Application of entropy production maximisation to evaporation of atoms

F. Kassubek [1*], J. Lehmann [1*]

[1] *ABB Switzerland, Corporate R&D, CH-5405 Baden-Dättwil, Switzerland*
[*] frank.kassubek@ch.abb.com, joerg.lehmann@ch.abb.com

We consider the evaporation (or condensation) of atoms without internal degrees of freedom from a solid surface. A relation between the properties of the gas near the surface and those in the equilibrium gas far away from the surface is found by means of an entropy-production-maximisation procedure, which yields the velocity distribution of the backscattered atoms. We compare the results to exact solutions of the Boltzmann equation obtained by Monte Carlo simulations.

Introduction Finite volume studies of plasma flow, e.g., inside high-voltage switching devices require correct boundary conditions. Apart from the arc root itself, especially the modeling of evaporation of insulation material, e.g., PTFE, requires some attention, since energy and mass flow can have a strong influence on the flow dynamics. Simple and efficient models are necessary to provide such boundary conditions.

In the present study, we restrict ourselves to the evaporation of neutral atoms without internal degrees of freedom. The dynamics in the non-equilibrium Knudsen layer can be determined by solving the Boltzmann equation (see Ref. [1]). For a flat surface, only the spatial coordinate z normal to the surface has to be considered. We introduce a simplified model where the complex dynamics is replaced by the general principle of entropy maximisation [2]: A system that can explore many degrees of freedom tries to evolve maximising the produced entropy while obeying the relevant conservation constraints. While this principle is exact near equilibrium, it provides an approximation in the general case.

Compared to the study [3] that also addresses processes in the solid and the chemistry of the evaporated material, we explicitly consider the role of non-equilibrium velocity distributions and include the full momentum balance.

Entropy maximisation In equilibrium, e.g. in the gas far away from the surface, the velocity distribution of the atoms is given by the Maxwell distribution

$$f^{n,T,u_z}(\vec{v}) = n\left(4/v_{\mathrm{T}}^2\right)^{3/2} e^{-4\pi|\vec{v}-\vec{u}|^2/v_T^2}, \tag{1}$$

where the parameters n, T, $\vec{u}$ denote gas density, temperature and velocity, respectively, and $v_{\mathrm{T}} = \sqrt{8kT/m\pi}$ is the mean thermal velocity with Boltzmann constant k and atom mass m. Directly at the surface, the outgoing atoms ($v_z > 0$) may be characterised by a half Maxwellian distribution, whereas for the backscattered atoms the distribution is at first unknown.

Typically, an ansatz for this distribution is used, e.g. that the distribution with $v_z < 0$ is equal to the distribution (1) in the gas multiplied with some reduction factor β (see [1] for further references). In [4], the entropy production as a function of β and also for another distribution has been investigated. Here, we fully generalise this approach by a variation of the whole distribution of the backscattered atoms for entropy production maximisation (and not a parameterized ansatz) under the constraint of conservation of particles, momentum and energy. This requires only the distributions at the solid surface and in the equilibrium gas. Appropriate integration over velocity space yields ,the fluxes of mass, momentum, energy, and entropy at these boundaries of the Knudsen layer. For the conserved quantites, the difference of the fluxes has to vanish, whereas for the entropy, it directly gives the entropy production rate.

Results and comparison to Monte-Carlo calculations The numerical maximisation gives the velocity distribution of backscattered atoms. In general, for subsonic evaporation, one has to fix one parameter on the gas side and two parameters on the hot surface. Hence, we scale all densities and temperatures by the respective parameters in the outgoing half-Maxwell distribution at the surface and use the Mach number M_g in the gas as additional free parameter. The left panel of Fig. 1 shows density and temperature (or pressure) as a function of the Mach number, illustrating the desired boundary condition that can be used for finite volume simulations. It is in good agreement with previous numerical studies of the Boltzmann equations [5].

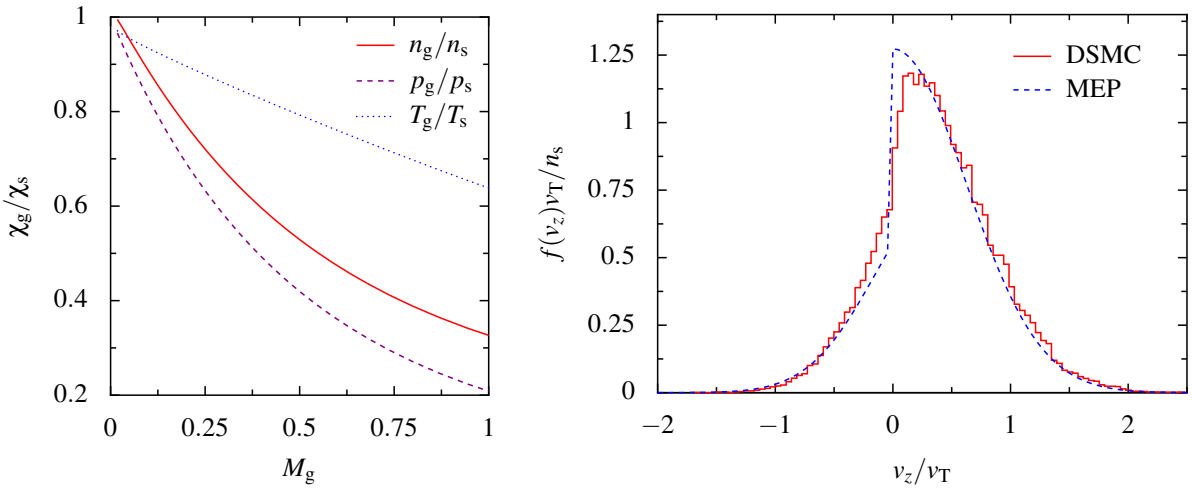

Fig. 1: Left: Density, pressure and temperature in the gas. Right: Distribution function of the velocity v_z near the surface (see text). Solid line: Numerical results from a DSMC simulation. Dashed: Results obtained from the maximum-entropy-production principle.

A more significant test of the result is given by a direct comparison of the calculated velocity distribution with numerical solutions of the Boltzmann equations. We consider a case analogous to [4], i.e., evaporation into vacuum; here, no constraint on the Mach number is imposed and a maximal entropy production is found for $M_g = 0.91$. The numerical solutions have been obtained by a Direct-Simulation-Monte-Carlo method similar to Ref. [6]. The comparison is shown in the right panel of Fig. 1. A good agreement of the simplified theory and the full numerical result has been obtained.

This demonstrates that entropy production maximisation is a good approach to develop simplified models for evaporation (and similarly condensation). In the future, more complex systems, e.g. with internal degrees of freedom are planned to be investigated similarly.

References

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