

A Marie-Curie-ITN



# DRAFT MIGRATE-XX

## A NUMERICAL STUDY OF INTERFACIAL TEMPERATURE JUMPS IN THE EVAPORATION OF WATER

Aldo Frezzotti

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

## **KEY WORDS**

Kinetic theory, vapor- liquid interface, boundary conditions.

## ABSTRACT

TIn 1999, Fang and Ward published a paper reporting measurements of large temperature jumps at the vapor-liquid interface, during the slow evaporation of purified water [1]. Temperature jumps in evaporation flows have also been observed in experiments adopting different setups [2] and working fluid [3]. The observed temperature jumps appeared as anomalous in that the vapor temperature, in proximity of the interface was found to be a few degrees *higher* than the liquid surface temperature, whereas it was expected to be slightly lower because of the vapor expansion in the evaporation flow. As pointed out in a few following papers [4, 2], such expectation is not correct, in principle. Actually, the temperature jump at the vapor-liquid interface is determined not only by evaporation mass flow rate but also by the heat flux [5]. The former gives a negative contribution to the temperature jump, in the case of evaporation. However, the latter gives a positive contribution when, as in the case of the experiment described in Ref. [1], a steep raise of the temperature is found outside the Knudsen layer, next to the interface. Although a clear, quantitative explanation of the observed jumps has not vet been given, the possible role of kinetic boundary conditions has been pointed out in Ref. [4] where a velocity dependent condensation coefficient, proposed by Tsuruta [6], has been adopted to study the influence of kinetic boundary conditions on temperature jumps. Although interesting, the analysis was affected by a few limitations. First of all, kinetic contributions have been taken into account only approximately, not by a consistent treatment of the Knudsen layer structure as done, for instance, by Soga [5] using a linearized kinetic model for a diatomic gas. Second, molecular internal degrees of freedom have not been taken into account. In principle, the latter approximation might have an important quantitative impact on the model predictions since the amount of internal energy stored in rotational motion of water molecules equals the translational contribution, in near equilibrium flows. The aim of the present work is to study the onset of temperature jumps at the vapor-liquid interface by a kinetic model, based on the Boltzmann equation [7] for a gas of rigid rotators with three rotational degrees of freedom. Molecular collisions are described by the Variable Soft Sphere (VSS) model [8] in combination with the Borgnakke-Larsen [9] statistical model to couple rotational and translational degrees of freedom. The (fundamental) role of boundary conditions at the interface is analyzed by a comparison of two different evaporation models. The first is a quite standard one, assuming an energy independent evaporation/condensation coefficient and Maxwellian distribution of spontaneously evaporated molecules [10]. The second one is Tsuruta's model, cited above, and already used by Bond and Struchtrup [4] to interpret experimental temperature jumps. The kinetic equation has

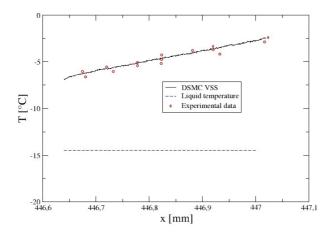




#### A Marie-Curie-ITN

Proceedings of the 2<sup>nd</sup> MIGRATE Workshop June 29-30, 2017 – Sofia, Bulgaria

been solved numerically with the necessary accuracy by the Direct Simulation Monte Carlo method [11] thus providing results which are not affected by additional approximations beyond those intrinsic in the underlying physical models and in the flow geometry simplifications. As shown in the Figure below, matching kinetic theory predictions and experimental results is possible, provided the evaporation/condensation coefficient of water is very small (around 0.05) and specular reflection of molecules is assumed to occur at the vapor-liquid interface. Moreover, it is found that Tsuruta's model results are very close to those of the more standard energy independent evaporation/condensation coefficient. Since the boundary conditions setting that leads to agreement with experimental data appears as unrealistic, a deeper analysis of the experimental results and of the theoretical models is necessary.



#### References

[1] G. Fang, C. Ward, Temperature measured close to the interface of an evaporating liquid, Physical Review E 59 (1) (1999) 417–428.

[2] V. Badam, V. Kumar, F. Durst, K. Danov, Experimental and theoretical investigations on interfacial temperature jumps during evaporation, Experimental Thermal and Fluid Science 32 (1) (2007) 276–292.

[3] E. Gatapova, I. Graur, O. Kabov, V. Aniskin, M. Filipenko, F. Sharipov, L. Tadrist, The temperature jump at water – air interface during evaporation, International Journal of Heat and Mass Transfer 104 (2017) 800–812.

[4] M. Bond, H. Struchtrup, Mean evaporation and condensation coefficients based on energy dependent condensation probability, Physical Review E - Statistical, Nonlinear, and Soft Matter Physics 70 (6 1) (2004) 061605–1–061605–21.

[5] T. Soga, A kinetic theory analysis of evaporation and condensation of a diatomic gas, Phys. Fluids 28 (1985) 1280–1285.

[6] T. Tsuruta, H. Tanaka, T. Masuoka, Condensation/evaporation coefficient and velocity distribution at liquid-vapor interface, Int. J. Heat and Mass Transf. 42 (1999) 4107–4116.

[7] C. Cercignani, The Boltzmann Equation and Its Applications, Springer-Verlag, Berlin, 1988.

[8] K. Koura, H. Matsumoto, Variable soft sphere molecular model for Inverse Power Law or Lennard–Jones potential, Physics of Fluids A: Fluid Dynamics 3 (10) (1991) 2459–2465.

[9] C. Borgnakke, P. S. Larsen, Statistical collision model for Monte Carlo simulation of polyatomic gas mixtures, J. Comput. Phys. 18 (1975) 405–420.

[10] A. Frezzotti, Boundary conditions at the vapor-liquid interface, Physics of Fluids 23 (3) (2011) 030609.

[11] G. A. Bird, Molecular Gas Dynamics and the Direct Simulation of Gas Flows, Clarendon Press, Oxford, 1994.