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Entropy Inequalities for Evaporation/Condensation Problem in Rarefied Gas Dynamics

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The present paper is devoted mainly to the half space problem for stationary Boltzmann-type equations. Using only conservation laws and the Boltzmann H-theorem we derive an inequality for unknown constant fluxes of mass, energy, and momentum. This inequality is expressed in terms of three parameters (pressure p, temperature T and the Mach number M) of the asymptotic Maxwellian at infinity. Geometrically the inequality describes a "physical" domain with positive entropy production in the 3-d space of the parameters. The domain appears to be qualitatively different for evaporation and condensation problems. We show that for given M, the curve $p = p(M)$, $T = T(M)$ of maximal entropy production practically coincides with the experimental evaporation curve obtained by Sone *et al.* on the basis of numerical solutions of BGK equation. Similar consideration for the condensation problem is also in qualitative agreement with known numerical results.

KEY WORDS: Boltzmann equation; BGK-model; entropy; evaporation/condensation problem; convex functional; asymptotic Maxwellian.

1. INTRODUCTION

The concept of entropy plays a central role in the thermodynamics of irreversible processes. However, for a majority of practically interesting systems of statistical physics we know not very much about strongly non-equilibrium states of such systems. A remarkable exception is a dilute gas (or plasma) for which one can use so powerful tool as the Boltzmann-type kinetic equation for a distribution function $f(x, v, t)$ (x, v and t denote

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respectively position, velocity and time variables). Unfortunately, this nonlinear multidimensional equation is rather complicated and therefore it can be solved only numerically for spatially inhomogeneous problems having physical interest. On the other hand, the Boltzmann-type equation implies the famous inequality for H-function (entropy with the minus sign):

$$\frac{\partial H}{\partial t} + \operatorname{div} \Psi \leqslant 0$$

where

$$H(x, t) = \int_{\mathbb{R}^3} dv\, f(x, v, t) \log f(x, v, t)$$

$$\Psi(x, t) = \int_{\mathbb{R}^3} dv\, vf(x, v, t) \log f(x, v, t)$$

This inequality can be considered as the main inequality of the thermodynamics of rarefied gas. We note that the entropy inequality is much weaker, however much more general, than the Boltzmann equation itself. It has obvious generalisations to mixtures, gases with internal degrees of freedom, etc. Moreover, it does not depend on external or self-consistent forces $F(x, v, t)$ (provided $\operatorname{div}_v F = 0$) and on particular form of the collision integral.

The aim of the present paper is to show that the entropy inequality can be successfully used for qualitative and quantitative estimates of strongly nonequilibrium steady states of a rarefied gas, without solving the Boltzmann equation. In this paper, we restrict our consideration to the plane evaporation/condensation problem (mostly in the half-space). This problem was previously studied by many authors (see ref. 1 for a review, this paper contains 55 related references). In particular, a very detailed numerical study was performed by Sone, Aoki and their collaborators. As we shall see below, some of the numerical results can be obtained with a good accuracy on the basis of the entropy inequality.

The paper is organised as follows. In Section 2 we discuss a statement of the evaporation/condensation problem and give a very short review of known results. Then we explain an idea of applying the entropy inequality to the problem of estimates of unknown parameters of asymptotic Maxwellian. The estimates are based on a simple generalisation of well-known properties of H-function (Lemma 1) and on representation of the entropy flux as a difference of two convex functionals (Section 3).

One of the functionals is given by boundary conditions, whereas the other one is estimated below in Section 4. Combining the results of

Sections 3–4, we prove in Section 5 our main inequalities for the unknown parameters of asymptotic Maxwellians in the half-space and in a slab. Then, in Section 6, we consider the half-space inequality in variables p (pressure), T (temperature) and M (Mach number). The inequality describes a "physical" domain of positive entropy production in the three dimensional space of the parameters. The domain appears to be qualitatively different for evaporation and condensation problems. In particular, it has a shape of closed narrow "pipe" for the evaporation problem. The curve of maximal (for given M) entropy production inside this "pipe" is in surprising agreement with the famous evaporation curve obtained by Sone *et al.* on the basis of numerical solutions of BGK equation. For the condensation problem, we have constructed the surface of maximal (for given M and p) entropy production and show that this surface is also very similar (at least qualitatively) to the well-known evaporation surface obtained by numerical methods (see ref. 1 for details). These and other concrete results are presented in Section 6.

2. STATEMENT OF THE PROBLEM AND MOTIVATION

Let $f(x, v)$ be a non-negative solution of the stationary plane problem for the Boltzmann-type kinetic equation

$$v_x \frac{\partial f}{\partial x} = Q(f, f), \qquad x \in \mathbb{R}_+, \quad v \in \mathbb{R}^3 \tag{1}$$

with given distribution of incoming particles at $x = 0$

$$f(0, v) = \varphi_+(v), \qquad v_x > 0 \tag{2}$$

One more boundary condition is stated at $x = L$, $L > 0$,

$$f(L, v) = \varphi_-(-v), \qquad v_x < 0 \tag{3}$$

In the asymptotic case $L \to \infty$ (half-space problem) we can demand the solution to be bounded at infinity. This means, roughly speaking, that

$$f(x, v) \to M(\rho, u, T) = \rho(2\pi T)^{-3/2} \exp\left[-\frac{(u-v)^2}{2T}\right] \tag{4}$$

with certain $\rho > 0$, $T > 0$, $u \in \mathbb{R}^3$, provided the three parameter family of Maxwellians $M(\rho, u, T)$ represents the whole class of non-negative (equilibrium) solutions to the equation $Q(f, f) = 0$.

Our aim is to present some very general estimates for functions satisfying the equation (1) and boundary conditions (2), (3) or (2), (4). The term "very general" means that we are not going to use any information concerning the operator $Q(f, f)$ except (a) conservation laws:

$$\int_{\mathbb{R}^3} dv\, \psi(v)\, Q(f, f) = 0 \qquad \text{if} \quad \psi = v_x, v_y, v_z, 1, |v|^2 \tag{5}$$

and (b) H-theorem

$$\int_{\mathbb{R}^3} dv[\log f(v)]\, Q(f, f) \leqslant 0 \tag{6}$$

The properties (a) and (b) are valid for Boltzmann's and Landau's equations, BGK-model, etc. For the sake of simplicity we assume also that there exists a class of solutions satisfying the symmetry condition

$$f(x, v) = f(x, v_x, r^2), \qquad r^2 = v_y^2 + v_z^2 \tag{7}$$

and consider such functions only.

The corresponding class of Maxwellians consists of functions

$$M(\rho, u, T) = \rho(2\pi T)^{-3/2} \exp\left[-\frac{(v_x - u)^2 + r^2}{2T}\right] \tag{8}$$

where all the three parameters ρ, $T \in \mathbb{R}_+$, $u \in \mathbb{R}$ are real numbers.

It is obvious that two main properties of $f(x, v)$ follow from Eqs. (5) and (6).

(A) There exist three numbers $\mathscr{L}_1$, $\mathscr{L}_2$, $\mathscr{L}_3$ such that

$$\int_{\mathbb{R}^3} dv\, f(x, v)\, v_x \begin{Bmatrix} 1 \\ v_x \\ |v|^2 \end{Bmatrix} = \begin{Bmatrix} \mathscr{L}_1 \\ \mathscr{L}_2 \\ \mathscr{L}_3 \end{Bmatrix} \tag{9}$$

(B)

$$\Psi[f(x_1, \cdot)] \leqslant \Psi[f(x_2, \cdot)] \qquad \text{if} \quad x_1 \geqslant x_2 \tag{10}$$

where

$$\Psi[f] = \int_{\mathbb{R}^3} dv\, v_x f(v) \log f(v) \tag{11}$$

Combining (A) with (4), (8), we obtain usual relations

$$\mathscr{L}_1 = \rho u, \qquad \mathscr{L}_2 = \rho(u^2 + T), \qquad \mathscr{L}_3 = \rho u(u^2 + 5T) \tag{12}$$

Using the physics terminology, we can say that we consider the evaporation/condensation problem.

The terminology becomes clear if we assume that the plane $x=0$ is the boundary between liquid ($x<0$) and gas ($x>0$) phases. The liquid phase is described very roughly by the boundary condition (2) at $x=0$, whereas the gas phase ($x>0$) is described by the kinetic equation (1). Parameters (ρ, u, T) represent density, bulk velocity and temperature respectively. The functional $[-\Psi(f)]$ is the entropy flux, whereas $\mathscr{L}_{1,2,3}$ are proportional to fluxes of mass, momentum and energy respectively. We speak about evaporation (of the liquid) if the fluxes of mass and energy are positive ($u>0$) and condensation (of the gas into liquid) otherwise ($u<0$). The plane half-space problem arises naturally as a nonlinear boundary layer problem in the neighbourhood of evaporating surface in R^3. Solutions to this problem define correct boundary conditions (at such surfaces) for the hydrodynamic equations.

Let us formulate now the specific problem we are going to study below. Note that each solution of the above stated boundary value problems implies the existence of three numbers $\mathscr{L}_1$, $\mathscr{L}_2$, $\mathscr{L}_3$. The numbers, however, are not known in advance. In case of finite interval (boundary conditions (2), (3)), the numbers are certain functionals $\mathscr{L}_\alpha(\varphi_+, \varphi_-)$, $\alpha=1,2,3$, on functions $\varphi_\pm(v)$. In case of the half-space problem, the fluxes $\mathscr{L}_\alpha$ are directly connected by Eq. (12) with parameters (ρ, u, T) which are also not necessary known (for brevity we omit a discussion of well-known peculiarities of the half-space problem for various cases of sub(super)sonic evaporation/condensation, see e.g., ref. 1).

There is a large number of publications on this topic based on numerical computations for the Boltzmann equation or the BGK model (see ref. 1 for a review). For example, we set

$$\varphi_+ = a_+ \exp[-b_+ |v|^2] \tag{13}$$

and study the half-space problem. That gives some "experimental" (in the sense of the computer experiment) knowledge of parameters (ρ, u, T) at infinity. A detailed investigation of the problem was done by Sone *et al.*[1, 2] The authors presented their results in the 3-d space of parameters (p, M, T) such that

$$p = pT, \qquad M^2 = 3u^2/(5T), \qquad T = T, \qquad c^2 = \frac{5T}{3} \tag{14}$$

(it is sufficient for many molecular models to consider the case $a_+=1$, $b_+=1$). They have obtained: (a) a curve for sub-sonic evaporation

$(0<u<c)$; (b) a surface for sub-sonic condensation $(-c<u<0)$; and (c) a 3d domain for supersonic condensation $(u<-c)$. The qualitative difference between cases (a), (b), (c) was explained long ago (see, for example, ref. 3) on the basis of the linearised Boltzmann equation. A recent discussion on transonic condensation[4] is interesting, but concerns only the case $M \approx 1$. Many interesting numerical results can be found also for the finite interval problem.[5] Moreover, the first rigorous results concerning the existence of solutions to the problems (1)–(4) for the Boltzmann equation in the strongly nonlinear case were recently obtained by Arkeryd and Nouri.[6]

In the following, we derive some inequalities which impose certain restrictions on parameters $\mathscr{L}_{1,2,3}$ or ρ, u, T for given functions $\varphi_{\pm}(v)$. The inequalities are rough enough since they use only general properties (9)–(10). They are however useful because of their rigorousity and generality.

3. GENERALISED H-FUNCTIONAL AND DECOMPOSITION OF THE ENTROPY FLUX

We consider first a straightforward generalisation of well-known properties of the Boltzmann's H-functional. Let $g(v) \geqslant 0$, $v \in \mathbb{R}^3$, be a fixed locally integrable function. We introduce the functional acting on v-variable

$$H_g(f) = \int_{\mathbb{R}^3} dv\, g(v)\, f(v) \log f(v) \tag{15}$$

and moments

$$\mu_0 = \int_{\mathbb{R}^3} dv\, g(v)\, f(v), \qquad \mu_1 = \int_{\mathbb{R}^3} dv\, g(v)\, f(v)\, v$$
$$\mu_2 = \int_{\mathbb{R}^3} dv\, g(v)\, f(v)\, |v|^2 \tag{15a}$$

where $\mu_{0,2} > 0$, $\mu_1 \in \mathbb{R}^3$.

Lemma 1. Let $f(v)$ be a function such that the integrals $H_g(f)$ and moments (15a) are finite. We assume that there exists a Maxwellian

$$f_M(v) = A \exp[-\beta\, |v|^2 - \gamma \cdot v], \qquad A, \beta \geqslant 0, \quad \gamma \in \mathbb{R}^3 \tag{16}$$

having the same moments (15a). Then

(i) the Maxwellian is defined uniquely and

(ii) satisfies the inequality

$$H_g(f_M) \leqslant H_g(f) \tag{17}$$

Proof. It is obvious that

$$H_g(f) - H_g(f_M) = \int_{\mathbb{R}^3} dv\, g(v) \left[f(v) \log \frac{f(v)}{f_M(v)} - (f(v) - f_M(v)) \right] \geqslant 0 \tag{18}$$

since $y \log(y/x) - (y - x) \geqslant 0$ for any positive x, y.

Thus, (ii) is proved. To prove (i), we assume that there exist two different Maxwellians $f_M^{(1,2)}(v)$ with the same moments (15a). Then $H_g(f_M^{(1)}) = H_g(f_M^{(2)})$ because of (ii). Therefore

$$f_M^{(1)} \log \frac{f_M^{(1)}}{f_M^{(2)}} = f_M^{(1)} - f_M^{(2)}$$

on a set of positive measure in $\mathbb{R}^3$ where $g(v) > 0$. Hence, $f_M^{(1)} = f_M^{(2)}$ for all $v \in \mathbb{R}^3$ and the proof is completed. ∎

Both assertions (i) and (ii) are wrong if we do not assume that $g(v) \geqslant 0$. In particular, we obtain (in the general case) two Maxwellians (sub- and supersonic) for $g(v) = v_x$.

Let us now return to the boundary value problems (1)–(4). In accordance with (10), we have a monotone functional (11). The functional, however, is not convex and does not satisfy the above lemma. In order to apply Lemma 1, we decompose $f(v)$ onto two parts $f^{\pm}(v)$: $\mathbb{R}^3_+ \to \mathbb{R}_+$ such that

$$f^{\pm}(v) = f(\pm v) \qquad \text{if} \quad v \in \mathbb{R}^3_+ = \{v \in \mathbb{R}^3, v_x > 0\} \tag{19}$$

(The plane $v_x = 0$ is irrelevant for our goals). The functional (11) can be written as difference of two convex functionals (or two values of the same convex functional)

$$\Psi(f) = \Psi_+(f^+) - \Psi_+(f^-), \qquad \Psi_+(f) = \int_{\mathbb{R}^3_+} dv\, v_x f \log f \tag{20}$$

Note that $\Psi_+(f) = H_g(f)$ where $H_g(f)$ is defined by Eq. (15) with the weight function

$$g(v) = v_x \qquad \text{if} \quad v_x > 0, \qquad g(v) = 0 \qquad \text{otherwise}$$

Therefore $\Psi_+(f)$ satisfies conditions of Lemma 1 (we always imply, if necessary, a trivial extension of $f^{\pm}(v)$ to the whole space $\mathbb{R}^3$ such that $f^{\pm}(v)=0$ if $v_x \leqslant 0$).

We denote

$$\int_{\mathbb{R}^3_+} dv\, f^{\pm}(v)\, v_x \begin{Bmatrix} 1 \\ v_x \\ |v|^2 \end{Bmatrix} = \begin{Bmatrix} m_1^{\pm} \\ m_2^{\pm} \\ m_3^{\pm} \end{Bmatrix} \tag{21}$$

for functions $f(v)$ satisfying (7) and explain a simple idea of applying Lemma 1 to boundary value problems (1)–(4). Let us, for example, consider the half-space problem (1), (2), (4). Combining Eqs. (2), (4), (10), (20), we obtain

$$\Psi_+(\varphi_+) - \Psi_+[f^-(0,\cdot)] \geqslant \Psi(M) \tag{22}$$

where

$$\Psi(M) = \rho u \log[\rho(2\pi e T)^{-3/2}] \tag{23}$$

The function $f^-(0,v)$ is unknown. However, we can express its moments $m_{1,2,3}$ through the same moments $m^+_{1,2,3}$ of the function $\varphi_+(v)$ and through (ρ, u, T) by using Eqs. (9), (12). Hence, we obtain

$$\begin{gathered} m_1^+ - m_1^- = \rho u, \qquad m_2^+ + m_2^- = \rho(u^2+T) \\ m_3^+ - m_3^- = \rho u(u^2+5T) \end{gathered} \tag{24}$$

On the other hand, Lemma 1 leads to the inequality

$$\Psi_+[f^-(0,\cdot)] \geqslant \Psi_+[f_M^-] \tag{25}$$

where the right-hand side can be expressed as certain function (see below its specific form) of the three moments $m^-_{1,2,3}$. Then we substitute Eq. (24) and finally obtain the inequality which directly connects the parameters (ρ, u, T) at infinity with the boundary condition (2) at $x=0$. To derive such inequalities in (almost) explicit form, we first study in the next section the lower estimates for $\Psi_+(f)$ in more detail.

4. AUXILIARY PROBLEM

We consider the following

Problem. Let (z, r, φ) denote cylindrical coordinates in $\mathbb{R}^3$, $f(z, r) \geqslant 0$ be an auxiliary symmetric function defined on the half-space $z > 0$. Find

$$F(m_1, m_2, m_3) = \text{Min } \Psi_+(f) \tag{26}$$

where

$$\begin{Bmatrix} m_1 \\ m_2 \\ m_3 \end{Bmatrix} = 2\pi \int_0^\infty dz \int_0^\infty dr\, rf(z, r) \begin{Bmatrix} z \\ z^2 \\ z(z^2 + r^2) \end{Bmatrix} \tag{27}$$

$$\Psi_+(f) = 2\pi \int_0^\infty dz \int_0^\infty dr\, rzf(z, r) \log f(z, r) \tag{28}$$

Solution. Following Lemma 1, we first construct the Maxwellian

$$f_M(z, r) = \frac{a\beta^3}{\pi} \exp[-\beta^2(z - w)^2 - \beta^2 r^2] \tag{29}$$

with parameters (a, β, w) satisfying (27) for $f = f_M$. The second step is to evaluate $F(m_1, m_2, m_3) = \Psi_+(f_M)$.

Substituting (29) into (27), we obtain three equations for (a, β, w)

$$\begin{aligned} m_n &= \frac{a}{\beta^n} [I_n(\beta w) + \delta_{n3} I_1(\beta w)] \\ I_n(s) &= \int_0^\infty dz\, z^n \exp[-(z - s)^2], \qquad n = 1, 2, 3 \end{aligned} \tag{30}$$

Their solution can be expressed in parametric form

$$a = \frac{m_1^2}{m_2} \frac{I_2(s)}{I_1^2(s)}, \qquad \beta = \frac{m_1}{m_2} \frac{I_2(s)}{I_1(s)}, \qquad w = \frac{m_2}{m_1} \frac{sI_1(s)}{I_2(s)} \tag{31}$$

where the parameter $s \in (-\infty, \infty)$ is a solution of the equation

$$\frac{m_1 m_3}{m_2^2} = \frac{I_1(s)[I_1(s) + I_3(s)]}{I_2^2(s)} \tag{32}$$

To apply Lemma 1, we need to prove that Eq. (32) has a solution for any given number $(m_1 m_3/m_2^2) > 1$. Then three numbers (a, β, w) are uniquely defined (Lemma 1, (i)).

We note that the function

$$\Phi(s) = \frac{I_1(s)[I_1(s) + I_3(s)]}{I_2^2(s)} \tag{33}$$

is continuous on $(-\infty, \infty)$. Moreover,

$$I_n(s) \simeq s^{n+1} \int_0^\infty dz\, e^{-s^2(z-1)^2} \simeq \sqrt{\pi}\, s^n, \qquad s \to \infty$$

therefore $\Phi(s) \to 1$ as $s \to \infty$. On the other hand,

$$I_n(s) = |s|^{n+1} \int_1^\infty dz (z-1)^n\, e^{-s^2 z^2}, \qquad s < 0 \tag{34}$$

By usual asymptotic consideration, we obtain

$$\begin{aligned} I_n(s) &= |s|^{n+1}\, e^{-s^2} \int_0^\infty dt\, e^{-s^2 t} \frac{(\sqrt{1+t} - 1)^n}{2\sqrt{1+t}} \\ &\approx 2^{-(n+1)}\, |s|^{n+1}\, e^{-s^2} \int_0^\infty dt\, t^n e^{-s^2 t} \\ &= n!\, (2\,|s|)^{-(n+1)}\, e^{-s^2}, \qquad s \to -\infty \end{aligned} \tag{35}$$

Hence

$$\Phi(s) \approx \frac{I_1^2(s)}{I_2^2(s)} \approx s^2 \to \infty, \qquad s \to -\infty \tag{36}$$

and therefore the continuous function $\Phi(s)$ attains all values on $(1, \infty)$. Hence, the equation has a root s for any $(m, m_3/m_2^2) > 1$. Moreover, the root is unique since $s = \beta w$ for uniquely defined (Lemma 1, (i)) numbers β and w.

Unfortunately, the parameter s cannot be expressed explicitly through $\tau = m_1 m_3/m_2^2 > 1$. One can construct, however, asymptotic formulae by using asymptotic expansions for $I_{1,2,3}(s)$. If $s > 0$, then

$$
\begin{aligned}
I_n(s) &= \int_{-s}^{\infty} dz(z+s)^n\, e^{-z^2} \\
&= \int_{-\infty}^{\infty} dz(z+s)^n\, e^{-z^2} - \int_{s}^{\infty} dz(s-z)^n\, e^{-z^2} \\
&= \sum_{k=0}^{[n/2]} \binom{n}{2k} s^{n-2k} \int_{-\infty}^{\infty} dz\, z^{2k} e^{-z^2} \\
&\quad + (-1)^{n+1}\, s^{n+1} \int_{1}^{\infty} dz(z-1)\, e^{-s^2 z^2} \\
&= (-1)^{n+1}\, I_n(-s) + \sqrt{\pi} \sum_{k=0}^{[n/2]} \binom{n}{2k} \frac{(2k-1)!!}{2^k}\, s^{n-2k}
\end{aligned}
\tag{37}
$$

where $(-1)!! \equiv 1$ by definition. The first integral was already studied above (Eqs. (34), (35)). Therefore we obtain

$$
\begin{aligned}
I_1(s) &= \sqrt{\pi}\, s + O(s^{-2} e^{-s^2}), \qquad s \to \infty \\
I_2(s) &= \sqrt{\pi}\, s^2(1 + \tfrac{3}{2} s^{-2}) + O(s^{-3} e^{-s^2}) \\
I_3(s) &= \sqrt{\pi}\, s^3(1 + \tfrac{9}{2} s^{-2}) + O(s^{-4} e^{-s^2})
\end{aligned}
\tag{38}
$$

and

$$
\Phi(s) \simeq 1 + \frac{3}{2s^2}, \qquad s \to \infty \tag{39}
$$

Hence, asymptotic values of the root s of the equation (32) are

$$
\begin{aligned}
s &\simeq \sqrt{\frac{3}{2}} \left(\frac{m_1 m_3}{m_2^2} - 1 \right)^{-1/2} \qquad \text{if} \quad \frac{m_1 m_3}{m_2^2} \to 1 \\
s &\simeq -\left(\frac{m_1 m_3}{m_2^2} \right)^{1/2} \qquad \text{if} \quad \frac{m_1 m_3}{m_2^2} \to \infty
\end{aligned}
\tag{40}
$$

It is clear also that s depends on $m_1 m_3 / m_2^2$ monotonically. Thus, the first part of the problem is solved and the properties of the solution are clarified.

Now we need to construct the function (26), i.e.,

$$
F(m_1, m_2, m_3) = \Psi_+(f_M) = 2\pi \int_0^{\infty} dz \int_0^{\infty} dr\, rz f_M(r, z) \log f_M(r, z)
$$

Noting that

$$\log f_M = \log \frac{a\beta^3}{\pi} - \beta^2(z^2 + r^2 + w^2 - 2zw), \qquad \beta w = s$$

we obtain

$$F(m_1, m_2, m_3) = m_1 \left(\log \frac{a\beta^3}{\pi} - s^2 \right) + 2s\beta m_2 + \beta^2 m_3 \tag{41}$$

where a and β are defined through s by Eq. (31). Sometimes it is more convenient to use slowly varying (for $s > 0$) functions $I_n(s)$ instead of s. To this goal we use the explicit formula

$$F(m_1, m_2, m_3) = m_1 \log \frac{a\beta^3}{\pi} - \frac{a}{\beta} F_1(s)$$

$$F_1(s) = \beta^4 \int_0^\infty dz\, z \int_0^\infty dt[\beta^2 t + (\beta z - s)^2]\, e^{-\beta^2 t - (\beta z - s)^2}$$

$$= \int_{-s}^\infty dz(z + s)(1 + z^2)\, e^{-z^2}$$

On the other hand,

$$a = \beta \frac{m_1}{I_1(s)}, \qquad I_1(s) = \int_{-s}^\infty dz(z + s)\, e^{-z^2}$$

in accordance with (31). Therefore

$$F(m_1, m_2, m_3) = m_1 \left[\log \frac{a\beta^3}{\pi} - 1 - \theta(s) \right] \tag{42}$$

where

$$\theta(s) = \frac{\int_{-s}^\infty d\mu\, z^2}{\int_{-s}^\infty d\mu} = \langle z^2 \rangle, \qquad d\mu = (z + s)_+\, e^{-z^2}\, dz \tag{43}$$

The function $\theta(s)$ is monotone on $s \in (-\infty, \infty)$ as one can verify by differentiation. Its typical values are:

$$\theta(0) = 1, \qquad \theta(s \to \infty) \to \tfrac{1}{2}, \qquad \theta(s \to -\infty) \approx s^2 \to \infty \tag{44}$$

Finally, we note that (see Eqs. (31), (32))

$$a\beta^3 = \frac{m_1^5}{m_2^4}\frac{I_2^4}{I_1^5} = \frac{1}{I_1}\frac{m_1^5}{m_2^4}\left(\frac{m_2^2}{m_1 m_3}\right)^2\left(1+\frac{I_3}{I_1}\right)^2 = \frac{m_1^3}{m_2^2}\frac{1}{I_1}\left(1+\frac{I_3}{I_1}\right)^2 \tag{45}$$

and present two "compact" formulae for $F(m_1, m_2, m_3)$ expressed through $I_n(s)$:

$$F(m_1, m_2, m_3) = m_1 \log\left[\frac{m_1^3(1+I_3/I_1)^2}{\pi e m_3^2 I_1}\, e^{-\theta(s)}\right] = m_1 \log\left[\frac{m_1^5 I_2^4}{\pi e m_2^4 I_1^5}\, e^{-\theta(s)}\right] \tag{46}$$

where all notations are defined by Eqs. (30), (32), (43). The practically convenient equalities (46) for $F(m_1, m_2, m_3)$ complete the solution of the problem stated at the beginning of this section.

5. ESTIMATES OF THE ENTROPY FLUX

We begin with obvious

Lemma 2. Assume that three moments

$$\int_{\mathbb{R}^3} dv\, f(v)\, v_x \begin{Bmatrix} 1 \\ v_x \\ |v|^2 \end{Bmatrix} = \begin{Bmatrix} \mathscr{L}_1 \\ \mathscr{L}_2 \\ \mathscr{L}_3 \end{Bmatrix} \tag{47}$$

of non-negative function $f(v)$: $\mathbb{R}^3 \to \mathbb{R}_+$ are given. Moreover one of two functions $\varphi_\pm(v)$: $\mathbb{R}^3_+ \to \mathbb{R}_+$

$$\begin{aligned} \varphi_+(v) &= f(v) \qquad \text{if} \quad v_x > 0 \\ \varphi_-(-v) &= f(v) \qquad \text{if} \quad v_x < 0 \end{aligned} \tag{48}$$

is also given, and

$$\int_{\mathbb{R}^3_+} dv\, v_x \varphi_\pm(v)[1 + |v|^2\, |\log \varphi_\pm(v)|] < \infty \tag{49}$$

Then the following inequalities are valid for the functional $\Psi(f)$ (11):

$$\begin{aligned} \Psi(f) &\leqslant \Psi_+(\varphi_+) - F(m_1^+ - \mathscr{L}_1, \mathscr{L}_2 - m_2^+, m_3^+ - \mathscr{L}_3) \\ \Psi(f) &\geqslant F(\mathscr{L}_1 + m_1^-, \mathscr{L}_2 - m_2^-, \mathscr{L}_3 + m_3^-) - \Psi_+(\varphi_-) \end{aligned} \tag{50}$$

where Ψ_+ and F are defined by Eqs. (20), (46), $m^\pm_{1,2,3}$ are given by equalities similar to Eq. (21).

Proof. It is already given in Section 3 (see inequalities (22), (25)), the only new element is the explicit expression (46) for $F(m_1, m_2, m_3)$ defined by Eq. (26). ∎

It is clear that Lemma 2 can be directly applied to the problem (1)–(3) (in a slab) in order to estimate unknown constant fluxes $\mathscr{L}_1, \mathscr{L}_2, \mathscr{L}_3$ (9) through given functions (2) and (3). To this goal, it is enough to combine the first and the second inequalities (50) at $x=0$ and $x=L$ respectively with the H-theorem (10). Thus we obtain

$$F(\mathscr{L}_1+m_1^-, \mathscr{L}_2-m_2^-, \mathscr{L}_3+m_3^-)-\Psi_+(\varphi_-) \\ \leqslant \Psi_+(\varphi_+)-F(m_1^+-\mathscr{L}_1, \mathscr{L}_2-m_2^+, m_3^+-\mathscr{L}_3) \tag{51}$$

This inequality is valid for arbitrary width L of the slab. One can find one more inequality by considering the hydrodynamic limit $L \to \infty$ (or, equivalently, the mean free path tends to zero whereas L is fixed). In such a case we assume that the asymptotic solution consists of two boundary layers at $x=0$ and $x=L$ and the intermediate constant Maxwellian with parameters (ρ, u, T) satisfying (12). Then

$$\Psi(M) = \rho u \log\left[\frac{\rho}{(2\pi e T)^{3/2}}\right] \tag{52}$$

and, by using again the H-theorem (10), and the inequality (51), we obtain two inequalities for unknown parameters (ρ, u, T):

$$F(\mathscr{L}_1+m_1^-, \mathscr{L}_2-m_2, \mathscr{L}_3+m_3^-)-\Psi_+(\varphi_-) \\ \leqslant \Psi(M) \leqslant \Psi_+(\varphi_+)-F(m_1^+-\mathscr{L}_1, \mathscr{L}_2-m_2^+, m_3^+-\mathscr{L}_3) \tag{53}$$

where $\mathscr{L}_{1,2,3}$ are expressed by Eq. (12).

Finally, we note that the parameters (ρ, u, T) of the Maxwellian at infinity in the half-space problem (1), (2), (4) obviously satisfy the second inequality (53), i.e.,

$$\Psi(M)+F(m_1^+-\mathscr{L}_1, \mathscr{L}_2-m_2^+, m_3^+-\mathscr{L}_3) \leqslant \Psi_+(\varphi_+) \tag{54}$$

with $\mathscr{L}_{1,2,3}$ given by Eq. (12).

Thus, we have proven the following

Theorem. We consider the boundary value problems (1)–(4) and assume that: (a) the operator $Q(f, f)$ satisfies conservation laws (5) and H-theorem (6); (b) the boundary functions $\varphi_\pm : \mathbb{R}_+^3 \to \mathbb{R}_+$ in (2), (3) satisfy (49); for each of the two boundary value problems there exists a non-negative solution $f(x, v)$ satisfying (7), (9), (10). Then

(i) parameters (ρ, u, T) of the Maxwellian (4) in the half-space problem (1), (2), (4) satisfy the inequality (54);

(ii) constant fluxes $(\mathscr{L}_1, \mathscr{L}_2, \mathscr{L}_3)$ in the slab problem (1)–(3) satisfy the inequality (51) for all $L > 0$;

(iii) parameters (ρ, u, T) of the asymptotic ($L \to \infty$ or mean free path tends to zero) Maxwellian (provided it exists) in the slab problem (1)–(3) satisfy two inequalities (53).

The proof is already given above.

All our inequalities define certain domains in three dimensional spaces of parameters $(\mathscr{L}_1, \mathscr{L}_2, \mathscr{L}_3)$ or (ρ, u, T). In the next section, we construct the domains numerically for a given function $\varphi_+(v)$ and compare them with well-known results (see the end of Section 1) obtained by direct numerical solution of BGK model and the Boltzmann equation.

The results can be reformulated in a stronger form, for brevity we do this below for the half-space problem only. Let the functional

$$\mathscr{D}(f) = -\int_0^\infty dx \int_{\mathbb{R}^3} dv[\log f(x, v)]\, Q(f, f) \geqslant 0 \tag{55}$$

denote the total entropy production. We rewrite the inequality (54) as

$$\begin{aligned} &\Delta[\rho, T, \theta, \varphi_+(v)] \\ &\qquad = \psi_+(\varphi_+) - F(m_1^+ - \mathscr{L}_1, \mathscr{L}_2 - m_2^+, m_3^+ - \mathscr{L}_3) - \psi(M) \geqslant 0 \end{aligned} \tag{56}$$

where $\theta = uT^{-1/2}$ is proportional to the Mach number, $\mathscr{L}_{1,2,3}(\rho, T, \theta)$ are given by Eq. (12).

What is actually proved above is the upper estimate of the total entropy production

$$0 \leqslant \mathscr{D}(f) \leqslant \Delta[\rho, T, \theta; \varphi_+(v)], \qquad \theta = uT^{-1/2} \tag{57}$$

through boundary conditions and parameters of the asymptotic Maxwellian. We omit simple calculations which show that

$$\Delta[\rho, T, \theta; \rho_0 T_0^{-3/2} \varphi_+(v T_0^{1/2})] = \rho_0 T_0^{1/2} \Delta\left[\frac{\rho}{\rho_0}, \frac{T}{T_0}, \theta; \varphi_+(v)\right] \tag{58}$$

for any positive constant ρ_0 and T_0. Therefore it is sufficient to consider boundary conditions normalised by equalities

$$\int_{\mathbb{R}^3_+} dv\, \varphi_+(v) = 1/2, \qquad \int_{\mathbb{R}^3_+} dv\, |v|^2\, \varphi_+(v) = 3/2 \tag{59}$$

Usual boundary conditions in the evaporation/condensation problem reduce in such a way to the normalised Maxwellian

$$\varphi_+(v) = (2\pi)^{-3/2} \exp\left(-\frac{|v|^2}{2}\right), \qquad v_x > 0 \tag{60}$$

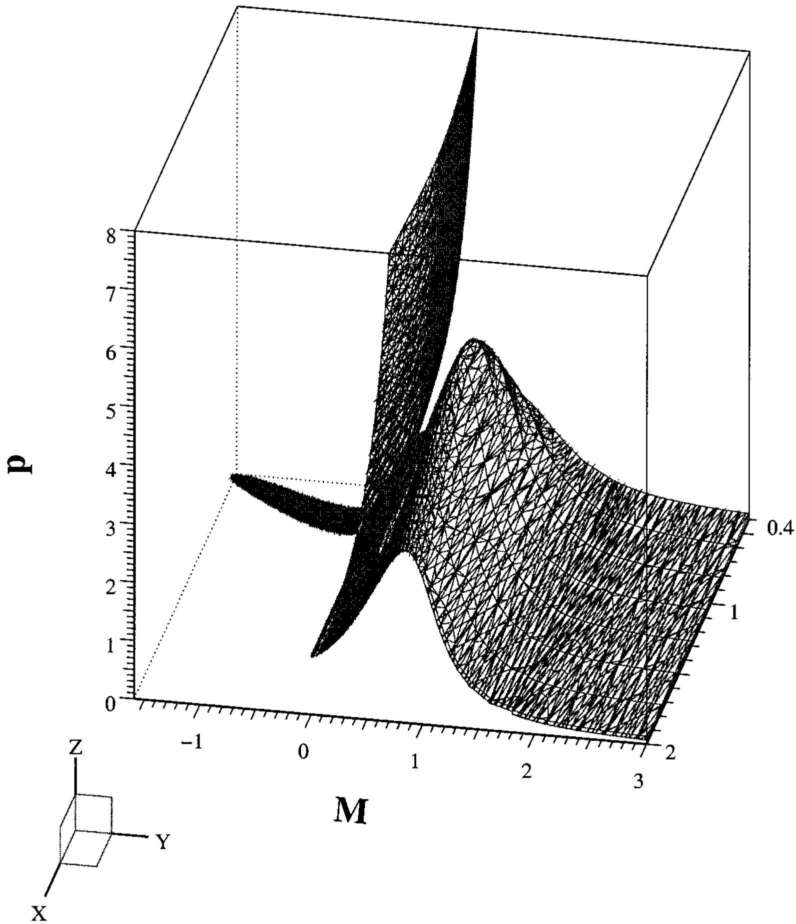

Fig. 1. Surface S defined by Eq. (65).

satisfying conditions (59). Just this case is studied in detail in the next section.

6. NUMERICAL RESULTS FOR HALF-SPACE PROBLEM

Elementary calculations lead in the special case (60) to equality

$$\Delta(\rho, T, \theta, \varphi_+) = \rho\theta\sqrt{T}\log\frac{(2\pi e T)^{3/2}}{\rho} - \frac{4+3\log 2\pi}{2\sqrt{2\pi}} - F(m_1, m_2, m_3) \tag{61}$$

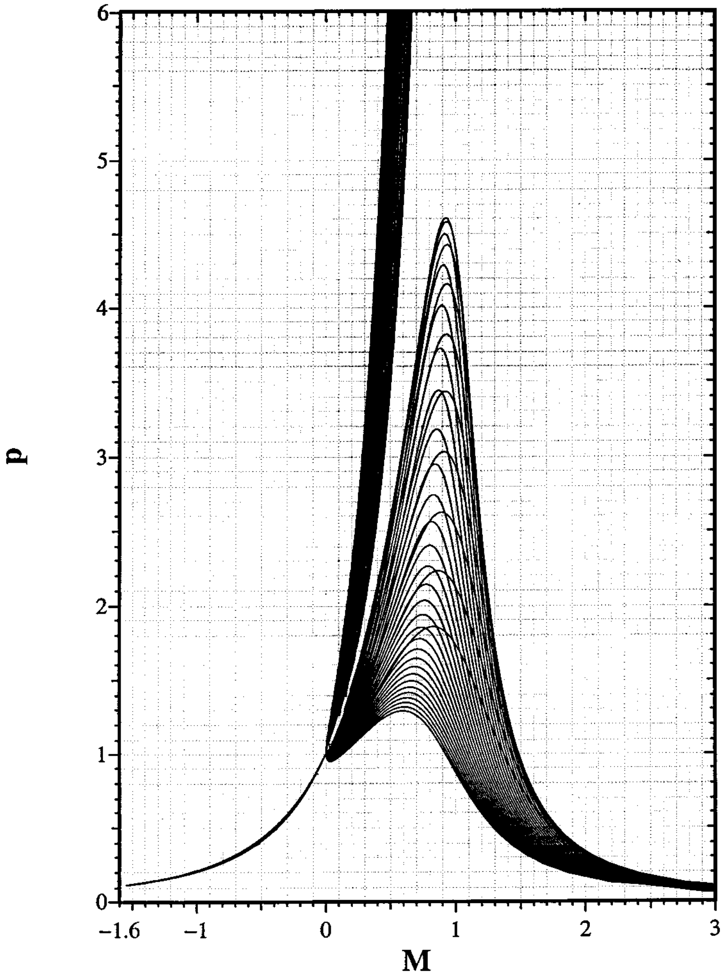

Fig. 2. The projection of the surface S on to the p-M plane.

where $F(\cdots)$ is defined by formula (46) with

$$m_1 = \frac{1}{\sqrt{2\pi}} - \rho\theta\sqrt{T}, \qquad m_2 = \rho T(1+\theta^2) - 1/2$$
$$m_3 = 2\sqrt{\frac{2}{\pi}} - \rho\theta T^{3/2}(5+\theta^2) \tag{62}$$

The inequality $\Delta \geqslant 0$ describes an allowed physical domain of positive entropy production in the three dimensional space of parameters $\rho > 0$, $T > 0$, $\theta \in (-\infty, \infty)$. In order to compare our results with results by Sone *et al.*,[1] we change variables (ρ, θ) to

$$p = \rho T, \qquad M = -\sqrt{\tfrac{3}{5}}\,\theta \tag{63}$$

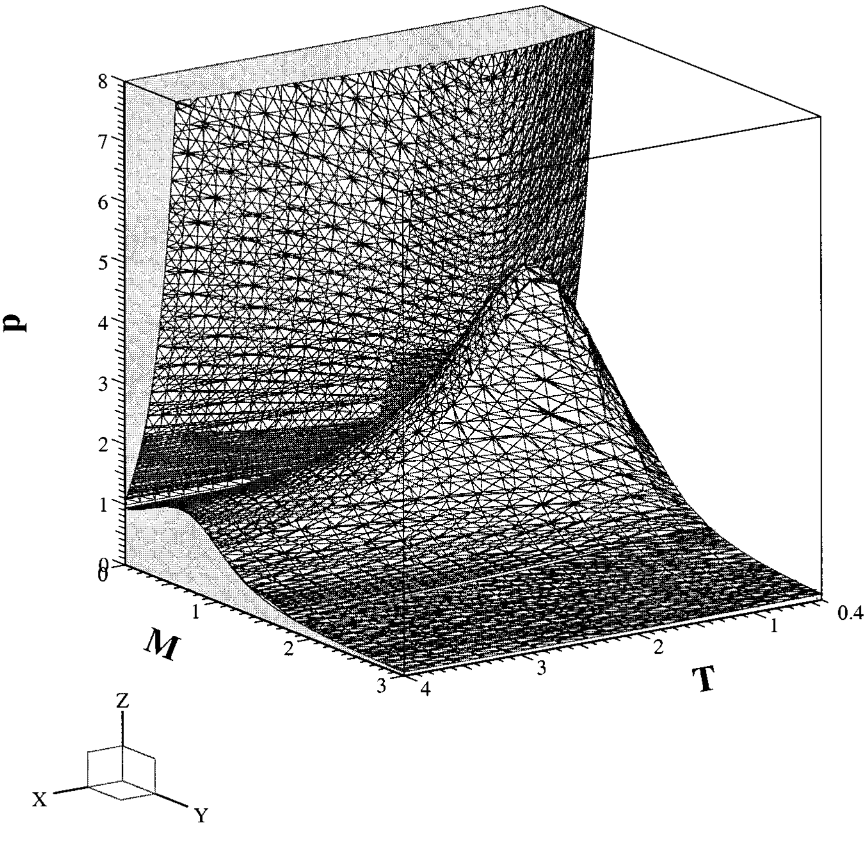

Fig. 3. The boundary surface S for condensation. The non-physical domain of negative entropy production is located below and behind S.

and rewrite Δ (61) as

$$\Delta(\rho, T, \theta, \varphi_+) = \Phi(p, T, M) \tag{64}$$

It is clear that $M > 0$ and $M < 0$ correspond to the condensation and evaporation problems respectively, whereas $|M|$ is the Mach number of the asymptotic Maxwellian. The surface

$$S : \Phi(p, T, M) = 0 \tag{65}$$

is a boundary of the physical space of (ρ, T, M) under additional conditions

$$\rho > 0, \qquad T > 0, \qquad -\infty < M < \infty, \qquad m_2 = \rho T(1 + \tfrac{5}{3}M^2) - \tfrac{1}{2} > 0$$

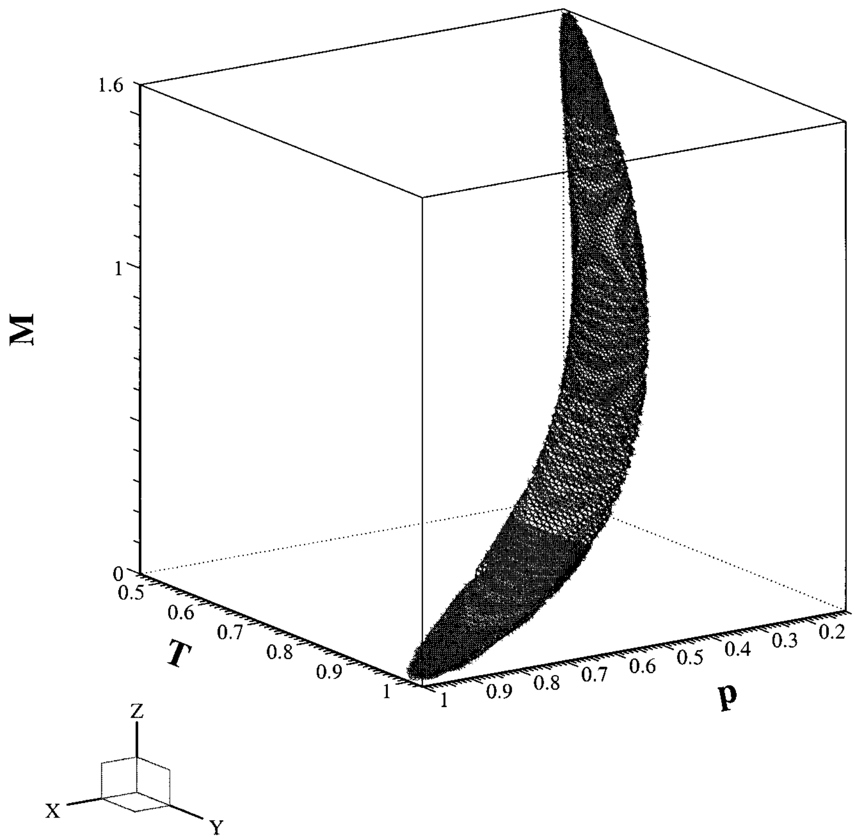

Fig. 4. Pipe-shaped boundary surface for evaporation.

The function $\Phi(\rho, T, M)$ is given by explicit formulae (except the parameter s defined by Eq. (33)). Therefore, it is relatively simple to construct the surface S (65) numerically and then to analyse it.

The resulting surface S is shown on Fig. 1 (we remind that two half-spaces $M > 0$ and $M < 0$ correspond to condensation and evaporation respectively). The surface consists of two qualitatively different parts ($M > 0$ and $M < 0$) which intersect at the only point $M = 0$, $\rho = T = 1$. The difference between the two parts is illustrated on Fig. 2 where a projection of S onto (p, M)-plane is shown. Figure 3 shows the condensation part ($M > 0$) of S in more detail. This part tends to a vertical plane $M = M_* \approx 0.8$ for $p \to \infty$. It is clear that such asymptotics corresponds to the absorption boundary conditions $\varphi_+ = 0$ for which the Mach number M becomes a unique parameter of the problem. Thus, there is no bounded solution of the half space problem with $\varphi_+ = 0$ and $M < M_* \approx 0.8$.

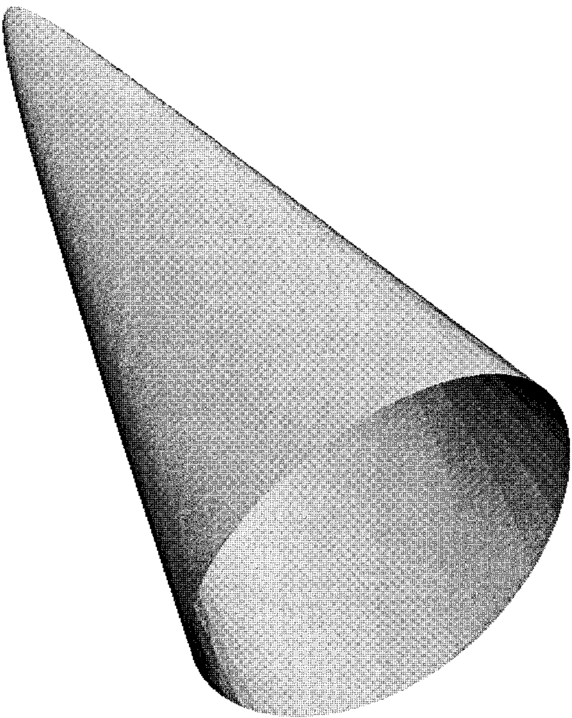

Fig. 5. The shape of S for M close to M_{cr}.

Figure 4 shows the evaporation part ($M<0$) of S. This part of S is closed and almost flat (look at its projection onto (p, M)-plane on Fig. 2). Figure 4 shows that there is no solution of the evaporation problem with Maxwellian boundary conditions (60) if $|M| > M_{cr} \simeq 1.6$. In a smaller scale this part ($M \simeq M_{cr}$) of S is shown on Fig. 5.

Numerical solutions of the Boltzmann and BGK equations[1] show that apparently $M_* = M_{cr} = 1$ ($M_{cr} = 1$ was conjectured by Cercignani[7] and supported at the linearised level by rigorous results obtained in ref. 3). Our simple and rough approach based on entropy inequalities leads to quite realistic rigorous estimates $M_* > 0.8$ and $M_{cr} < 1.6$ which do not

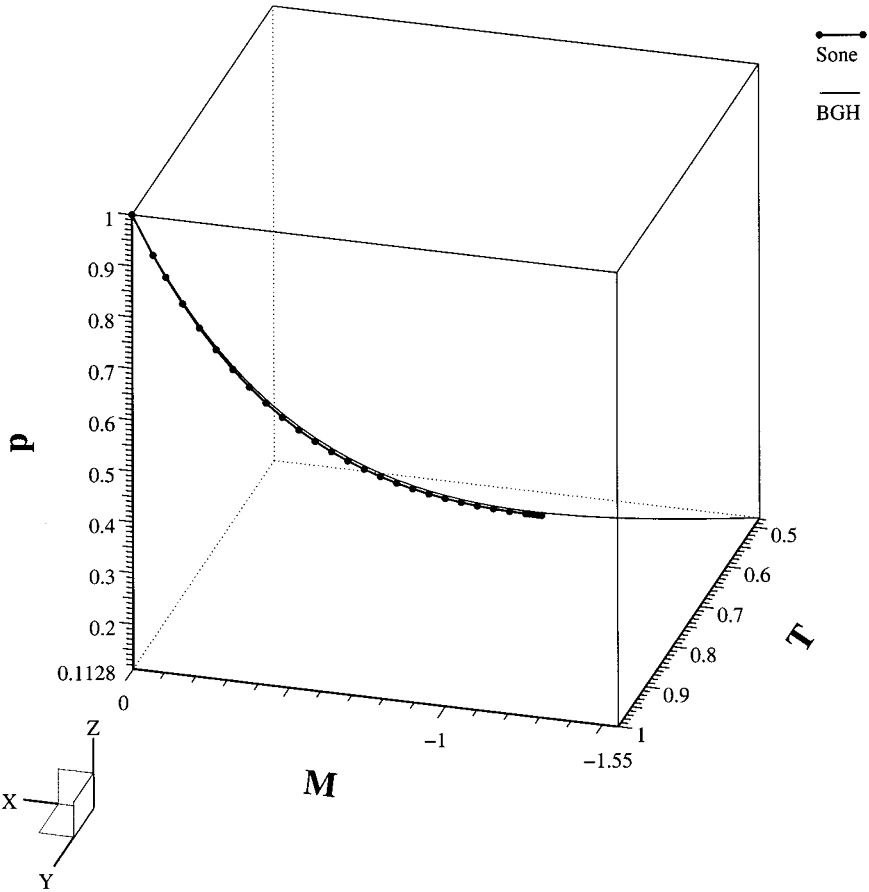

Fig. 6. Evaporation. 3-d picture of the maximal entropy production line compared with the numerical results by Sone.[1]

depend on specific form of the collision integrals. This can be considered as by product rigorous results of the present paper.

Until now all our considerations were quite rigorous (a priori estimates based on entropy inequalities), we have studied only the surface S of zero entropy production (65). On the other hand, we know that there exists the evaporation curve $p = p(M)$, $T = T(M)$ $(-1 \leqslant M \leqslant 0$ in our notations) and the condensation surface $p = p(M, T)$ $(0 \leqslant M \leqslant 1)$ which correspond to true solutions of the half-space problem (see the end of Section 2). How to find them?

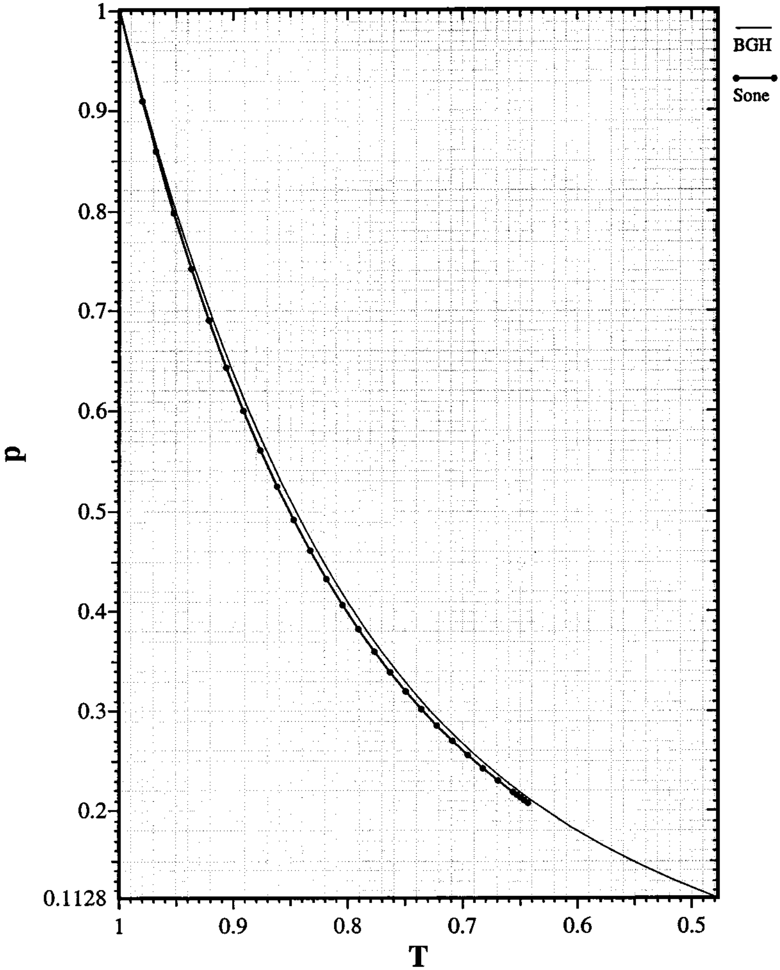

Fig. 7. Evaporation. T-p projection of the maximal entropy production line.

Let us consider the inequality (57) for the total entropy production

$$0 \leqslant D(f) \leqslant \Phi(p, T, M)$$

in notations (63), (64). Suppose that $-1 \leqslant M \leqslant 0$ (evaporation) is fixed. It is clear from Fig. 4 that there exist $p = p_0(M)$ and $T = T_0(M)$ such that

$$\Phi[p_0(M), T_0(M), M] = \mathrm{Max}_{p,\,T}\, \Phi(p, T, M), \qquad -1 \leqslant M \leqslant 0$$

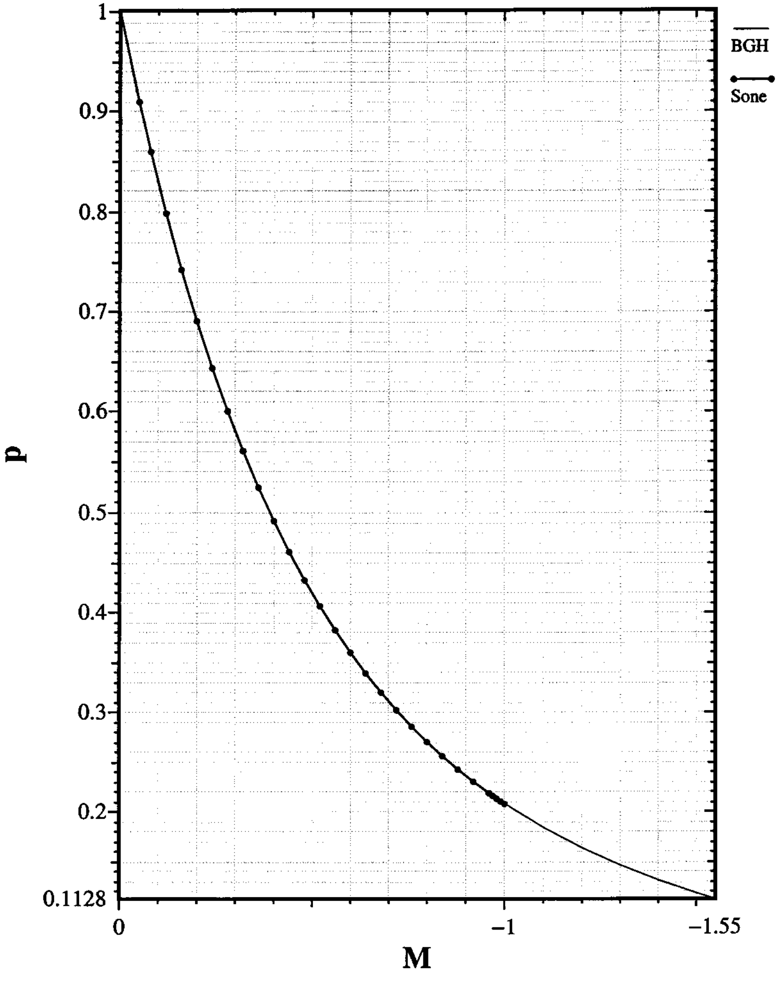

Fig. 8. Evaporation. M-p projection of the maximal entropy production line.

To prove this rigorously, it is enough to show that $\Phi(p, T, M)$ is continuous. We construct in such a way a curve

$$p = p_0(M), \qquad T = T_0(M), \qquad M \in [-M_{cr}, 0], \qquad M_{cr} \approx 1.6$$

of maximal entropy production and compare this curve (for $|M| \leqslant 1$) with the evaporation curve tabulated by Sone *et al.*[1,2] on the basis of a large number of numerical solutions of BGK-equation. Surprisingly, the two curves coincide with accuracy up to a few percents! A comparison of two curves is shown on Fig. 6, Fig. 7 (pT-projection), Fig. 8 (pM-projection) and Fig. 9, where the boundary surface S is also slightly sketched. For reader's convenience, we denote by M a "true" (positive) Mach number on Figs. 6–8.

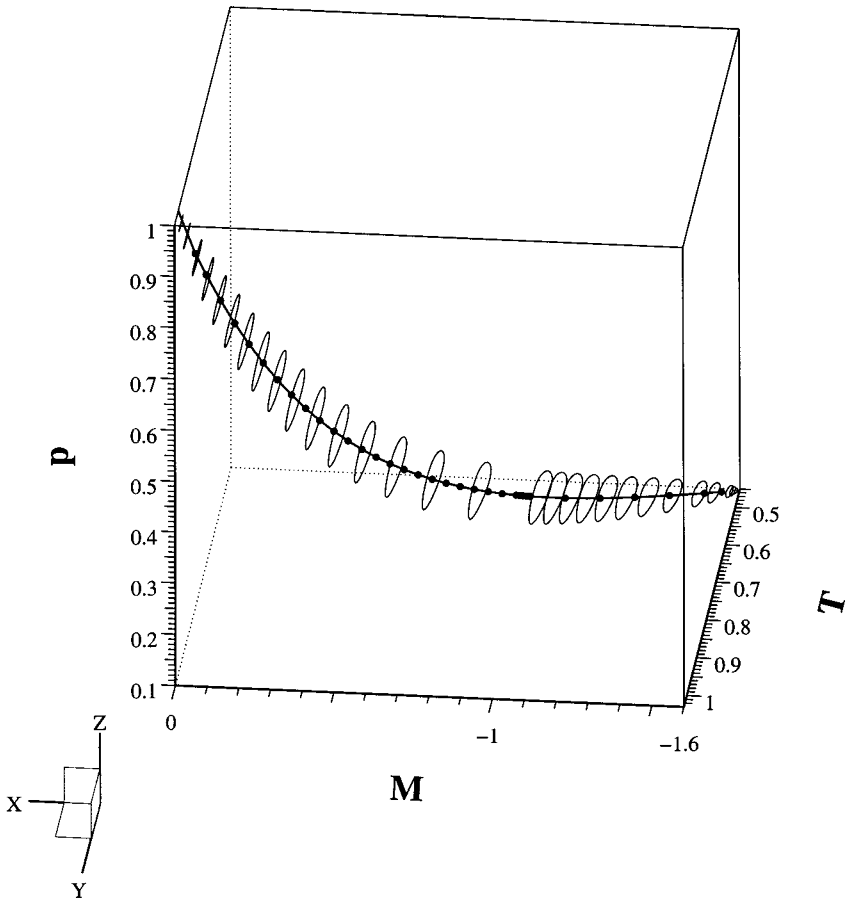

Fig. 9. Evaporation. Maximal entropy production line and sections of the boundary surface.

A similar procedure can be used for the condensation problem ($M \geqslant 0$) if we fix two values $M > 0$ and $T > 0$. Then there exist $p = p_*(T, M)$ such that

$$\Phi[p_*(T, M), T, M] = \mathrm{Max}_p\, \Phi(p, T, M), \qquad M > 0$$

Therefore we obtain for $M > 0$ the surface

$$p = p_*(T, M)$$

of maximal entropy production (Fig. 10). This surface is qualitatively very closed to the condensation surface by Sone *et. al.*,[1] but the quantitative difference (of order of 10%) is less impressive in this case.

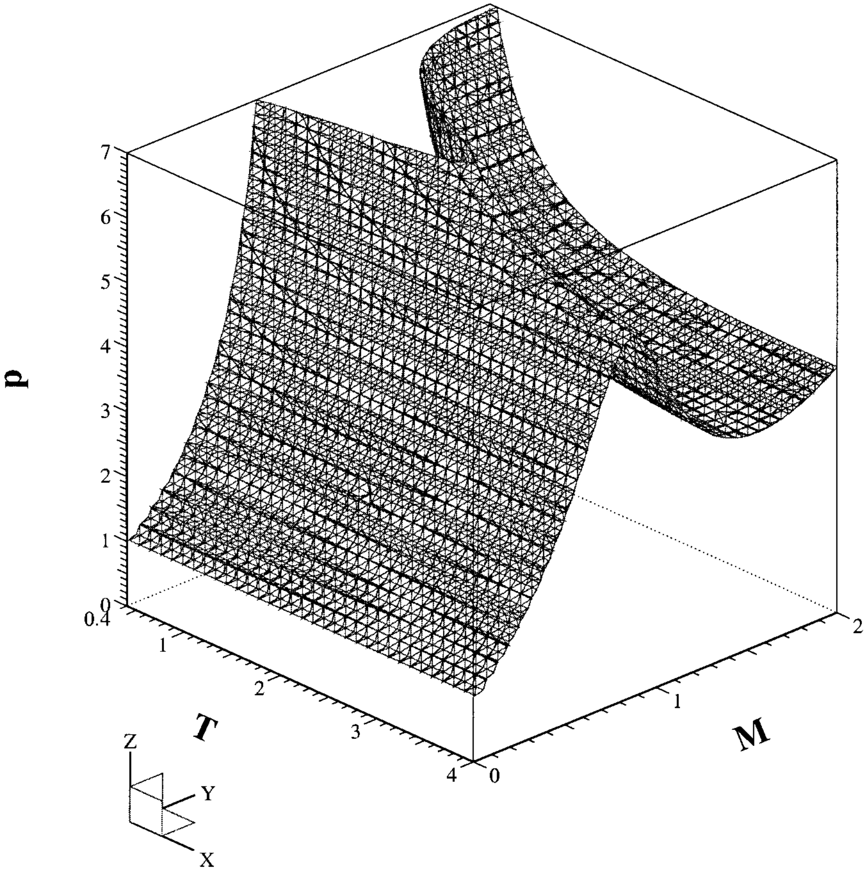

Fig. 10. Condensation. Maximal entropy production surface.

Anyway, our study clearly shows that solutions of the half-space problem (at least, for BGK-model) approximately satisfy a variational principle of maximal total entropy production.

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