled by (fitted) Lennard-Jones potentials. Another problem is that large computational time is needed when the walls are modeled explicitly in MD simulations. Therefore, we will propose a solution method in which novel wall potentials are derived and used.

Steele's wall potential has been used in studies of fluid-solid interface for a long time [1]. However, this approach is limited to van der Waals force interaction between an electrically neutral surface and argon-like molecules (Lennard-Jones potential). In semiconductor industry, one of the most common gas-surface interactions are air-silica or water-silica interactions. To describe these interactions, novel and more detailed wall potential functions are needed. Recently, a new wall potential model is developed based on electronegativity-equalization method (EEM) based ReaxFF empirical force field

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[2]. In this paper, water-silica interactions were studied and contact angle simulations were performed in order to validate the wall potential model. The paper showed that the computed contact angles were in good agreement with experimental values, indicating that the gas-wall interaction forces are modelled correctly without additional experimental fitting.

Within MIGRATE (project ESR14) we aim to investigate the conjugate heat transfer behavior from various solids (Si, polymer composites) to nozzle gas micro flows for different rarefaction levels. Therefore we will use a similar approach as described by Kim et al. [2] and will extend this model such that it can be used to study heat flows as well. These results will be validated by experiments conducted at Bell Labs and at Aix-Marseille University [3,4].

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