

Molecular Dynamics and Kinetic Modeling of the Evaporation of a Binary Mixture

Aldo Frezzotti¹ and Livio Gibelli²

¹ Politecnico di Milano, Dipartimento di Scienze & Tecnologie Aerospaziali
Via La Masa 34, Milano, 20156, Italy
aldo.frezzotti@polimi.it

² University of Edinburgh, School of Engineering
Mayfield Road, Edinburgh, EH93JL, Scotland UK
livio.gibelli@ed.ac.uk

Evaporation/condensation processes in single component fluids have been the subject of a huge number of studies, aimed at understanding and modeling transport phenomena across the liquid-vapor interface [1,2]. On the modeling side, most studies have focused on the gas dynamics properties of the vapor in the kinetic layer next to the liquid-vapor interface, where macroscopic properties suffer jumps across the Knudsen layer [3]. Kinetic models of the vapor phase are based on boundary conditions, to be prescribed at the liquid-vapor interface, which have a phenomenological nature and whose accuracy has been assessed/questioned in a number of studies based on Molecular Dynamics (MD)[4]. Although less studied, evaporation/condensation phenomena in multi-component fluids are relevant in many fields, which include distillation processes, laser induced ablation of materials and meteors entry flows. Kinetic theory studies of the evaporation of binary mixtures [5] have shed some light on how jumps of macroscopic quantities are affected by the mixture composition. However, all of the kinetic theory based investigations use simple extensions of the boundary conditions formulated for a single component fluid. A preliminary MD study of the evaporation of a binary Lennard-Jones fluid into vacuum [6] has shown that both components evaporate with a distribution function which is very close to a Maxwellian. However, the same study

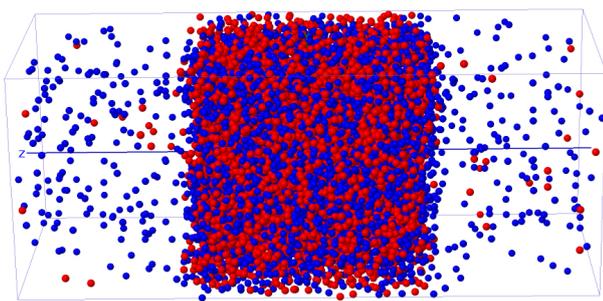


Figure 1: MD Simulation of evaporation of an initially equimolar Ar-Kr liquid film.

suggests that defining an evaporation coefficient for a multi-component fluid presents some difficulties, connected with the strong composition gradient in the interface region. The present work aims at extending the study presented in Ref. [6] to consider quasi-steady evaporation of a binary liquid film into a half-space (See Fig. 1). The study is mainly based on MD simulations of a Lennard-Jones binary fluid from which it is possible to obtain the structure of the Knudsen layer in

the vapor, as well as the evolution of the liquid bulk and interface compositions (See Fig. 2). The latter play a fundamental role in the determination of the evaporation coefficients. MD results are compared with companion results obtained by a hybrid model which couples the Boltzmann equations for a binary ideal gas to a continuum description of the liquid phase through kinetic boundary conditions.

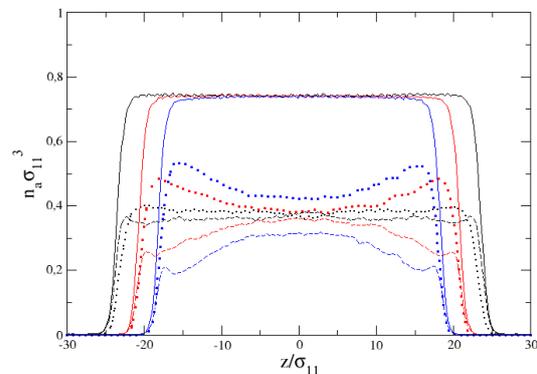


Figure 2: Time evolution of total and partial densities profiles, during the evaporation of a liquid Ar-Kr mixture.

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