



**ΑΝΑΚΟΙΝΩΣΗ - ΠΡΟΣΚΛΗΣΗ  
ΔΗΜΟΣΙΑ ΥΠΟΣΤΗΡΙΞΗ ΔΙΔΑΚΤΟΡΙΚΗΣ ΔΙΑΤΡΙΒΗΣ**

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Προσκαλούμε τους μεταπτυχιακούς και προπτυχιακούς φοιτητές μας, τα μέλη Δ.Ε.Π., τους διδάσκοντες του Τμήματος και κάθε ενδιαφερόμενο, στη δημόσια υποστήριξη της Διδακτορικής Διατριβής του κ. Αθανάσιου Μπασδάνη με τίτλο:

**INVESTIGATION OF GAS-SURFACE INTERACTION AND  
INTERMOLECULAR POTENTIAL EFFECTS IN RAREFIED GAS FLOWS VIA  
THE LINEARIZED BOLTZMANN EQUATION**

Rarefied gas flows, i.e., gas flows in low pressure/density conditions or in micro- and nano-scale systems, are far from local equilibrium and they have great theoretical and technological interest with numerous applications (vacuum technology, micro-electromechanical systems, high altitude aerodynamics, porous media, etc.). Under these conditions, the laws of molecular interaction must be considered. Thus, the typical continuum-type fluid mechanics approach is not valid and the flow must be treated based on kinetic theory via the Boltzmann equation or simplified kinetic model equations.

In the present thesis, the objectives include the investigation of the effects of the type of interaction between particles, as well as between particles and surfaces, on the overall quantities characterizing specific non-equilibrium transport phenomena, providing highly accurate results, free, as much as possible, from modeling errors. Therefore, the investigation is based on the computational solution of the Boltzmann equation, which is computationally very intensive, in order to introduce realistic potentials, with classical and quantum scattering. In addition to *ab initio*, hard sphere, variable hard sphere and Lennard-Jones potentials are considered, while gas-surface scattering kernels include the ones proposed by Maxwell, Cercignani-Lampis and Epstein. Targeted prototype rarefied monatomic gas flow setups, covering certain transport processes, are examined. They include the computation of the transport coefficients of dynamic viscosity and thermal conductivity, the estimation of the so-called velocity slip and temperature jump coefficients and the solution of pressure and temperature driven flow and heat transfer configurations. It is noted that in the extended hydrodynamics theory, the slip and jump coefficients are equally important with the transport coefficients.

In all cases, the Boltzmann integro-differential equation is solved, in a very computationally efficient manner, via the discrete velocity method in the molecular velocity space and finite differencing in the physical space, using marching schemes. It has been found that the intermolecular potential is of major importance in transport phenomena caused by temperature gradients imposed parallel to the wall (e.g., thermal creep type flows, velocity thermal slip coefficient), where quantum effects must be considered in light gases at low temperatures. For example, differences in the transport coefficients of helium between classical and quantum scattering, start to appear at 300K and reach 40% at 1K. The

corresponding differences in the velocity thermal slip coefficient reach 15%. On the contrary, the effect of the potential is rather small in pressure driven flows (e.g., Poiseuille type flows, velocity viscous slip coefficient), as well as in heat transfer configurations, with temperature gradients normal to the wall (e.g., Fourier type flow, temperature jump coefficient). When the hard sphere potential is not adequate, it is recommended, instead of the widely-used Lennard – Jones potentials, to apply, at any temperature, ab initio potentials, since they are free of any adjustable parameters and the computational effort is similar. Concerning the gas – surface interaction models, it is concluded that, in the present stage, the Cercignani – Lampis (CL) kernel is the most reliable one to capture simultaneously, both momentum and energy accommodation modes. It is noted however, that even with the CL model, it was not possible to match available experimental data with a unique pair of accommodation coefficients in the whole range of the gas rarefaction and further work on this issue is required.

It is believed that the present dissertation provides some new theoretical and computational insights in rarefied gas dynamics and also supports the design optimization of devices in microfluidics and vacuum technology.

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