Kinetic theory analysis of a binary mixture reacting on a surface

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ABSTRACT

A mixture of two rarefied gases is considered between two parallel planes. On one side of the domain evaporation/condensation conditions are imposed, while on the other side accommodation at the temperature of the wall and chemical equilibrium conditions are considered. The small Knudsen number asymptotics of this problem is performed at the formal level, and fluid-dynamic equations are derived and then solved numerically. We discuss the possible appearance of a ghost effect in this situation.

1 Introduction

Kinetic theory of gases plays an important role in microfluidics, since the mean free path of gas molecules is comparable to the characteristic length in micro-scale systems and thus the gas is not in a local equilibrium state [5, 6, 7, 8]. On the other hand, one expects the validity of fluid-dynamic (or macroscopic) approach when the mean free path is much shorter than the

characteristic length, i.e., near continuum regime including the continuum (or fluid-dynamic) limit. In general, however, it is not clear from macroscopic or phenomenological considerations what type of fluid-dynamic equations and boundary conditions are appropriate when surface phenomena, such as phase transition and chemical reaction, take place on the boundary. Most of such problems can be solved by considering the continuum limit and its neighborhood on the basis of kinetic theory. In other words, careful asymptotic analyses for small values of the Knudsen number (the ratio of the mean free path to the characteristic length) based on the Boltzmann equation and its kinetic boundary condition [3, 4, 9, 12, 13] lead to fluid-dynamic-type equations and their boundary conditions appropriate to the considered physical situations (see [12]). A good example is the fluid-dynamic-type systems for the vapor flows around its condensed phases, on the surface of which evaporation and condensation of the vapor are taking place (see [12, 13]). These fluid-dynamic-type systems have been extended to the case where another gas that neither evaporates nor condenses (noncondensable gas) is contained in the domain (e.g., [1, 21, 22, 23]). For instance, the behavior of a mixture of vapors and noncondensable gases in the continuum limit has been studied systematically in a one-dimensional setting (that is, for the mixture confined between two parallel planes) in [1, 22, 23]. It should also be mentioned that a mathematical study of the same setting was carried out recently [2].

In the present paper, we wish to extend somewhat the study in [22, 23] by considering the possibility that two gases can react at (part of) the boundary of the domain. We present here the simplest possible case when such a situation occurs. That is, we consider two species A, B of gases evolving in the domain $[0, D] \times \mathbb{R}^2$, which undergo a reversible reaction $A \rightleftharpoons B$ (or $M + A \rightleftharpoons N + B$, where M, N are in excess and are not considered in the modeling), supposed to occur only at the boundary $X_1 = 0$ ($X_2, X_3 \in \mathbb{R}$) and to be instantaneous. After having performed the reaction, the molecules are reflected diffusively (still at $X_1 = 0$). On the other boundary (that is, $X_1 = D$), evaporation/condensation conditions are imposed for both species A and B.

We are looking for solutions of the steady Boltzmann equation (including hard-sphere type collisions for couples of molecules $A - A$, $A - B$ and $B - B$) with the boundary condition described above. The set of kinetic equations (and boundary conditions) modeling the mixture is presented in section 2

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in its original form, and then in section 3 in non-dimensional form. The asymptotic analysis when the Knudsen number tends to 0 is performed in section 4. We obtain in this way a set of ODEs which models the mixture at the fluid-dynamical level. When the molecules of species A and B have same radius and same mass, this set of ODEs becomes particularly simple and can be solved explicitly. This is done in section 5. It is however not easy to extend this explicit computation in the more general case when the mass and/or the radius of the molecules of species A and B are different. Once all the possible explicit integrals of the ODEs have been used, one ends up with a boundary value problem for two first-order ODEs. The computations describing how to reach this problem are described in section 6. The final section 7 is devoted to the presentation of the numerical procedure and of typical results for the system of ODEs obtained in section 6. We use for this the database on transport coefficients in binary gas mixtures presented in [24]. We also comment there the appearance of a ghost effect [13] (that does not occur in the case of equal masses and radii).

2   Presentation of the model

We use here the notations of [22] for our presentation of the problem at the kinetic level. We denote by $F^\alpha := F^\alpha(X_1, \xi) \geq 0$ (with $\alpha = A$ or B) the number density of molecules of species α which at point $X_1 \in [0, D]$ ($D > 0$) have velocity ξ. The steady Boltzmann equation for this problem writes

$$\xi_1 \frac{\partial F^\alpha}{\partial X_1} = \sum_{\beta = A, B} J^{\beta\alpha}(F^\beta, F^\alpha), \tag{1}$$

where $J^{\beta\alpha}$ is the collision operator for hard-sphere interactions between molecules of species β, α :

$$J^{\beta\alpha}(F, G)(X_1, \xi) = \frac{(d^{\beta\alpha})^2}{2} \int_{\omega \in S^2} \int_{\xi_* \in \mathbb{R}^3} \tag{2}$$

$$\left(F(X_1, \xi_*^{\beta\alpha}) \, G(X_1, \xi^{\beta\alpha}) - F(X_1, \xi_*) \, G(X_1, \xi) \right) |\omega \cdot (\xi_* - \xi)| \, d\xi_* d\omega,$$

the pre-collisional velocities $\xi_*^{\beta\alpha}$ and $\xi^{\beta\alpha}$ are given by the formulas

$$\xi^{\beta\alpha} = \xi + \frac{\mu^{\beta\alpha}}{m^\alpha} \left[\omega \cdot (\xi_* - \xi) \right] \omega, \qquad \xi_*^{\beta\alpha} = \xi_* - \frac{\mu^{\beta\alpha}}{m^\beta} \left[\omega \cdot (\xi_* - \xi) \right] \omega, \tag{3}$$

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where m^α is the mass of a molecule of species α, and $\mu^{\beta\alpha} = \frac{2m^\alpha m^\beta}{m^\alpha + m^\beta}$ is the reduced mass. At last, in (2) $d^{\beta\alpha} = (d^\alpha + d^\beta)/2$, where d^α is the diameter of a molecule of species α, is the mean diameter.

Then, we impose on the wall $X_1 = D$ the following evaporation/condensation boundary condition:

$$F^\alpha(D, \xi) = \frac{n_R^\alpha}{(2\pi k T_R / m^\alpha)^{3/2}} \, e^{-\frac{m^\alpha |\xi|^2}{2kT_R}}, \qquad \text{when} \qquad \xi_1 \le 0, \qquad (4)$$

where k is Boltzmann's constant, T_R is the temperature of the wall $x_1 = D$, and $n_R^\alpha = p_R^\alpha/(kT_R)$, where p_R^α is the pressure given by the modified Raoult's law (Cf. [22]).

The main novelty of this work is that we impose on the wall $X_1 = 0$ a specific boundary condition, which expresses the fact that through a (infinitely fast) chemical reversible reaction, species A and B are at chemical equilibrium on this wall. Therefore, there exists a fixed number $a \in]0, 1[$ (proportion of molecules of species A at chemical equilibrium given by the mass action law) such that when $\xi_1 > 0$, defining the incoming flux of molecules

$$J = \int_{\xi \in \mathbb{R}^3, \xi_1 < 0} (-\xi_1) \left[F^A(0, \xi) + F^B(0, \xi) \right] d\xi,$$

one has

$$F^A(0, \xi) = \frac{a}{2\pi} \frac{\sqrt{m^B}}{a\sqrt{m^B} + (1-a)\sqrt{m^A}} \left(\frac{m^A}{kT_L} \right)^2 J \exp(-\frac{m^A |\xi|^2}{2kT_L}), \qquad (5)$$

$$F^B(0, \xi) = \frac{1-a}{2\pi} \frac{\sqrt{m^A}}{a\sqrt{m^B} + (1-a)\sqrt{m^A}} \left(\frac{m^B}{kT_L} \right)^2 J \exp(-\frac{m^B |\xi|^2}{2kT_L}).$$

Those formulas are best understood in two special cases:

1. When $a = 1$ (resp. $a = 0$), the reaction will in fact become the irreversible reaction $B \to A$ (resp. $A \to B$) and only molecules of species A (resp. B) are emitted, with the usual law of diffuse reflection.

2. When the masses m^A and m^B are equal, it is easy to see that the proportion of molecules of species A emitted (with any velocity) by the wall is a and corresponds to the proportion of molecules of species A present on the wall.

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In this boundary condition, the net flux of molecules across the boundary is zero ($\int_{\xi \in \mathbb{R}^3} \xi_1 \left[F^A(0,\xi) + F^B(0,\xi) \right] d\xi = 0$) whereas that of the mass does not vanish (except when $m^a = m^B$).

Finally, the problem that we consider at the kinetic level is (1)-(5).

3 Non dimensional form of the equations and macroscopic quantities

Introducing (in addition to the parameters already considered) various reference quantities (including the mean free path), we end up with the following non dimensional form of the equation (most of the computations leading to these equations are done in [22]).

The function $f^\alpha(x,\zeta)$ is the unknown and depends upon the new variables $x \in [0,1]$ and $\zeta \in \mathbb{R}^3$. It satisfies

$$\zeta_1 \frac{\partial f^\alpha}{\partial x_1} = \frac{2}{\sqrt{\pi}} Kn^{-1} \sum_{\beta=A,B} K^{\beta\alpha} \, \hat{J}^{\beta\alpha}(f^\beta, f^\alpha), \tag{6}$$

with

$$\hat{J}^{\beta\alpha}(f,g)(x,\zeta) = \frac{1}{4\sqrt{2\pi}} \int_{\omega \in S^2} \int_{\zeta_* \in \mathbb{R}^3} \tag{7}$$

$$\left(f(x,\zeta_*^{\beta\alpha}) \, g(x,\zeta^{\beta\alpha}) - f(x,\zeta_*) \, g(x,\zeta) \right) \left| \omega \cdot (\zeta_* - \zeta) \right| d\zeta_* d\omega,$$

and

$$\zeta^{\beta\alpha} = \zeta + \frac{\hat{\mu}^{\beta\alpha}}{\hat{m}^\alpha} \left[\omega \cdot (\zeta_* - \zeta) \right] \omega, \qquad \zeta_*^{\beta\alpha} = \zeta_* - \frac{\hat{\mu}^{\beta\alpha}}{\hat{m}^\beta} \left[\omega \cdot (\zeta_* - \zeta) \right] \omega. \tag{8}$$

Here, $K^{\beta\alpha}$, $\hat{\mu}^{\beta\alpha}$, $\hat{m}^\alpha$, Kn (Knudsen number) are non dimensional parameters whose precise definition can be found in [22].

The boundary condition at $x = 1$ becomes in non dimensional form

$$f^\alpha(1,\zeta) = \frac{\hat{p}_{II}^\alpha}{\hat{T}_{II}^{5/2}} \left(\frac{\hat{m}^\alpha}{\pi} \right)^{3/2} e^{-m^\alpha \frac{|\zeta|^2}{\hat{T}_{II}}} \qquad \text{for} \qquad \zeta_1 \le 0, \qquad \alpha = A, B \tag{9}$$

while at $x = 0$, by defining

$$\hat{J} = \int_{\zeta \in \mathbb{R}^3, \zeta_1 < 0} (-\zeta_1) \left[f^A(0, \zeta) + f^B(0, \zeta) \right] d\zeta,$$

it becomes (for $\zeta_1 > 0$)

$$f^A(0, \zeta) = \frac{2a}{\pi} \frac{\sqrt{\hat{m}^B}}{a\sqrt{\hat{m}^B} + (1-a)\sqrt{\hat{m}^A}} (\hat{m}^A)^2 \, \hat{J} \, e^{-\hat{m}^A |\zeta|^2}, \qquad (10)$$

$$f^B(0, \zeta) = \frac{2(1-a)}{\pi} \frac{\sqrt{\hat{m}^A}}{a\sqrt{\hat{m}^B} + (1-a)\sqrt{\hat{m}^A}} (\hat{m}^B)^2 \, \hat{J} \, e^{-\hat{m}^B |\zeta|^2}.$$

Here, T_{II} ($= \frac{T_R}{T_L}$ in [22]) and $\hat{p}_{II}^{\alpha}$ ($= \frac{n_R^{\alpha}}{n_0} T_{II}$ in [22], where n_0 is a reference molecular number density) are two extra non dimensional parameters.

Finally, we present the macroscopic quantities in non dimensional form:

$$\hat{n}^{\alpha} := \int_{\zeta \in \mathbb{R}^3} f^{\alpha}(x, \zeta) \, d\zeta, \qquad \hat{n}^{\alpha} \hat{u}_i^{\alpha} := \int_{\zeta \in \mathbb{R}^3} \zeta_i \, f^{\alpha}(x, \zeta) \, d\zeta, \quad i = 1, .., 3 \quad (11)$$

$$\frac{3}{2} \hat{n}^{\alpha} \hat{T}^{\alpha} := \int_{\zeta \in \mathbb{R}^3} \hat{m}^{\alpha} |\zeta - \hat{u}^{\alpha}(x)|^2 \, f^{\alpha}(x, \zeta) \, d\zeta.$$

We also define the mean velocity:

$$\left(\sum_{\alpha = A, B} \hat{m}^{\alpha} \, \hat{n}^{\alpha} \right) \hat{u}_i := \sum_{\alpha = A, B} \hat{m}^{\alpha} \, \hat{n}^{\alpha} \hat{u}_i^{\alpha}. \qquad (12)$$

4 Hilbert expansion

We now expand the solution f^{α} of problem $(6) - (10)$ in powers of $\varepsilon = \frac{\sqrt{\pi}}{2} Kn$, in order to investigate the behavior of the solution in the case when the gas is not rarefied any more.

We introduce for this the power series (at the formal level)

$$f^{\alpha} = f_{H0}^{\alpha} + \varepsilon \, f_{H1}^{\alpha} + \varepsilon^2 \, f_{H2}^{\alpha} + \dots, \qquad (13)$$

and we use the same notations (that is $\hat{n}_{H0}^{\alpha}$, $\hat{u}_{iH0}^{\alpha}$, etc.) for the corresponding macroscopic quantities.

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Identifying the terms of the same order in ε in formula (6), one ends up with the following hierarchy of equations (all linear, except the first one):

$$\sum_{\beta=A,B} K^{\beta\alpha} \, \hat{J}^{\beta\alpha}(f_{H0}^{\beta}, f_{H0}^{\alpha}) = 0, \tag{14}$$

$$\sum_{\beta=A,B} K^{\beta\alpha} \left[\hat{J}^{\beta\alpha}(f_{H0}^{\beta}, f_{H1}^{\alpha}) + \hat{J}^{\beta\alpha}(f_{H1}^{\beta}, f_{H0}^{\alpha}) \right] = \zeta_1 \frac{\partial f_{H0}^{\alpha}}{\partial x}, \tag{15}$$

$$\sum_{\beta=A,B} K^{\beta\alpha} \left[\hat{J}^{\beta\alpha}(f_{H0}^{\beta}, f_{Hm}^{\alpha}) + \hat{J}^{\beta\alpha}(f_{Hm}^{\beta}, f_{H0}^{\alpha}) \right] =$$

$$\zeta_1 \frac{\partial f_{H(m-1)}^{\alpha}}{\partial x} - \sum_{n=1}^{m-1} \sum_{\beta=A,B} K^{\beta\alpha} \, \hat{J}^{\beta\alpha}(f_{Hn}^{\beta}, f_{H(m-n)}^{\alpha}), \qquad m \geq 2. \tag{16}$$

Thanks to eq. (14), we obtain (this is the case of equality of Boltzmann's H theorem for mixtures) for f_{H0}^{α} a Maxwellian function of ζ whose parameters (velocity $\hat{u}_{1H0}$ and temperature $\hat{T}_{H0}$) are the same for the two species (and are therefore not written with the superscript α). This means that

$$f_{H0}^{\alpha}(x, \zeta) = \hat{n}_{H0}^{\alpha}(x) \left(\frac{\hat{m}^{\alpha}}{\pi \hat{T}_{H0}(x)} \right)^{3/2} e^{-\frac{\hat{m}^{\alpha}}{\hat{T}_{H0}(x)} (|\zeta_1 - \hat{u}_{1H0}(x)|^2 + |\zeta_2|^2 + |\zeta_3|^2)}. \tag{17}$$

Then, we observe that the compatibility condition for solving eq. (15) is related to the conservation of number density (of each species), of global momentum, and global energy for the kernel $\hat{J}^{\beta\alpha}$. It reads

$$\int_{\zeta \in \mathbb{R}^3} \zeta_1 \frac{\partial f_{H0}^{\alpha}}{\partial x} \, d\zeta = 0 \ (\alpha = A, B), \qquad \sum_{\alpha=A,B} \int_{\zeta \in \mathbb{R}^3} \zeta_1 \left(\hat{m}^{\alpha} \zeta_1, \hat{m}^{\alpha} |\zeta|^2 \right) \frac{\partial f_{H0}^{\alpha}}{\partial x} \, d\zeta = 0, \tag{18}$$

and can be rewritten (in terms of macroscopic quantities)

$$\frac{d}{dx} (\hat{n}_{H0}^{\alpha} \, \hat{u}_{1H0}) = 0, \qquad \alpha = A, B, \tag{19}$$

$$\frac{d}{dx} \left(\frac{1}{2} (\hat{n}_{H0}^A + \hat{n}_{H0}^B) \, \hat{T}_{H0} + [\hat{m}^A \, \hat{n}_{H0}^A + \hat{m}^B \, \hat{n}_{H0}^B] \, \hat{u}_{1H0}^2 \right) = 0, \tag{20}$$

$$\frac{d}{dx} \left(\{ [\hat{m}^A \, \hat{n}_{H0}^A + \hat{m}^B \, \hat{n}_{H0}^B] \, \hat{u}_{1H0}^2 + \frac{5}{2} (\hat{n}_{H0}^A + \hat{n}_{H0}^B) \, \hat{T}_{H0} \} \, \hat{u}_{1H0} \right) = 0. \tag{21}$$

Next we observe that thanks to the boundary condition (10), the flux of molecules (of both species A, B) at $x = 0$ is

$$\sum_{\alpha=A,B} \hat{n}^\alpha(0)\, \hat{u}_1^\alpha(0) = \sum_{\alpha=A,B} \int_{\zeta \in \mathbb{R}^3} \zeta_1\, f^\alpha(0, \zeta)\, d\zeta \tag{22}$$

$$= \sum_{\alpha=A,B} \int_{\zeta \in \mathbb{R}^3, \zeta_1 < 0} \zeta_1\, f^\alpha(0, \zeta)\, d\zeta + \frac{2}{\pi} \hat{J}$$

$$\times \int_{\zeta \in \mathbb{R}^3, \zeta_1 > 0} \left[\frac{a\,(\hat{m}^A)^2 \sqrt{\hat{m}^B}\, e^{-\hat{m}^A |\zeta|^2} + (1-a)\,(\hat{m}^B)^2 \sqrt{\hat{m}^A}\, e^{-\hat{m}^B |\zeta|^2}}{a\sqrt{\hat{m}^B} + (1-a)\sqrt{\hat{m}^A}} \right] \zeta_1\, d\zeta = 0.$$

In particular, the zero-th order of the expansion of this quantity is 0 so that

$$\sum_{\alpha=A,B} \hat{n}^\alpha_{H0}(0)\, \hat{u}^\alpha_{1H0}(0) = \left[\sum_{\alpha=A,B} \hat{n}^\alpha_{H0}(0) \right] \hat{u}_{1H0}(0) = 0. \tag{23}$$

Then, eq. (19) together with the boundary condition (23) implies that

$$\forall x \in [0, 1], \qquad \hat{u}_{1H0}(x) = 0. \tag{24}$$

As a consequence, the system of fluid-dynamic equations (19) – (21) reduces to

$$\frac{d}{dx} \left[(\hat{n}^A_{H0} + \hat{n}^B_{H0})\, \hat{T}_{H0} \right] = 0. \tag{25}$$

In order to obtain a set of equations for $\hat{n}^\alpha_{H0}$ and $\hat{T}_{H0}$, we need to solve the compatibility conditions given by eq. (16) for $m = 2$. This leads to (Cf. [20], and Appendix A in [22])

$$\frac{d}{dx} (\hat{n}^\alpha_{H0}\, \hat{u}^\alpha_{1H1}) = 0, \qquad \alpha = A, B \tag{26}$$

$$\frac{d}{dx} \left(-\hat{\lambda}\, \hat{T}^{1/2}_{H0}\, \frac{d\hat{T}_{H0}}{dx} + k_T\, (\hat{n}^A_{H0} + \hat{n}^B_{H0})\, \hat{T}_{H0}\, (\hat{u}^A_{1H1} - \hat{u}^B_{1H1}) + \frac{5}{2}\, \hat{T}_{H0}\, [\hat{n}^A_{H0}\, \hat{u}^A_{1H1} + \hat{n}^B_{H0}\, \hat{u}^B_{1H1}] \right) = 0. \tag{27}$$

This system is closed by the use of (25) and by the formula (Cf. [20] again)

$$\hat{u}^A_{1H1} - \hat{u}^B_{1H1} = -\hat{T}^{1/2}_{H0}\, \hat{D}_{AB} \left(\frac{\hat{n}^A_{H0} + \hat{n}^B_{H0}}{\hat{n}^A_{H0}\, \hat{n}^B_{H0}} \right) \left\{ \frac{d}{dx} \left(\frac{\hat{n}^A_{H0}}{\hat{n}^A_{H0} + \hat{n}^B_{H0}} \right) + \frac{k_T}{\hat{T}_{H0}}\, \frac{d\hat{T}_{H0}}{dx} \right\}. \tag{28}$$

Here, $\hat{\lambda}$, k_T and $\hat{D}_{AB}$ are functions of $\frac{\hat{n}_{H0}^A}{\hat{n}_{H0}^A + \hat{n}_{H0}^B}$ whose functional forms are not explicit [22]. Using now eq. (22) at first order, we see that

$$\sum_{\alpha=A,B} \hat{n}_{H0}^\alpha(0)\, \hat{u}_{1H1}^\alpha(0) = 0.$$

Then, thanks to eq. (26), we obtain

$$\forall x \in [0,1], \qquad \sum_{\alpha=A,B} \hat{n}_{H0}^\alpha(x)\, \hat{u}_{1H1}^\alpha(x) = 0. \tag{29}$$

We can therefore simplify (27) in

$$\frac{d}{dx}\left(-\hat{\lambda}\,\hat{T}_{H0}^{1/2}\,\frac{d\hat{T}_{H0}}{dx} + k_T\,(\hat{n}_{H0}^A + \hat{n}_{H0}^B)\,\hat{T}_{H0}\,(\hat{u}_{1H1}^A - \hat{u}_{1H1}^B)\right) = 0. \tag{30}$$

The boundary conditions corresponding to the system (25), (26), and (30) are obtained by matching (17) and (24) with (9) and (10). They are

$$\hat{T}_{H0}(0) \;=\; 1, \qquad \frac{\hat{n}_{H0}^A(0)}{\hat{n}_{H0}^A(0) + \hat{n}_{H0}^B(0)} = a,$$

$$\hat{T}_{H0}(1) \;=\; \hat{T}_{II} \qquad \hat{n}_{H0}^\alpha(1) = \frac{\hat{p}_{II}^\alpha}{\hat{T}_{II}} \;\; (\alpha = A, B). \tag{31}$$

5   Coloring problem

It happens that the system described above, in the special case when masses and diameters of molecules are equal, can be solved explicitly. This is due to the fact that in this case (sometimes called the coloring problem), $k_T = 0$, and $\hat{D}_{AB}$, $\hat{\lambda}$ do not depend on $\frac{\hat{n}_{H0}^A}{\hat{n}_{H0}^A + \hat{n}_{H0}^B}$ [21].

Using the fact that $k_T = 0$, eq. (30) becomes

$$\frac{d}{dx}\left(\hat{T}_{H0}^{1/2}\,\frac{d\hat{T}_{H0}}{dx}\right) = 0. \tag{32}$$

Taking into account boundary conditions (31) we get

$$\hat{T}_{H0}(x) = \left[(\hat{T}_{II}^{3/2} - 1)\,x + 1\right]^{2/3}. \tag{33}$$

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Then, recalling that one has (26),

$$\frac{d}{dx}\Big[-\hat{T}_{H0}^{1/2}\,\hat{D}_{AB}\,\frac{d}{dx}\Big(\frac{\hat{n}_{H0}^A}{\hat{n}_{H0}^A + \hat{n}_{H0}^B}\Big)\Big]$$

$$= \frac{d}{dx}\Big(\frac{\hat{n}_{H0}^A\,\hat{n}_{H0}^B}{\hat{n}_{H0}^A + \hat{n}_{H0}^B}\,(\hat{u}_{1H1}^A - \hat{u}_{1H1}^B)\Big)$$

$$= -(\hat{n}_{H0}^A\,\hat{u}_{1H1}^A + \hat{n}_{H0}^B\,\hat{u}_{1H1}^B)\,\frac{d}{dx}\Big(\frac{\hat{n}_{H0}^A}{\hat{n}_{H0}^A + \hat{n}_{H0}^B}\Big) = 0.$$

This leads (after using the boundary conditions (31)) to

$$\frac{\hat{n}_{H0}^A(x)}{\hat{n}_{H0}^A(x) + \hat{n}_{H0}^B(x)} = \frac{1}{\hat{T}_{II} - 1}\Big\{\hat{T}_{II}\,a - \frac{\hat{p}_{II}^A}{\hat{p}_{II}^A + \hat{p}_{II}^B} - (a - \frac{\hat{p}_{II}^A}{\hat{p}_{II}^A + \hat{p}_{II}^B})\,[(\hat{T}_{II}^{3/2}-1)\,x+1]^{2/3}\Big\}. \tag{34}$$

Using eq. (25) and the boundary conditions (31), we get

$$\hat{n}_{H0}^A(x) + \hat{n}_{H0}^B(x) = (\hat{p}_{II}^A + \hat{p}_{II}^B)\,[(\hat{T}_{II}^{3/2} - 1)\,x + 1]^{-2/3}.$$

Those last two equations can be summarized in the following formulas:

$$\hat{n}_{H0}^A(x) = \frac{1}{\hat{T}_{II} - 1}\Big\{[a\,\hat{T}_{II}\,(\hat{p}_{II}^A + \hat{p}_{II}^B) - \hat{p}_{II}^A]\,[(\hat{T}_{II}^{3/2}-1)\,x+1]^{-2/3} - [a\,(\hat{p}_{II}^A + \hat{p}_{II}^B) - \hat{p}_{II}^A]\Big\},$$

$$\hat{n}_{H0}^B(x) = \frac{1}{\hat{T}_{II} - 1}\Big\{[(1-a)\,\hat{T}_{II}\,(\hat{p}_{II}^A + \hat{p}_{II}^B) - \hat{p}_{II}^B]\,[(\hat{T}_{II}^{3/2}-1)\,x+1]^{-2/3} - [(1-a)\,(\hat{p}_{II}^A + \hat{p}_{II}^B) - \hat{p}_{II}^B]\Big\}.$$

This gives a complete description of the macroscopic problem (at order 0) related to our initial problem.

The results presented in this section will be compared with the case of different masses and diameters in Sec. 7.2.

6   Case of different masses and/or different diameters of molecules

It does not seem possible to extend this explicit computation to the general case (that is, when masses or diameters of the species A, B are not the same). It is nevertheless possible to write the equations under a simple form which makes not too tedious the numerical computation of their solution. In

particular, it is possible to write a closed system of two equations (each of the second order) for the quantities $\hat{T}_{H0}$ and $\hat{\chi}_{H0}^A = \frac{\hat{n}_{H0}^A}{\hat{n}_{H0}^A + \hat{n}_{H0}^B}$.

Combining eq. (30) and (28), we can write

$$\frac{d}{dx}\Big[-\hat{\lambda}\,\hat{T}_{H0}^{1/2}\,\frac{d\hat{T}_{H0}}{dx} - k_T\,\hat{D}_{AB}\,\hat{T}_{H0}^{3/2}\,\frac{1}{\hat{\chi}_{H0}^A(1-\hat{\chi}_{H0}^A)}$$

$$\times \Big(\frac{d\,\hat{\chi}_{H0}^A}{dx} + \frac{k_T}{\hat{T}_{H0}}\,\frac{d\hat{T}_{H0}}{dx} \Big) \Big] = 0. \tag{35}$$

Then, we observe that

$$\frac{d}{dx}\Big[\hat{D}_{AB}\,\hat{T}_{H0}^{1/2}\,\Big(\frac{d\,\hat{\chi}_{H0}^A}{dx} + \frac{k_T}{\hat{T}_{H0}}\,\frac{d\hat{T}_{H0}}{dx} \Big) \Big]$$

$$= -\frac{d}{dx}\Big[\frac{\hat{n}_{H0}^A\,\hat{n}_{H0}^B}{\hat{n}_{H0}^A + \hat{n}_{H0}^B}\,(\hat{u}_{1H1}^A - \hat{u}_{1H1}^B) \Big]$$

$$= (\hat{n}_{H0}^A\,\hat{u}_{1H1}^A + \hat{n}_{H0}^B\,\hat{u}_{1H1}^B)\,\frac{d\,\hat{\chi}_{H0}^A}{dx} = 0.$$

This leads to the second equation

$$\frac{d}{dx}\Big[\hat{D}_{AB}\,\hat{T}_{H0}^{1/2}\,\Big(\frac{d\,\hat{\chi}_{H0}^A}{dx} + \frac{k_T}{\hat{T}_{H0}}\,\frac{d\hat{T}_{H0}}{dx} \Big) \Big] = 0. \tag{36}$$

This system is complemented with the set of boundary conditions coming out of (31), namely

$$\hat{\chi}_{H0}^A(0) = a, \quad \hat{\chi}_{H0}^A(1) = \frac{\hat{p}_{II}^A}{\hat{p}_{II}^A + \hat{p}_{II}^B}, \quad \hat{T}_{H0}(0) = 1, \quad \hat{T}_{H0}(1) = \hat{T}_{II}. \tag{37}$$

The system (35)-(37) cannot be solved explicitly; we propose however in next section a procedure allowing to compute numerically the solution.

7   Numerical approximation

The system (35)-(37) can be written in the equivalent form

$$\frac{d\,\hat{\chi}_{H0}^A}{dx} = \frac{\gamma_1}{\sqrt{\hat{T}_{H0}}}\Big[\frac{1}{\hat{D}_{AB}} + \frac{(k_T)^2}{\hat{\lambda}}\,\frac{1}{\hat{\chi}_{H0}^A(1-\hat{\chi}_{H0}^A)} \Big] + \gamma_2\frac{k_T}{\lambda\hat{T}_{H0}^{3/2}}, \tag{38}$$

$$\frac{d\hat{T}_{H0}}{dx} = -\frac{\gamma_2}{\hat{\lambda}\sqrt{\hat{T}_{H0}}} - \frac{\gamma_1 k_T\sqrt{\hat{T}_{H0}}}{\hat{\lambda}}\,\frac{1}{\hat{\chi}_{H0}^A(1-\hat{\chi}_{H0}^A)}, \tag{39}$$

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where the two constants γ_1, γ_2 have the following expressions

$$\gamma_1 = \hat{D}_{AB}|_{x=0} \sqrt{\hat{T}_{H0}(0)} \left[\frac{d\,\hat{\chi}_{H0}^A}{dx}|_{x=0} + \frac{k_T|_{x=0}}{\hat{T}_{H0}(0)} \frac{d\hat{T}_{H0}}{dx}|_{x=0} \right], \qquad (40)$$

$$\gamma_2 = -\hat{\lambda}|_{x=0} \sqrt{\hat{T}_{H0}(0)} \frac{d\hat{T}_{H0}}{dx}|_{x=0} - \frac{\gamma_1 \, k_T|_{x=0} \, \hat{T}_{H0}(0)}{\hat{\chi}_{H0}^A(0)(1 - \hat{\chi}_{H0}^A(0))}. \qquad (41)$$

7.1   Description of the method

We use an inductive procedure (quasi-Newton method) in order to solve numerically (38)-(39), the first step of the fixed point procedure being given by the results of the coloring problem with the same data (that is, the problem in which all parameters are the same except that the ratio of masses is 1.0 and the ratio of diameters is also 1.0).

More precisely, we define $\hat{T}_{H0}^{(0)}$, $\hat{\chi}_{H0}^{A\,(0)}$ as the solution of the Cauchy problem (38)-(39), treated thanks to a standard second order RK method, with initial data:

$$\hat{\chi}_{H0}^{A\,(0)}(0) = a, \qquad \frac{d\,\hat{\chi}_{H0}^{A\,(0)}}{dx}(0) = \frac{d\,\hat{\chi}_{H0\,\mathrm{col}}^A}{dx}(0), \qquad (42)$$

$$\hat{T}_{H0}^{(0)}(0) = 1, \qquad \frac{d\hat{T}_{H0}^{(0)}}{dx}(0) = \frac{d\hat{T}_{H0\,\mathrm{col}}}{dx}(0),$$

where $\dfrac{d\,\hat{\chi}_{H0\,\mathrm{col}}^A}{dx}(0)$, $\dfrac{d\hat{T}_{H0\,\mathrm{col}}}{dx}(0)$ are the values obtained explicitly for the coloring problem, thanks to formulas (33), (34).

Then, for $m \geq 1$, if $\hat{\chi}_{H0}^{A\,(m-1)}$, $\hat{T}_{H0}^{(m-1)}$ are given, we define $\hat{\chi}_{H0}^{A\,(m)}$, $\hat{T}_{H0}^{(m)}$ as the solution of the Cauchy problem (38)-(39), treated thanks to a standard second order RK method, with initial data:

$$\hat{\chi}_{H0}^{A\,(m)}(0) = a, \qquad \hat{T}_{H0}^{(m)}(0) = 1, \qquad (43)$$

$$\begin{bmatrix} \dfrac{d\,\hat{\chi}_{H0}^{A\,(m)}}{dx}(0) \\[3ex] \dfrac{d\hat{T}_{H0}^{(m)}}{dx}(0) \end{bmatrix} = \begin{bmatrix} \dfrac{d\,\hat{\chi}_{H0}^{A\,(m-1)}}{dx}(0) \\[3ex] \dfrac{d\hat{T}_{H0}^{(m-1)}}{dx}(0) \end{bmatrix} + [M^{(m-1)}]^{-1} \begin{bmatrix} \hat{\chi}_{H0}^{A\,(m-1)}(1) - \dfrac{\hat{p}_{II}^A}{\hat{p}_{II}^A + \hat{p}_{II}^B} \\[3ex] \hat{T}_{H0}^{(m-1)}(1) - \hat{T}_{II} \end{bmatrix}.$$

$$(44)$$

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Here, $M^{(m-1)}$ is an approximation of the Jacobian matrix of the function
$\Phi : \mathbb{R}^2 \to \mathbb{R}^2$

$$
\Phi : \begin{bmatrix} \dfrac{d\,\hat{\chi}_{H0}^A}{dx}(0) \\[2ex] \dfrac{d\hat{T}_{H0}}{dx}(0) \end{bmatrix} \mapsto \begin{bmatrix} \hat{\chi}_{H0}^A(1) \\[2ex] \hat{T}_{H0}(1) \end{bmatrix},
$$

where $\hat{\chi}_{H0}^A$, $\hat{T}_{H0}$ satisfy equations (38)-(39) with $\hat{\chi}_{H0}^A(0) = a$, $\hat{T}_{H0}(0) = 1$.

This matrix $M^{(m-1)}$ is computed by using a finite difference approximation of the Jacobian matrix previously described; this means that, for each step of the iterative procedure, the RK method has to be used twice in order to compute the entries of such a matrix. More precisely, two components of the matrix are given by the finite difference approximation

$$
\frac{1}{h}\left\{ \Phi\left(\begin{array}{c} \dfrac{d\,\hat{\chi}_{H0}^{A\,(m-1)}}{dx}(0) + h \\[2ex] \dfrac{d\hat{T}_{H0}^{(m-1)}}{dx}(0) \end{array} \right) - \Phi\left(\begin{array}{c} \dfrac{d\,\hat{\chi}_{H0}^{A\,(m-1)}}{dx}(0) \\[2ex] \dfrac{d\hat{T}_{H0}^{(m-1)}}{dx}(0) \end{array} \right) \right\}
$$

and the other two are given by

$$
\frac{1}{h}\left\{ \Phi\left(\begin{array}{c} \dfrac{d\,\hat{\chi}_{H0}^{A\,(m-1)}}{dx}(0) \\[2ex] \dfrac{d\hat{T}_{H0}^{(m-1)}}{dx}(0) + h \end{array} \right) - \Phi\left(\begin{array}{c} \dfrac{d\,\hat{\chi}_{H0}^{A\,(m-1)}}{dx}(0) \\[2ex] \dfrac{d\hat{T}_{H0}^{(m-1)}}{dx}(0) \end{array} \right) \right\}
$$

with h a given (small) parameter. The iteration procedure is stopped when the difference (of derivatives of temperature and concentration at point 0) between two successive steps is smaller than a fixed tolerance τ.

In the computation, the values of the transport coefficients $\hat{\lambda}$, k_T and $\hat{D}_{AB}$ as a function of the concentration fraction $\hat{\chi}_{H0}^A$ are obtained by using the database proposed in [24]. Cubic splines are also employed to interpolate such functions in points $\hat{\chi}_{H0}^A$ different from those given in the database.

7.2 Results

In the simulation, one can choose freely the following parameters of the problem: a, $\hat{T}_{II}$, $\hat{p}_{II}^A$, $\hat{p}_{II}^B$. Then the mass ratio $\hat{m}^B/\hat{m}^A$ and the diameter

ratio $\hat{d}^B/\hat{d}^A$ can be taken in the set of the possible parameters of the database [24].

We now present some numerical results for

$$\hat{T}_{II} = 3.0, \quad \hat{p}_{II}^A = 1, \quad \hat{p}_{II}^B = 5, \quad \hat{m}^B/\hat{m}^A = 2, \quad \hat{d}^B/\hat{d}^A = 0.5,$$

and for two different values of a:

$$\text{Case I}: \quad a = 0.5, \qquad \text{Case II}: \quad a = 0.8.$$

In this parameter setting, the heavy species (species B) is dominant in the evaporating gas from the wall at $x = 1$. In Case II, because of relatively large value of a, substantial part of the heavy species is converted to the light species (species A) at the wall at $x = 0$.

Figure 1 shows the result for Case I: (a) shows the number densities of the individual species, $\hat{n}_{H0}^A$, $\hat{n}_{H0}^B$, versus x; (b) the temperature $\hat{T}_{H0}$ vs x; (c) the flow velocities of the individual species at order 1, $\hat{u}_{1H1}^A$, $\hat{u}_{1H1}^B$, vs x; and (d) the barycentric flow velocity at order 1, $\hat{u}_{1H1}$, vs x. Figure 2 is the corresponding figure for Case II. In Figs. 1(a), 1(b), 2(a), and 2(b), the corresponding results for the coloring problem, i.e., for $\hat{m}^B/\hat{m}^A = \hat{d}^B/\hat{d}^A = 1$ with other parameters being the same, are also shown. In both cases, the deviation from the coloring problem, that is, the effect of different masses and diameters, is not large. Since the total particle flow is zero [eq. (29)] in the present problem, the barycentric flow velocity $\hat{u}_{1H1}$ (or equivalently, the total mass flow) is also small in contrast to the fact that the flow velocities of the individual species $\hat{u}_{1H1}^A$, $\hat{u}_{1H1}^B$ are relatively large. The barycentric velocity $\hat{u}_{1H1}$ vanishes in the coloring problem.

Here, we give a remark on the continuum limit ($\varepsilon \to 0$). In this limit, the flow of gases vanishes because of $\hat{u}_{1H0}^\alpha = \hat{u}_{1H0} = 0$ for all $x \in [0, 1]$. It is widely accepted that the temperature field in a gas at rest is described by the steady heat-conduction equation in the continuum limit. In fact, it is true in the coloring problem because the temperature field is given by (32), which is nothing but the (steady) heat-conduction equation. However, in the general case, the temperature field is given by (35) and (36), which are not the heat-conduction equation. As one can see from (30), the difference from the heat-conduction equation is caused by the first-order velocity field $\hat{u}_{1H1}^A - \hat{u}_{1H1}^B$, more specifically, by the diffusion. This means that, although the velocity field is infinitesimal ($\hat{u}_{1H}^\alpha = \hat{u}_{1H1}^\alpha \varepsilon + \cdots$) in the continuum limit,
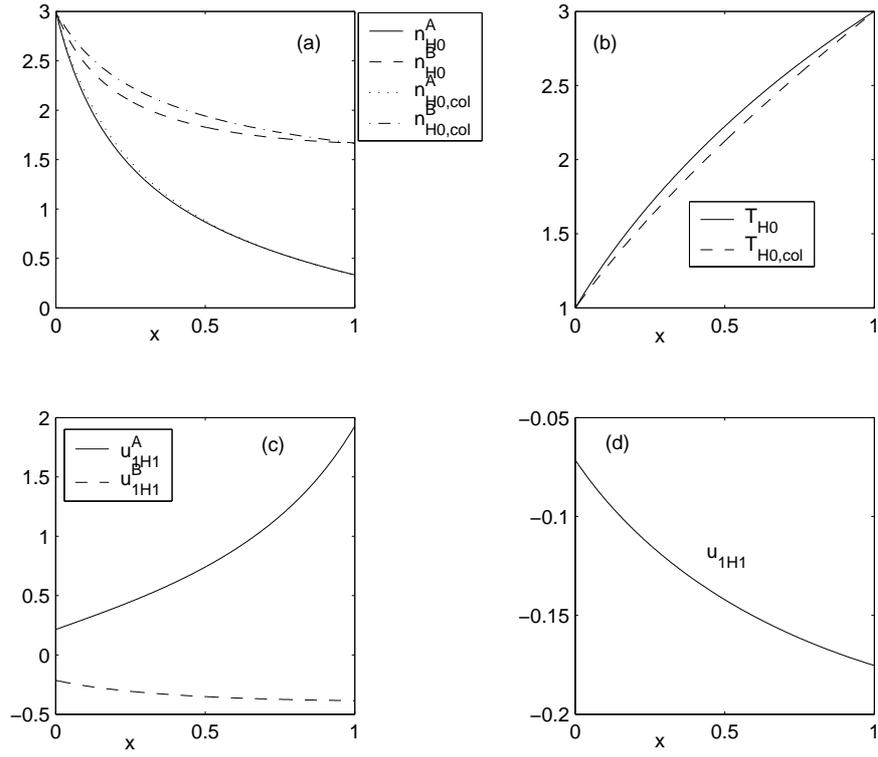
Figure 1: Profiles of the number densities, temperature, and flow velocities in Case I.
(a) $\hat{n}_{H0}^A$ and $\hat{n}_{H0}^B$, (b) $\hat{T}_{H0}$, (c) $\hat{u}_{1H1}^A$ and $\hat{u}_{1H1}^B$, (d) $\hat{u}_{1H1}$. In (a) and (b), the corresponding results for the coloring problem are also shown for comparison.
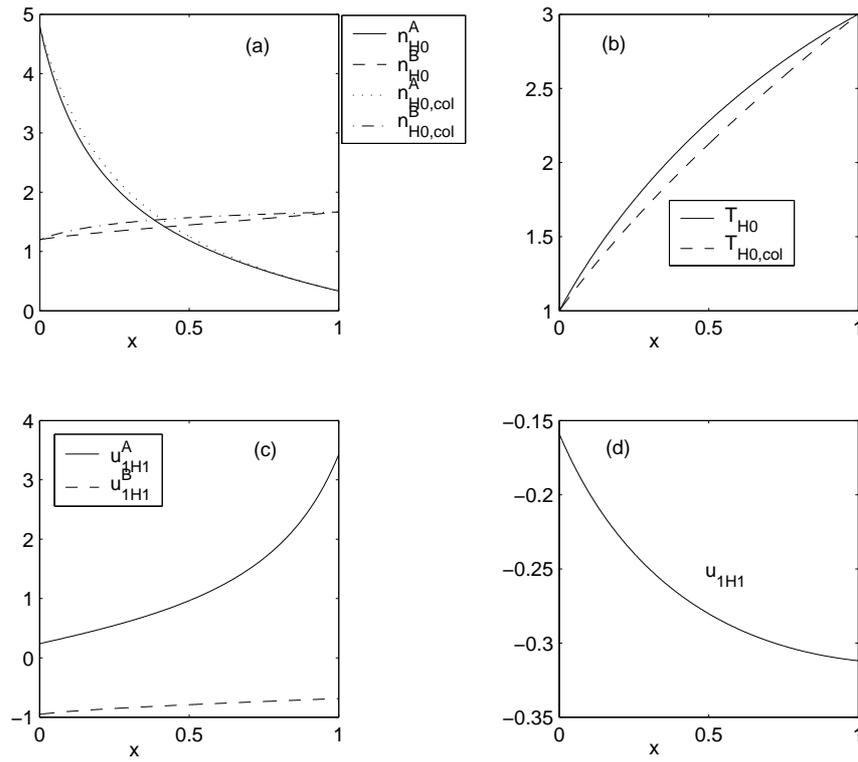
Figure 2:   Profiles of the number densities, temperature, and flow velocities in Case II.
(a) $\hat{n}_{H0}^A$ and $\hat{n}_{H0}^B$, (b) $\hat{T}_{H0}$, (c) $\hat{u}_{1H1}^A$ and $\hat{u}_{1H1}^B$, (d) $\hat{u}_{1H1}$. In (a) and (b), the corresponding
results for the coloring problem are also shown for comparison.

it still has a finite effect on the temperature field $\hat{T}_{H0}$ in this limit. This is a manifestation of the ghost effect that was pointed out in [14] and discussed in detail in subsequent papers by Sone [10, 11, 19] (see [20, 21, 22, 23] for the ghost effect in a gas mixture).

As seen from the original equation (27), the deviation from the heat-conduction equation is caused by two terms, one is $k_T \, (\hat{n}_{H0}^A + \hat{n}_{H0}^B) \, \hat{T}_{H0} \, (\hat{u}_{1H1}^A - \hat{u}_{1H1}^B)$ and the other is $(5/2) \, \hat{T}_{H0} \, [\hat{n}_{H0}^A \, \hat{u}_{1H1}^A + \hat{n}_{H0}^B \, \hat{u}_{1H1}^B]$. Since the latter is zero and k_T is rather small, we do not expect a significant manifestation of the ghost effect in the present problem. In fact, the temperature distribution given by the heat-conduction equation almost coincides with $\hat{T}_{H0}$ in Figs. 1(b) and 2(b). We note here that the heat-conduction equation has been solved with the same density distributions as given in Figs. 1(a) and 2(a), under the no-jump condition $\hat{T}_{H0}(0) = 1$, $\hat{T}_{H0}(1) = \hat{T}_{II}$ [eq. 31]. In order to demonstrate the effect, we also consider a rather extreme case:

Case III: $\quad a = 0.95, \qquad \hat{T}_{II} = 3.0, \qquad \hat{p}_{II}^A = 0.1, \qquad \hat{p}_{II}^B = 10,$
$\qquad\qquad \hat{m}^B/\hat{m}^A = 10, \qquad \hat{d}^B/\hat{d}^A = 1.$

In this case, the gas evaporating from the wall at $x = 1$ contains a very small fraction of the light species (species A), but most of the heavy species is converted to the light species at the wall at $x = 0$. Since the mass ratio is large, one can expect that $\hat{u}_{1H1} < 0$.

Figure 3 shows the results for this case: (a) shows the distribution of the temperature $\hat{T}_{H0}$, together with that of the solution $\hat{T}_{cond}$ of the heat-conduction equation; (b) the difference $\hat{T}_{H0} - \hat{T}_{cond}$ versus x; (c) $\hat{u}_{1H1}^A$ and $\hat{u}_{1H1}^B$ vs x; and (d) $\hat{u}_{1H1}$ vs x. Although the difference is still small, one can observe the deviation of the temperature field from that given by the heat-conduction equation. There is a sharp increase of $\hat{u}_{1H1}^A$ in the vicinity of the wall at $x = 1$. We observe $\hat{u}_{1H1} < 0$, as mentioned in the previous paragraph.

In recent years, the ghost effect has been viewed more comprehensively as a consequence of the singular nature of the continuum limit, and new types of ghost effect, such as the surprising effect of infinitesimal curvature of the boundary, have been pointed out and clarified [15, 16, 17, 18]. The reader is referred to [13] for the detailed description of the ghost effect.

It is not obvious to verify rigorously that system (38), (39), and (37) admits a unique (physically admissible) solution. However, our insight based on numerical simulation would be that such an existence and uniqueness re-
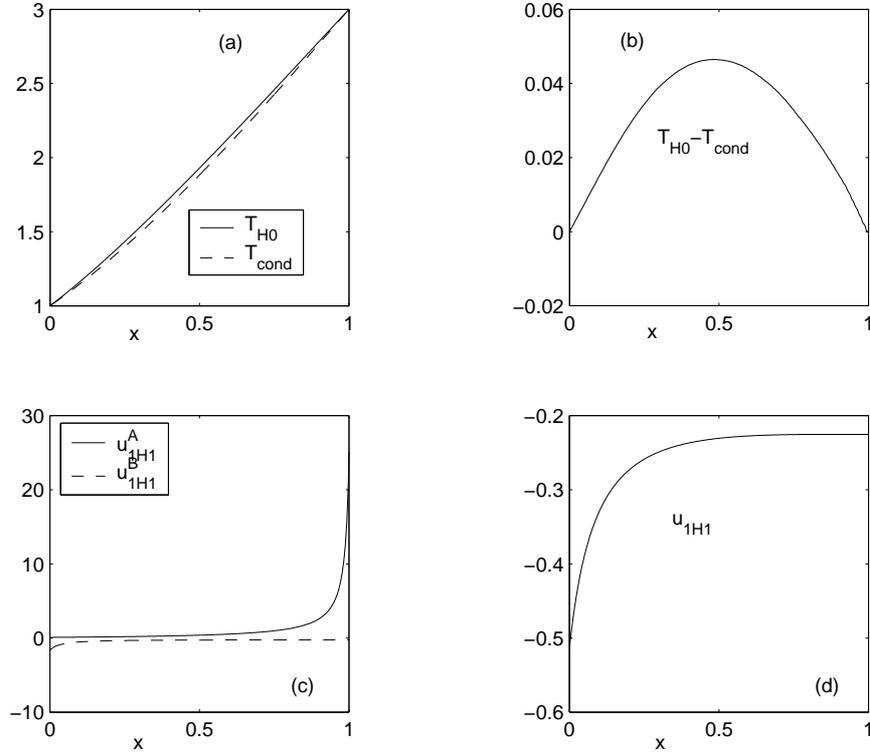
Figure 3: Profiles of the temperature and flow velocities in Case III. (a) $\hat{T}_{H0}$ and $\hat{T}_{cond}$, (b) the difference $\hat{T}_{H0} - \hat{T}_{cond}$, (c) $\hat{u}_{1H1}^A$ and $\hat{u}_{1H1}^B$, (d) $\hat{u}_{1H1}$.

sult might hold. In Fig. 4, we provide a picture of the possible concentration and temperature at point 1 starting from various derivatives of concentration and temperature at point 0. Note that only the points corresponding to an admissible trajectory (that is, when the concentration remains between 0 and 1 at all points, and the temperature is nonnegative at all points) are represented. It seems that all concentrations between 0 and 1 and nonnegative temperatures can be reached.

In the present computation, the spatial domain $[0, 1]$ is divided in $N = 400$ grid points; the parameter h needed in the quasi-Newton scheme is set equal to 0.3; the tolerance is fixed as $\tau = 10^{-3}$.
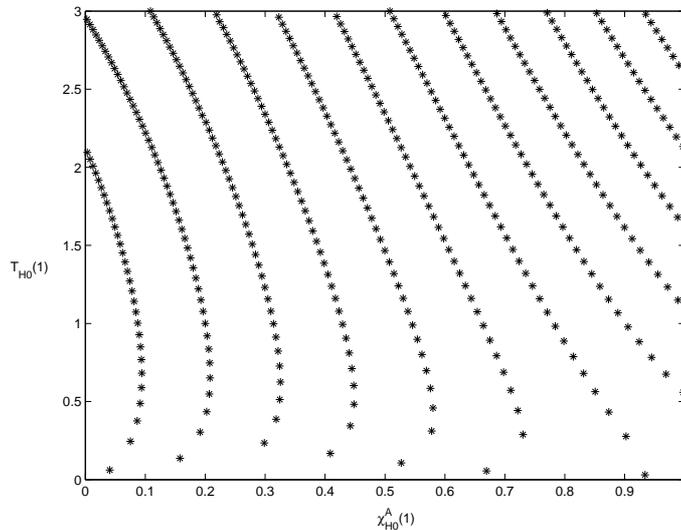
Figure 4: Final points $(\hat{\chi}^A_{H0}(1), \hat{T}_{H0}(1))$ for various Cauchy data.

References

[1] K. Aoki, S. Takata, and S. Kosuge, Vapor flows caused by evaporation and condensation on two parallel plane surfaces: Effect of the presence of a noncondensable gas, *Phys. Fluids* **10**, 1519–1533 (1998).

[2] S. Brull, Problem of evaporation-condensation for a two component gas in the slab, *Kinetic and Related Models* **1**, 185–221 (2008).

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

[4] C. Cercignani, "Rarefied Gas Dynamics, From Basic Concepts to Actual Calculations," Cambridge Univ. Press, Cambridge, 2000.

[5] C. Cercignani, "Slow Rarefied Flows: Theory and Application to Micro-Electro-Mechanical Systems," Birkhäuser, Basel, 2006.

[6] N. G. Hadjiconstantinou, The limits of Navier–Stokes theory and kinetic extensions for describing small-scale gaseous hydrodynamics, *Phys. Fluids* **18**, 111301 (2006).

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[7] G. M. Karniadakis and A. Beskok, "Micro Flows: Fundamentals and Simulation," Springer-Verlag, New York, 2002.

[8] G. M. Karniadakis, A. Beskok, and N. Aluru, "Microflows and Nanoflows: Fundamentals and Simulation," Springer Science+Business Media, New York, 2005.

[9] M. N. Kogan, "Rarefied Gas Dynamics," Plenum, New York, 1969.

[10] Y. Sone, Continuum gas dynamics in the light of kinetic theory and new features of rarefied gas flows, in "Rarefied Gas Dynamics", edited by C. Shen, Peking University Press, Beijing, 3–24 (1997).

[11] Y. Sone, Flows induced by temperature fields in a rarefied gas and their ghost effect on the behavior of a gas in the continuum limit, *Annu. Rev. Fluid Mech.* **32**, 779–811 (2000).

[12] Y. Sone, "Kinetic Theory and Fluid Dynamics,"Birkhäuser, Boston, 2002.

[13] Y. Sone, "Molecular Gas Dynamics: Theory, Techniques, and Applications", Birkhäuser, Boston (2007).

[14] Y. Sone, K. Aoki, S. Takata, H. Sugimoto, and A. V. Bobylev, Inappropriateness of the heat-conduction equation for description of a temperature field of a stationary gas in the continuum limit: Examination by a asymptotic analysis and numerical computation of the Boltzmann equation, *Phys. Fluids* **8**, 628–638 (1996); Erratum: *ibid.* **8**, 841 (1996).

[15] Y. Sone and T. Doi, Bifurcation and ghost effect on the temperature field in the Bénard problem of a gas in the continuum limit, *Phys. Fluids* **15**, 1405–1423 (2003).

[16] Y. Sone and T. Doi, Ghost effect of infinitesimal curvature in the plane Couette flow of a gas in the continuum limit, *Phys. Fluids* **16**, 952–971 (2004).

[17] Y. Sone and T. Doi, Instability of the plane Couette flow by the ghost effect of infinitesimal curvature, in "Rarefied Gas Dynamics", edited by M. Capitelli, AIP, Melville, 258–263 (2005).

[18] Y. Sone, M. Handa, and T Doi, Ghost effect and bifurcation in a gas between coaxial circular cylinders with different temperatures, *Phys. Fluids* **15**, 2903–2915 (2003).

[19] Y. Sone, S. Takata, and H. Sugimoto, The behavior of a gas in the continuum limit in the light of kinetic theory: The case of cylindrical Couette flows with evaporation and condensation, *Phys. Fluids* **8**, 3403–3413 (1996); Erratum: *ibid.* **10**, 1239 (1998).

[20] S. Takata, Kinetic theory analysis of the two-surface problem of a vapor-vapor mixture in the continuum limit, *Phys. Fluids* **16**, 2182–2198 (2004).

[21] S. Takata and K. Aoki, The ghost effect in the continuum limit for a vapor-gas mixture around condensed phases: Asymptotic analysis of the Boltzmann equation, *Transp. Theory Stat. Phys.* **30**, 205-237 (2001); **31**, 289–290(E) (2002).

[22] S. Takata and K. Aoki, Two-surface problems of a multicomponent mixture of vapors and noncondensable gases in the continuum limit in the light of kinetic theory, *Phys. Fluids* **11**, 2743-2756 (1999).

[23] S. Takata, K. Aoki, and T. Muraki, Behavior of a vapor-gas mixture between two parallel plane condensed phases in the continuum limit, in "Rarefied Gas Dynamics", edited by R. Brun, R. Campargue, R. Gatignol, and J.-C. Lengrand, Cépaduès–Éditions, Toulouse, Vol. 1, 479–486 (1999).

[24] S. Takata, S. Yasuda, K. Aoki, and T. Shibata, Various transport coefficients occurring in binary gas mixtures and their database, in "Rarefied Gas Dynamics", edited by A. D. Ketsdever and E. P. Muntz, AIP, New York, 106–113 (2003).