A Numerical Investigation of the Steady Evaporation of a Polyatomic Gas

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Abstract

In many situations, both of theoretical and practical interest, it is required to model the transfer of mass, momentum and energy between the vapor phase and its condensed phase (liquid or solid) coexisting in the same flowfield. Although hydrodynamic equations (Euler or Navier-Stokes) generally provide an adequate description of flow properties far from the vapor-liquid or vapor-solid interface, it is well known that there exists a narrow region (Knudsen layer) where the mechanical interaction between the vapor and the condensed phase is to be treated by the microscopic approach of the kinetic theory of gases. The Knudsen layer formed during evaporation or condensation processes is only a few mean free paths wide, but the macroscopic quantities appearing in hydrodynamic equations may suffer strong jumps across this kinetic region. The necessity of describing the structure of the Knudsen layer and providing jump relationships to be used as boundary conditions for a hydrodynamic treatment of multi-phase flows has triggered the production of a huge number of papers where the problem has been extensively investigated. However, most of the research activity has been concentrated on studying monatomic substances whereas evaporation or condensation of a polyatomic vapor in contact with its condensed phase has not attracted the same attention, in spite of their importance for many applications. In this paper we investigate the structure of the Knudsen layer formed in the steady evaporation of a vapor whose molecules behave as rigid rotators. The vapor motion is obtained by the numerical solution of the Boltzmann equation by the Direct Simulation Monte Carlo (DSMC) method. The obtained result are also compared with the solutions of a simplified kinetic BGK-like model equation. It is shown that density and temperature drops across the Knudsen layer are reasonably well reproduced by approximate methods proposed in the literature.