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Temperature and pressure criteria for half-space discrete velocity models

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Abstract

For discrete velocity models (DVMs), we present a criterion which predicts the nonmonotonic behaviour of the pressure in the half-space problem of evaporation and condensation, and we extend a criterion for the internal energy previously given for the problem with two interfaces. We study the profiles of these quantities and their inversion. © 2002 Éditions scientifiques et médicales Elsevier SAS. All rights reserved.

1. Introduction

A long time ago, a paradoxical result was found in the kinetic treatment of a gas between two interfaces. The temperature of the vapor at the warm interface can be below the one at the cold wall (inverted gradient). Experiments, numerical and theoretical results using the continuous [1–3] and discrete [4–7] kinetic theory were presented. In our previous work [7] extending a criterion [8,9] for temperature overshoots of shock waves to a gas between two plates, we have studied both the inverted gradient and overshoot effects for the temperature.

Here we consider the steady flow of a semi-infinite expanse of gas in contact with its condensed phase. Condensation and evaporation can take place at the interface between the two phases. This is called the half-space problem of evaporation and condensation and for DVMs models, we seek the possible inversion or overshoots of the macroscopic variables of the flow. As in the continuum treatment of the problem [10–16] the flow is assumed one-dimensional depending upon the spatial variable $z > 0$. The interface is located at $z = 0$.

The first change with respect to our previous work [7] is that one interface is replaced by a Maxwellian state of the gas at $z \rightarrow +\infty$. Let us consider a macroscopic quantity $Y(z)$, like the temperature (or internal energy [17] for DVMs). We can have different aspects concerning respectively its value Y_w in the wall at $z = 0$ and the two gas values $Y_0 = Y(z \rightarrow 0_+)$ and $Y_\infty = Y(z \rightarrow +\infty)$.

Recently [18] (review in [16]) the half-space for condensation was studied in continuous kinetic theory. There were considered, for the flow in a transonic regime, both the temperature and the pressure; in the studies of $Y(z)/Y_w$, they found either monotonic $z \in (z_0, \infty)$ (z_0 small) domains or nonmonotonic ones with a center curve for $Y_0 = Y_\infty$. *The second change with respect to Ref. [7] is that we introduce the pressure and give a new criterion for nonmonotonic effects.* We explain also why the nonmonotonic domains are divided by central $Y_0 = Y_\infty$ curves.

In our DVMs, the densities with velocities symmetric with respect to the z -axis are equal. Consequently, the momentum is reduced to $J \neq 0$ along the z -axis. Here we restrict our boundary conditions to a plane at rest at $z = 0$ (perpendicular to the z -axis) with a condensed phase. We retain only the densities with emerging velocities, for the other (impinging) velocities we

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associate new densities such that the whole set at the wall represents a fictitious Maxwellian state with a zero momentum and all collisions vanishing.

In Section 2 we recall briefly the DVMs boundary conditions for our DVMs and introduce the boundary conditions at infinity. In Section 3 we give the criteria for the inversion of the internal energy E_I and the pressure P in the flow. These criteria are independent of explicit collisions.

In Sections 4 and 5, Figs. 1(a)–2(a), for models with four independent densities, we first study the restrictions for possible nonmonotonic pressure, while second, the densities N_i satisfy scalar integrable Riccati equations [8,9,19,20]. With exact solutions, we study different domains where either P or E_I have overshoots. In Sections 6 and 7, Figs. 3(a)–4(a), we study models with five and six independent densities, giving first the restrictions of the criterion for nonmonotonic P and second, with exact solutions, examples of really nonmonotonic P or E_I . In these sections, the steady densities satisfy a system of 2×2 , 3×3 Riccati equations. In all Sections 4–7, we make the conditions for fictitious Maxwellians at the wall, give the $Y_0 = Y_\infty$ values and compare those at the wall and in the gas.

2. Half-space DVMs and boundary conditions [4–6]

We give a brief survey while a complete study is made in Refs. [1–6]. We restrict the class of DVMs studied in the paper: each velocity \vec{v}_i has another \vec{v}_j symmetric with respect to the z -axis. Then $N_i = N_j$ and along the z -axis it remains only the momentum J . For a DVMs with p velocities $\vec{v}_i, i = 1, \dots, p$, we denote by number $N_i(m, t)$ the density of the particles of velocity \vec{v}_i at time t and point m . The macroscopic variables denoting mass, velocity and energy (M, J, E) are [4–6,21,22]:

$$M = \sum_{i=1}^p N_i, \quad J = \sum_{i=1}^p N_i \vec{v}_{iz}, \quad E = \sum_{i=1}^p N_i \vec{v}_i^2 / 2. \quad (2.1)$$

We assume that a DVMs is in equilibrium with a wall or a condensed phase when the microscopic densities N_{iw} of the Maxwellian state are associated with M, J, E . At the interface we assume that the particles leaving the condensed phase are in Maxwellian equilibrium with it. At infinity the gas is assumed to be uniform and in a Maxwellian equilibrium associated with the macroscopic variables of the flow.

Let $\mathcal{B} = (\vec{i}_x, \vec{i}_y, \vec{i}_z) \in R^3$ be an orthonormal base for the x, y, z coordinates. We denote by u_i, v_i and $\lambda_i \neq 0$ the components of the velocity \vec{v}_i in \mathcal{B} and we assume that the interface is the plane $z = 0$ and the gaseous phase fills the half-space $z > 0$. When we assume that the flow is steady one-dimensional and depends only upon z , the modelling of the half-space problem of evaporation and condensation using a p velocity discrete model yields the following boundary value problem for $1 \leq k \leq p$:

$$\lambda_k dN_k/dz = \mathcal{F}_k(N), \quad N_k(0) = N_{k0}, \quad \lambda_k > 0, \quad N_{z \rightarrow \infty} = N_{k\infty}, \quad (2.2a)$$

$$\mathcal{F}_k(N) = \sum_{r=2}^S \sum_{I_r, J_r} \in \mathcal{E}_r \delta(k, J_r, I_r) A_{I_r}^{J_r} N_{I_r}, \quad (2.2b)$$

where $\mathcal{F}_k(N)$ is the k th component of the collision operator for r -collisions, $2 \leq r \leq S$. In the paper we take into account only binary and ternary collisions, so $r = 2$ or $r = 3$. We define: $\partial X / \partial z = X'$ for any $X(z)$ and l_i for the evolution equation of N_i . We write the mass, momentum and energy conservation laws for a steady z -dependent one-dimensional flow:

$$l_i = \lambda_i N'_i, \quad \sum l_i = 0, \quad \sum \lambda_i l_i = 0, \quad \sum \vec{v}_i^2 l_i = 0. \quad (2.3)$$

We integrate and obtain three constants $K_i, i = 1, 2, 3$. The conservation equations, written at infinity are the DVM's Euler equations [21,22]. We thus can obtain the three K_i constants as functions of only the macroscopic variables of the flow at infinity. Rewriting the relations obtained by the integration at $z = 0$ with these constants expressed in terms of the macroscopic variables of the flow at infinity, we derive the relations linking the macroscopic variables at the boundaries of the flow.

3. Criteria for the inversion of macroscopic quantities: E_I, P

To the variables $M(z), J, E(z)$ (mass, momentum and energy) we add $E_I(z)$ and $P(z)$:

$$\text{internal energy: } E_I(z) = 2E(z)/M(z) - [J/M(z)]^2 = P/M; \quad P: \text{ pressure.} \quad (3.1)$$

However, as discussed by Cercignani [17], owing to the discretisation, the definitions of temperature given by the theory of real gases are no longer valid in DVMs. We thus use the internal energy E_I for the temperature.

We consider two- and three-dimensional models ($d = 2, 3$) admitting only three physical invariants. The particles undergo binary, ternary... collisions which lead to quadratic, cubic... polynomials in the collision terms. By using the symmetry properties of the model, we can sometimes reduce the order of these terms and obtain linear, quadratic... polynomials, leading to known integrable solutions for the microscopic densities $N_i(z)$:

$$N_i(z) = n_{0i} + n_i F(z), \quad 1 \leq i \leq p, \quad F = 1/D^{1/(v-1)}, \quad D = 1 + \bar{\lambda} e^{\gamma z}; \quad (3.2)$$

v is the degree of the reduced collision operator and $v = 2$ in Sections 4–7. n_{0i} , n_i , γ and $\bar{\lambda}$ are constants, $\bar{\lambda}$ such that $D(z) > 0$ for $z \in (0, \infty)$. We compute $M(z)$ and $E(z)$ at the boundaries $z \rightarrow 0$ and $z \rightarrow \infty$, introduce the values $M_0, M_\infty, E_0, E_\infty$ as well as F_0, F_∞ and define $X_{0,\infty}^- = X_0 - X_\infty$. With $F(z) > 0$ monotonic, $M(z)$ and $E(z)$ are monotonic functions of z .

$$M = M_a + M_b F(z), \quad M_a = \sum n_{0i} = [F_0 M_\infty - F_\infty M_0]/F_{0,\infty}^-, \quad M_b = \sum n_i, \quad (3.3)$$

$$M_b = M_{0,\infty}^-/F_{0,\infty}^-, \quad E = E_a + E_b F(z), \quad E_a = [F_0 E_\infty - F_\infty E_0]/F_{0,\infty}^-, \quad E_b = E_{0,\infty}^-/F_{0,\infty}^-, \quad (3.4)$$

$$M_0 = M_a + M_b F_0, \quad E_0 = \dots, \quad M_\infty = M_a + M_b F_\infty, \quad E_\infty = \dots$$

3.1. Criterion for the internal energy E_I

We recall this criterion [7,8], initiated for shock waves, here with constant J along the z -axis. We write E'_I , $F' \neq 0$ for the derivatives with respect to z and deduce from (3.1), (3.2) and (3.4):

$$M^3 E'_I / 2F' = Q_1[F(z)] = J^2 M_b + (E_b M_a - E_a M_b)[M_a + M_b F(z)]. \quad (3.5a)$$

Lemma 1. With Q_1 monotonic, a condition for E_I to be nonmonotonic is:

$$Q_1[F_0]Q_1[F_\infty] < 0 \quad \text{or} \quad E'_I(z \rightarrow 0)E'_I(z \rightarrow \infty) < 0, \quad F' \neq 0. \quad (3.5b)$$

With $M_0, E_0, M_\infty, E_\infty$ we write the constants in $Q_1(z)$ and define:

$$\Lambda_\mu = J^2 M_{0,\infty}^- + \mu(E_0 M_\infty - M_0 E_\infty). \quad (3.5bis)$$

Lemma 1bis. A sufficient condition for E_I to be nonmonotonic is $\Lambda_{M_0} \Lambda_{M_\infty} < 0$. If $\Lambda_{M_0} \Lambda_{M_\infty} \geq 0$, then $E_I(z)$ is monotonic and we cannot have $E_{I,0} = E_{I,\infty}$ when $z \rightarrow 0, \infty$. There is a strict inversion if and only if:

$$(E_{I,w} - E_{I,\infty})(E_{I,0} - E_{I,\infty}) < 0. \quad (3.5c)$$

3.2. Criterion for the pressure $P = E_I M$

We write the derivative P' :

$$\begin{aligned} P' M^2 / F' &= 2E_b M^2 + J^2 M_b = Q_2[F] = A F^2 + B F + C, \quad A = 2E_b M_b^2, \quad B = 4E_b M_a M_b, \\ C &= 2E_b M_a^2 + J^2 M_b, \quad B^2 - 4AC = -8J^2 E_b M_b^3. \end{aligned} \quad (3.6)$$

Lemma 2. With $F' \neq 0$ a necessary (not sufficient) condition for P to be nonmonotonic is $B^2 - 4AC > 0$ or $M_b E_b < 0$ or equivalently $M_{0,\infty}^- E_{0,\infty}^- < 0$ ($P' = 2E' + J^2 M' / M^2$, M and E cannot be both increasing or decreasing). $Q_2[F_0]Q_2[F_\infty] < 0$ is a sufficient (not necessary) condition. We define

$$\bar{\Lambda}_\mu = J^2 M_{0,\infty}^- + 2\mu^2 E_{0,\infty}^-. \quad (3.6bis)$$

Lemma 2bis. A sufficient condition for P to be nonmonotonic is $\bar{\Lambda}_{M_0} \bar{\Lambda}_{M_\infty} < 0$. If $P(z)$ is monotonic, then $P_0 \neq P_\infty$. If $M_{0,\infty}^- E_{0,\infty}^- > 0$, then $Q_2[F(z)]$ has no roots, $\bar{\Lambda}_\mu / E_{0,\infty}^- > 0 \rightarrow \bar{\Lambda}_{M_0} \bar{\Lambda}_{M_\infty} > 0$, P is monotonic and $P_0 \neq P_\infty$. If $\bar{\Lambda}_{M_0} \bar{\Lambda}_{M_\infty} < 0$, then $Q_2[F]$ and $\bar{\Lambda}_\mu$ have one root between the two z limits: (F_0, F_∞) and (M_0, M_∞) , P is nonmonotonic and $P_0 = P_\infty$ is possible.

In all our numerical examples, with a parameter varying, we find P nonmonotonic in domains limited by the values where $Q_2[F_0]Q_2[F_\infty] = \bar{\Lambda}_{M_0} \bar{\Lambda}_{M_\infty} = 0$.

Let us call F_\pm , the roots of $A F^2 + B F + C = 0$ with $M_{0,\infty}^- E_{0,\infty}^- < 0$ and $F_0 = (1 + \bar{\lambda})^{1/(1-v)}$ (see (3.2)), $F_\infty = 0, 1$ if $\gamma \geq 0$. A condition for P to be nonmonotonic is either $F_\pm \in [F_0, F_\infty]$ and for P to be monotonic: both $F_\pm \notin [F_0, F_\infty]$.

4. DVMs with four independent densities (none velocity along z), Fig. 1

We present a class of models in Fig. 1(a), $d = 2$, with arbitrary parameters λ (along z -axis), α, β (along x, y axes), and, if $d_* := (d - 1)$, with $8d_*$ velocities \bar{v}_i . Here we discuss the $d = 2$ models ($d = 3$ in Appendix A.1). We write the $\bar{v}_i(x, z)$ in the x, z plane:

$$\bar{v}_1 : (\alpha, 1) = -\bar{v}_3, \quad \bar{v}_5 : (\beta, \lambda) = -\bar{v}_7, \quad \bar{v}_{i+1}(x, z) = \bar{v}_i(-x, z), \quad i = 1, 3, 5, 7. \quad (4.1)$$

Due to the symmetries with respect to the z -axis, only four independent $N_i(z) = N_{i+1}(z)$, i odd densities and associated evolution equations I_i remain. In Sections 4.1 and 4.2, we present results without explicit collisions.

4.1. Conservation laws and macroscopic quantities

Contrary to $N_{1,3}^+$, $N_{5,7}^+$ and $N_5\lambda + N_1$, all N_i and conservation laws cannot be written only with M , E , J (mass, energy and momentum):

$$\begin{aligned} M/2 &= N_{1,3}^+ + N_{5,7}^+, & E &= (\alpha^2 + 1)N_{1,3}^+ + (\beta^2 + \lambda^2)N_{5,7}^+, & J/2 &= N_{1,3}^- + \lambda N_{5,7}^-, \\ C &:= (\beta^2 + \lambda^2 - 1 - \alpha^2), & N_{5,7}^+ &= B = [E - M(\alpha^2 + 1)/2]/C, \end{aligned} \quad (4.2)$$

$$\begin{aligned} N_{1,3}^+ &= A = [(\beta^2 + \lambda^2)M/2 - E]/C \rightarrow N_5\lambda + N_1 = J/4 + (A + \lambda B)/2, \\ 0 &= \partial_z[(\lambda^2 - 1)E + (\beta^2 - \lambda^2\alpha^2)M/2] = \partial_z[(\beta^2 + \lambda^2)J/2 - CN_{1,3}^-]. \end{aligned} \quad (4.3)$$

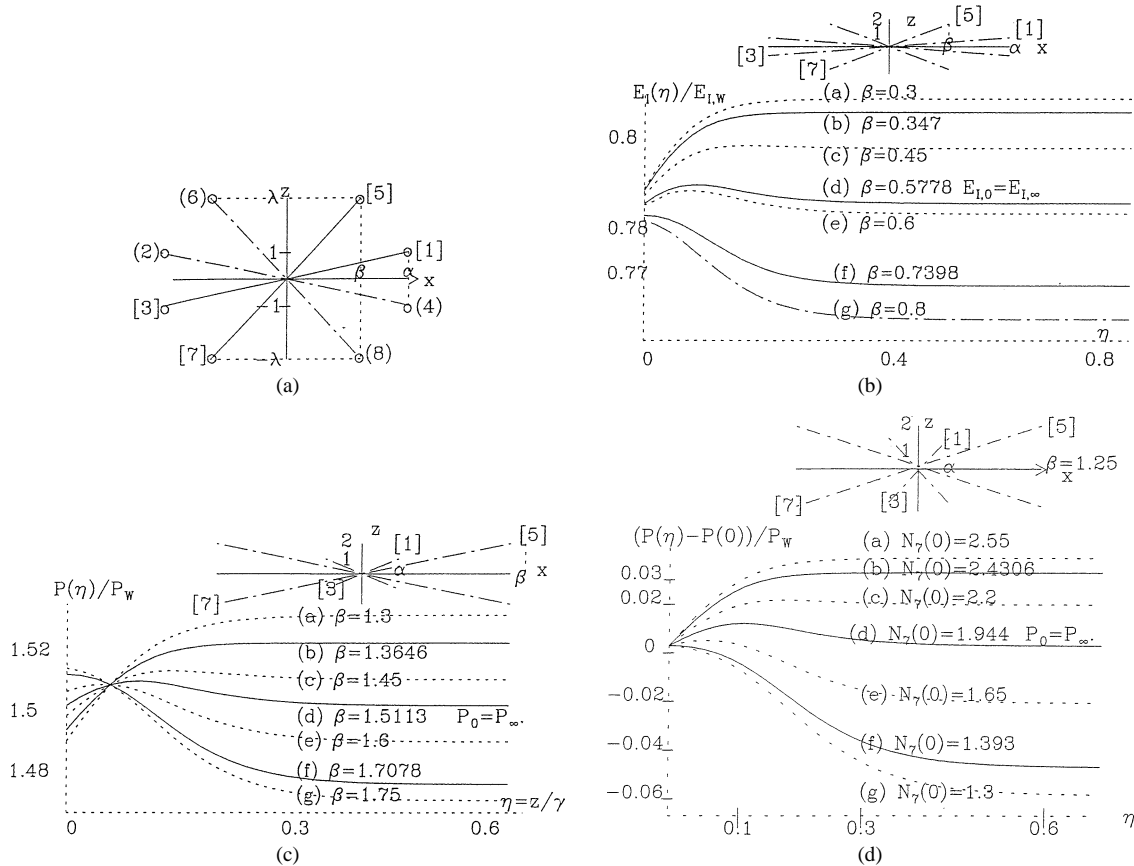


Fig. 1. (a) $d = 2$; model: four independent N_i , eight v_i , none along z , $N_{i+1} = N_i$, $i = 1, 3, 5, 7$. (b) $d = 2$, $\alpha = 1.5$: four independent N_i ; internal energy E_I . (b)–(f) Transition monotonic and nonmonotonic; (a)–(g) monotonic; (c), (d), (e) nonmonotonic; (d) $E_{I,0} = E_{I,\infty}$, $E_{I,w} > \sup(E_{I,0}, E_{I,\infty})$. (c) $d = 2$, $\alpha = 1/2$: four independent N_i , pressure P . (b)–(f) Transition monotonic and nonmonotonic; (a)–(g) monotonic; (c), (d), (e) nonmonotonic; (d) $P_0 = P_\infty$, $P_w < \inf(P_0, P_\infty)$. (d) $d = 2$, $\alpha = 1/2$: four independent N_i , pressure P . (b)–(f) Transition monotonic and nonmonotonic; (a)–(g) monotonic, (c), (d), (e) nonmonotonic; (d) $P_0 = P_\infty$, $P_w < \inf(P_0, P_\infty)$.

4.2. Possible P nonmonotonic, $M_b E_b < 0$ if $\lambda \geq 1$ and $\beta \geq \alpha\lambda$

From the three conservation laws, we get three relations between the four l_i :

$$0 = l_{1,3}^+ + l_{5,7}^+ = l_{1,3}^- + \lambda l_{5,7}^- = (\alpha^2 + 1)l_{1,3}^+ + (\beta^2 + \lambda^2)l_{5,7}^+, \quad (4.4)$$

$$X' := dX/dz \rightarrow l_1 = N_1' = -l_3 = N_3' = -\lambda l_5 = -\lambda^2 N_5' = \lambda l_7 = -\lambda^2 N_7'. \quad (4.5)$$

We integrate N_i' , obtain all N_i , M , J , E as functions of N_1 with constants a_i :

$$\begin{aligned} N_i(z) &= n_{0i} + n_i F(z), & N_3 &= N_1 + a_3, & N_j &= -N_1/\lambda^2 + a_j \rightarrow n_1 = n_3 = -\lambda^2 n_5 = -\lambda^2 n_7, & j &= 5, 7, \\ M/2 &= 2N_1(\lambda^2 - 1)/\lambda^2 + a_{3,5}^+ + a_7, & J/2 &= -a_3 + \lambda a_{5,7}^-, \\ E &= 2N_1(\alpha^2 - \beta^2/\lambda^2) + (\alpha^2 + 1)a_3 + (\beta^2 + \lambda^2)a_{5,7}^+, \end{aligned} \quad (4.6)$$

M_b , E_b given in (3.3), $\lambda \neq 1$, $\beta \neq \lambda\alpha \rightarrow M_b/4n_1 = 1 - \lambda^{-2}$, $E_b/2n_1 = \alpha^2 - (\beta/\lambda)^2$.

4.3. Collisions $N_5 N_3^\lambda - N_7 N_1^\lambda$ with $\lambda > 1$ integer

4.3.1. Gas

From $N_{i+1} = N_i$, i odd and (4.6) it is sufficient to study l_1 for N_1 :

$$\begin{aligned} l_1 &= N_1' = n_1 F' = \Theta[(N_5 N_3^\lambda - N_8 N_1^\lambda) + (N_6 N_3^\lambda - N_7 N_2^\lambda)] = 2\Theta(N_5 N_3^\lambda - N_7 N_1^\lambda) \\ &= 2\Theta[(a_5 - N_1/\lambda^2)(N_1 + a_3)^\lambda - N_1^\lambda(a_7 - N_1/\lambda^2)], \end{aligned} \quad (4.7)$$

where Θ is the collision rate, in fact a scaling parameter for z . The highest $N_1^{\lambda+1}$ term disappears in (4.7) and the $N_1(z)$ polynomial is of order λ .

4.3.2. Wall, Appendix A.1

From the emerging densities $N_{w,i}$, $i = 1, 5$, we obtain the equality with the impinging $N_{w,i+2}$.

4.3.3. Appendix A.2

$N_i(\eta) = n_{0i} + n_i/D(\eta)$ for $\lambda = 2$. The cubic collisions $N_5 N_3^2 - N_7 N_1^2$ leads to a quadratic integrable Riccati equation for N_1 .

4.3.4. Numerical calculations

$d = \lambda = 2$, $\eta = z/2\gamma\Theta$, Figs. 1(b)–1(d)				
Fig. 1	$N_{7,0}$	α	β	Y nonmonotonic
(b)	2.9	1.5	$0.3 < \beta < 0.8$	E_I : $0.347 < \beta < 0.7398$
(c)	2.9	0.5	$1.3 < \beta < 1.75$	P : $1.3646 < \beta < 1.7078$
(d)	$1.3 < N_{7,0} < 2.55$	0.5	1.25	P : $1.393 < N_{7,0} < 2.4306$

$N_{7,0}$ in Fig. 1(d) (β in Figs. 1(a) and 1(b)) are varying. With $J < 0$ and $M(z)$ decreasing from ∞ , we have evaporation from ∞ . The macroscopic quantities Y (E_I , P) in Figs. 1(b)–1(d) are nonmonotonic in intervals (limited by the $\Lambda_{M_0} \Lambda_{M_\infty} = 0$, $\bar{\Lambda}_{M_0} \bar{\Lambda}_{M_\infty} = 0$ values), including $Y_0 = Y_\infty$ and monotonic outside. We find $E_{I,w} > \sup(E_{I,0}, E_{I,\infty})$ in Fig. 1(b), $P_w < \inf(P_0, P_\infty)$ in Figs. 1(c) and 1(d); and in Fig. 1(b), $\beta < 0.5778$, the condition (3.5c) for a *strict inversion* is satisfied.

4.4. Euler with cubic collisions, $\lambda = d = 2$

First, we rewrite (4.2):

$$N_1 = (A + N_{1,3}^-)/2, \quad N_{7,5}^- = B - 2N_5, \quad N_5 = (B - N_1)/2 + J/8 + A/4. \quad (4.8)$$

With the Maxwellian, we get a cubic equation for $N_{1,3}^-$ and deduce all N_i :

$$N_5 N_3^2 = N_7 N_1^2 \rightarrow N_1^2 N_{7,5}^- = N_5 N_{3,1}^- N_{3,1}^+, \quad (N_{1,3}^-)^3 - J(N_{1,3}^-)^2/2 + N_{1,3}^- A(A + 4B) - A^2 J/2 = 0, \quad (4.9)$$

as functions of J, M, E with (4.8). *Second*, we integrate the conservation laws:

$$\begin{aligned} J &= \text{const.}, \quad 3E(z) + (\beta^2 - 4\alpha^2)M(z)/2 = CK_J = \text{const.}, \\ C &:= \beta^2 + 3 - \alpha^2 - CN_{1,3}^-(z) + (\beta^2 + 4)J/2 = 2CN_{5,7}^-(z) + (\alpha^2 + 1)J/2 = K_E = \text{const.} \end{aligned} \quad (4.10)$$

From $z \rightarrow \infty$, $N_{i,j}^- = N_{i,j}^-(\infty)$, $(i, j) = (1, 3), (5, 7)$ in (4.9), $CK_J = 3E_\infty + (\beta^2 - 4\alpha^2)M_\infty/2$ and from $z \rightarrow 0_+$, $N_{i,0}$ giving the impinging densities ($i = 3, 7$) from the known emerging ones ($i = 1, 5$), we get a link between the interface and the asymptotic variables:

$$\begin{aligned} N_{3,0} &= N_{1,0} + [K_E - (\beta^2 + 4)J/2]/C, \quad N_{7,0} = N_{5,0} + (K_E - (1 + \alpha^2)J/2)/2C, \\ N_{7,0} &= -N_{5,0} - N_{1,0}/2 + K_J/4 + [(\beta^2 + 4)J/2 - K_E]/4C. \end{aligned} \quad (4.11)$$

5. DVMs with four independent densities (two \bar{v}_i along z), Fig. 2

We present a class of models (Fig. 2(a)) with $\lambda > 1$ integer, with number $(4d_* + 2)$ of velocities \bar{v}_i , $\eta_i^2 = 1$:

$$\eta_i = 1: (\eta_1\alpha_x, \eta_2\alpha_y, \lambda) = \bar{v}_1 = -\bar{v}_3, \quad \bar{v}_5: (0, 0, 1) = -\bar{v}_6, \quad d = 2 \rightarrow \alpha_y = 0.$$

We have four independent N_i , $i = 1, 3, 5, 6$ (four l_i : evolution equations) associated to \bar{v}_i . For any \bar{v}_i we have another $-\bar{v}_i$. In Section 5.1, we give results without explicit collisions. In Section 5.3, the necessary condition $\lambda > 1$ for P to be nonmonotonic is satisfied, but the sufficient one gives a small interval limited by $\bar{A}_{M0} \bar{A}_{M\infty} = 0$.

5.1. Conservation laws and macroscopic quantities

All N_i (except $N_{1,3}^+$ and $N_{5,6}^+$) and conservation laws are not written with M, E, J :

$$\begin{aligned} C: \alpha_x^2 + \alpha_y^2 + \lambda^2 - 1, \quad M &= 2d_*N_{1,3}^+ + N_{5,6}^+, \quad E = d_*(C + 1)N_{1,3}^+ + N_{5,6}^+/2, \quad J = 2d_*\lambda N_{1,3}^- + N_{5,6}^-, \\ N_{1,3}^+ &= A = [E - M/2]/d_*C, \end{aligned} \quad (5.1)$$

$$N_{5,6}^+ = B = [(C + 1)M - 2E]/C \rightarrow N_5 = d_*\lambda(A - 2N_1) + J/2 + B/2, \quad (5.2)$$

$$0 = \partial_z [2(\lambda^2 - 1)E + (\alpha_x^2 + \alpha_y^2)M] = \partial_z [d_*\lambda(C + 1)N_{1,3}^- + N_{5,6}^+/2]. \quad (5.3)$$

From the three conservation laws we get three l_i relations that we integrate:

$$\begin{aligned} 0 &= 2d_*l_{1,3}^+ + l_{5,6}^+ = 2d_*\lambda l_{1,3}^- + l_{5,6}^- = d_*(C + 1)l_{1,3}^+ + l_{5,6}^+/2 \rightarrow l_{1,3}^+ = l_{5,6}^+ = 0, \\ l_1 &= \lambda N_1' = -l_3 = \lambda N_3' = -l_5/2\lambda d_* = -2N_5'/2\lambda d_* = -N_6'/2d_*\lambda, \end{aligned} \quad (5.4)$$

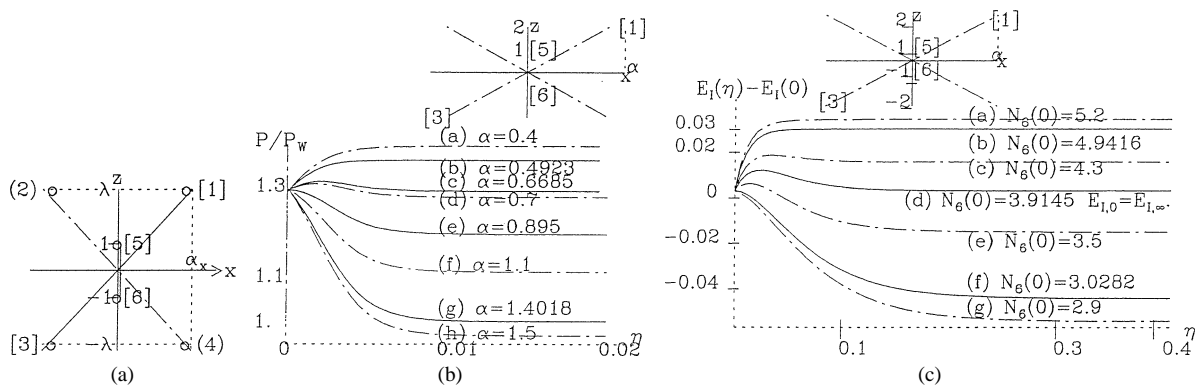


Fig. 2. (a) $d = 2$; model: four independent N_i , six v_i , two along z , $N_{i+1} = N_i$, $i = 1, 3$. (b) $d = 3$; model with four independent N_i , $\lambda = 2$, pressure P . (b)–(e) Transition monotonic and nonmonotonic P ; (a)–(f)–(g)–(h) monotonic; (c), (d) nonmonotonic; (g) $P_W = P_\infty$; (c) $P_0 < P_\infty$, $\alpha > 0.6685$, $P_w < P_0 < P_\infty$, $\alpha > 1.4018$, $P_\infty < P_w < P_0$, $0.668 < \alpha < 1.4018$, $P_w < P_\infty < P_0$. (c) $d = 3$, $\alpha = 0.4$: four independent N_i , internal energy E_I . (b)–(f) Transition monotonic and nonmonotonic; (a)–(g) monotonic; (c), (d), (e) nonmonotonic; (d) $E_{I,0} = E_{I,\infty}$, $E_{I,w} < \inf(E_{I,0}, E_{I,\infty})$.

$$A' = 2N_1', \quad B' = 2N_5', \quad N_{1,3}^- = N_{5,6}^- \equiv 0, \quad J' = 0, \quad N_i = n_{0i} + n_i F(z), \quad (5.5)$$

$$N_3(z) = N_1(z) + a_3, \quad N_j = -2d_*\lambda^2 N_1 + a_j, \quad j = 5, 6, \quad J = -2\lambda d_* a_3 + a_{5,6}^-, \quad (5.6)$$

$$n_3 = n_1, \quad n_5 = -2\lambda^2 d_* n_1 = n_6, \quad M_b/4d_* n_1 = (1 - \lambda^2), \quad E_b/2d_* n_1 = \alpha_x^2 + \alpha_y^2.$$

Possible P nonmonotonic, $M_{0,\infty}^- E_{0,\infty}^- < 0$ or $M_b E_b < 0$ if $\lambda > 1$.

5.2. Wall at $z = 0$, Appendix B

With collisions of the type $I_1 = \Theta(N_3 N_5^\lambda - N_1 N_6^\lambda)$ and emerging densities $N_{w,j}$, $j = 1, 5$, we deduce $N_{w,i}$, $i = 3, 6$, M_w and E_w .

5.3. Explicit $N_i(z)$ solutions for the model with $\lambda = 2$ and $d = 2, 3$

5.3.1. Gas, Appendix B

For $\lambda = 2$, we have cubic collisions, reducing to quadratic collisions with (5.6) (scalar Riccati integrable equation).

5.3.2. Numerical calculations

$d = 3, \lambda = 2$, Fig. 2b (c) for $P(E_I)$						
Fig.	$N_{1,0}$	$N_{5,0}$	$N_{3,0}$	$N_{6,0}$	$\alpha = \alpha_x = \alpha_y$	Y nonmonotonic
2(b)	0.85	0.5	1.37	9.7	$0.4 < \dots < 1.5$	$P: 0.4923 < 0.895$
2(c)	0.05	0.075	0.057	$2.9 < \dots < 5.2$	0.4	$E_I: 3.0282 < 4.9416$

The macroscopic quantities Y (P in Fig. 2(b), E_I in Fig. 2(c)) are nonmonotonic in intervals $(\alpha, N_{6,0})$ including $Y_0 = Y_\infty$ (monotonic outside) and with $J = -13.8$, $J \in (-5.38, -3.08)$, $M(z) \leq M(\infty)$, evaporation from ∞ . In Fig. 2(b), we have another transition $\alpha = 1.4018$ for $P_w = P_\infty$ and three domains: $P_w < P_0 < P_\infty$ if $\alpha > 0.6685$, $P_w < P_\infty < P_0$ if $0.6685 < \alpha < 1.4018$ and $P_\infty < P_w < P_0$ for $\alpha > 1.4018$ and in Fig. 2(c): $E_{I,w} < \inf(E_{I,0}, E_{I,\infty})$.

5.4. Euler with cubic collisions, $\lambda = 2$

First, we rewrite (5.1) and (5.2):

$$2N_1 = A - N_{3,1}^-, \quad N_{6,5}^- = B - 2N_5, \quad N_5 = 2d_* N_{3,1}^- + (J + B)/2. \quad (5.7)$$

With the Maxwellian, we get a cubic equation for $N_{3,1}^-$ and deduce all N_i :

$$N_3 N_5^2 = N_1 N_6^2 \rightarrow N_5^2 N_{3,1}^- = N_1 N_{6,5}^- N_{6,5}^+, \quad N_1 = (A - N_{3,1}^-)/2, \quad (5.8)$$

$$8d_*^2 (N_{3,1}^-)^3 + 4Jd_* (N_{3,1}^-)^2 + N_{3,1}^- (J^2 + B^2 + 8d_* BA)/2 + BJA = 0,$$

as functions of J, M, E with (5.9). Second, we integrate the conservation laws:

$$J = \text{const.}, \quad 6E(z) + (\alpha_x^2 + \alpha_y^2)M(z) = CK_J = \text{const.}, \quad (5.9)$$

$$2d_* C N_{1,3}^-(z) + J/2 = -C N_{5,6}^-(z)/2 + (C + 1)J/2 = K_E = \text{const.}$$

From $z \rightarrow \infty$, $N_{i,j}^- = N_{i,j}^-(\infty)$, $(i, j) = (3, 1), (5, 6)$ in (5.8), $CK_J = 6E_\infty + (\alpha_x^2 + \alpha_y^2)M_\infty/2$ and from $z \rightarrow 0_+$, $N_{i,0}$ giving the impinging densities ($i = 3, 6$) from the known emerging ones ($i = 1, 5$), we get a link between the interface and the asymptotic variables:

$$N_{3,0} = N_{1,0} + [J/2 - K_E]/2d_* C, \quad N_{6,0} = N_{5,0} + [2K_E - (C + 1)J]/C, \quad (5.10)$$

$$N_{6,0} = -N_{5,0} - 16d_* N_{1,0}/2 + K_J - 2J + 4K_E.$$

6. A class of DVMs with five independent densities $N_i(z)$, Fig. 3

We present a class of models, Fig. 3(a), with $(2 + 6d_*)$ velocities \vec{v}_i and two arbitrary parameters, λ , β along the z , x axes, which enter into the \vec{v}_i coordinates:

$$\begin{aligned} d = 2: & \text{ eight } \vec{v}_i(x, y = 0, z), & d = 3: & \text{ add with } x \rightleftharpoons y, \text{ six } \vec{v}_i(x = 0, y, z), \\ d = 2, & \vec{v}_1 : (\lambda + 1, 0, -1), & \vec{v}_3 : (\beta, 0, \lambda), & \vec{v}_7 : (\beta, 0, -2 - \lambda), \quad \lambda > 0, \\ x \rightarrow -x, & \vec{v}_i \rightarrow \vec{v}_{i+1}, \quad i = 1, 3, 7, & \vec{v}_6 : (0, 0, \lambda), & \vec{v}_5 : (0, 0, -\lambda - 2). \end{aligned} \quad (6.1)$$

These models with five independent $N_i(z)$, $i = 1, 3, 5, 6, 7$, are symmetric with respect to the z -axis but not for any \vec{v}_i we have the opposite $-\vec{v}_i$. First, with only the conservation relations, we study the necessary condition for P to be nonmonotonic. Second, we introduce binary collisions and study the exact solutions for any λ value. We solve the equations for the microscopic densities (a 2×2 Riccati system) which are independent of β . From a set of $N_i(z) > 0$, varying β , only macroscopic densities $E(z)$, $E_I(z)$, $P(z)$ will vary with β .

6.1. Possible nonmonotonic pressures $E_{0,\infty}^- M_{0,\infty}^- < 0$, if $n_7/n_1 < 0$

Study of $N_i = n_{0i} + n_i F(z)$, without explicit collisions. We write the evolution equations l_i , the three linear conservation laws (Appendix C), deduce three linear l_i relations giving the $N_i(z)$ as functions of N_1 , N_7 and constants a_i :

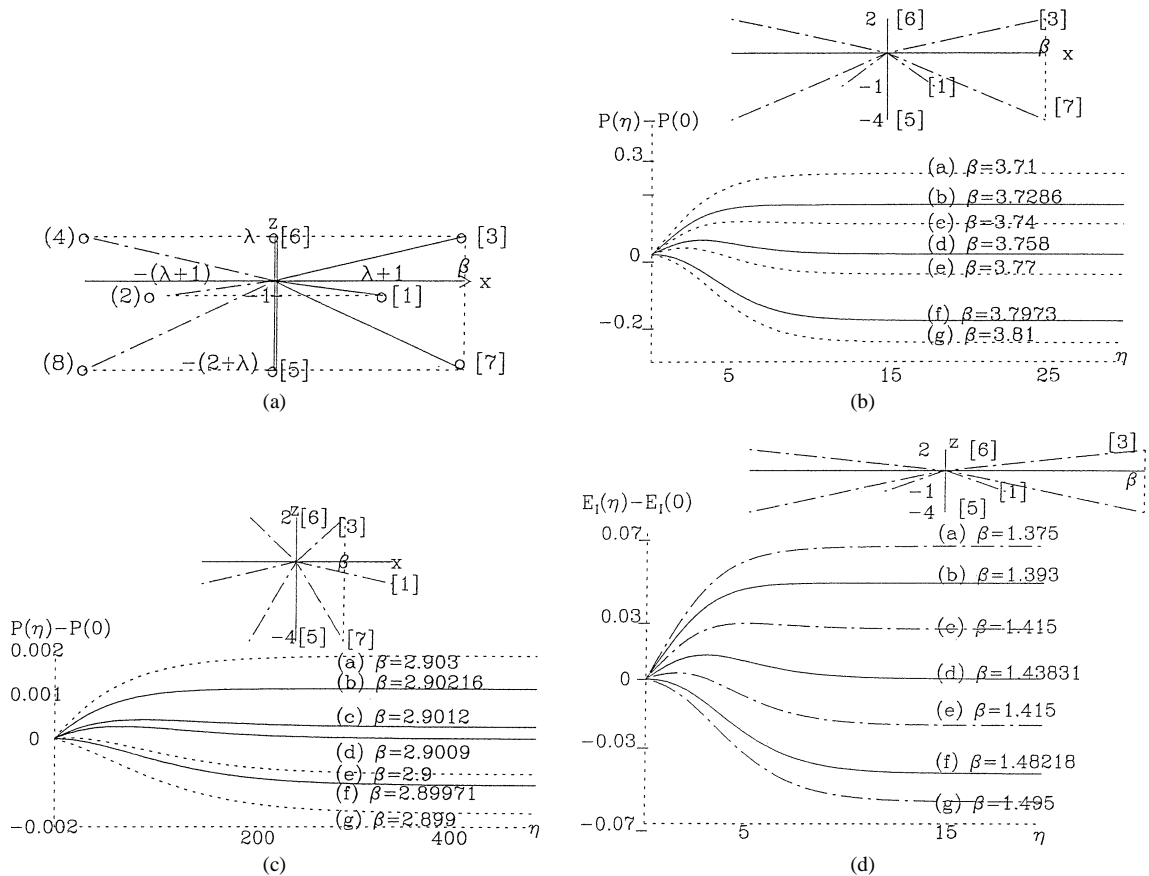


Fig. 3. (a) $d = 2$; model: five independent N_i , $i = 1, 3, 5, 6, 7$, eight v_i , two along the z -axis, $N_{i+1} = N_i$, $i = 1, 3, 7$. (b) $d = 2$; model with five independent N_i , pressure $P(\eta)$. (b)–(f) Transition monotonic and nonmonotonic; (a)–(f) monotonic; (c)–(d)–(e) nonmonotonic; (d) $P_0 = P_\infty$, $P_w > \sup(P_0, P_\infty)$. (c) $d = 2$; model with five independent N_i , pressure $P(\eta)$. (b)–(f) Transition monotonic and nonmonotonic; (a)–(f) monotonic; (c)–(d)–(e) nonmonotonic; (d) $P_0 = P_\infty$, $P_w < \inf(P_0, P_\infty)$. (d) $d = 2$; model with five independent N_i , internal energy E_I . (b)–(g) Transition monotonic and nonmonotonic; (a)–(g) monotonic; (c)–(d)–(e) nonmonotonic; (d) $E_{I,0} = E_{I,\infty}$, $E_{I,w} > \sup(E_{I,0}, E_{I,\infty})$.

$$\begin{aligned}
l_1 &= -N'_1, & l_j &= \lambda N'_j, & j &= 3, 6, & l_k &= -(2 + \lambda)N'_k, & k &= 5, 7, & d_* &= d - 1, & l_{3,7}^+ &= 0, \\
l_1 - 2l_7 + l_6/d_* &= 0, & l_1 + 2l_7 + l_5/d_* &= 0, & N_3 &= (\lambda + 2)N_7/\lambda + a_3, \\
N_5 &= -d_*[N_1/(2 + \lambda) + 2N_7] + a_5, & N_6 &= d_*[N_1 - 2(2 + \lambda)N_7]/\lambda + a_6.
\end{aligned} \tag{6.2}$$

With M , E , J , we deduce: it is possible for P to be nonmonotonic if $\bar{n}_7 := n_7/n_1 < 0$.

$$\begin{aligned}
M &= 2d_*(N_{1,3}^+ + N_7) + N_{5,6}^+, \\
E &= d_*[N_1(1 + (\lambda + 1)^2) + (\beta^2 + \lambda^2)N_3 + (\beta^2 + (2 + \lambda)^2)N_7] + \lambda^2 N_6/2 + (\lambda + 2)^2 N_5/2, \\
J &= \lambda(2d_*a_3 + a_6) - (2 + \lambda)a_5, & n_3 &= (\lambda + 2)n_7/\lambda, & n_5/d_* &= -n_1/(\lambda + 2) - 2n_7, \\
\lambda n_6/d_* &= n_1 - 2(2 + \lambda)n_7, & M_b/d_*n_1 &= 2(\lambda + 1)^2/\lambda(\lambda + 2) > 0, \\
E_b/n_1d_*(\lambda + 1) &= \lambda + 1 + 2\beta^2\bar{n}_7/\lambda \rightarrow E_bM_b < 0 \quad \text{or} \quad M_{0,\infty}^- E_{0,\infty}^- < 0 \quad \text{if} \quad \bar{n}_7 < -\lambda(\lambda + 1)/2\beta^2 < 0.
\end{aligned} \tag{6.3}$$

6.2. Explicit binary collisions (Appendix C), $\lambda > 0$

$$\begin{aligned}
X_1 &= N_5N_6 - N_1^2, & X_3 &= \Theta(N_7N_6 - N_5N_3), & \Theta &> 0 \text{ (collision rate)}, \\
l_1 &= X_1, & l_3 &= X_3 = -l_7, & l_5/d_* &= -X_1 + 2X_3, & l_6/d_* &= -X_1 - 2X_3.
\end{aligned} \tag{6.4}$$

6.2.1. Gas

We start with $N_j(z) = n_{0,j} + n_j/D$, $D = 1 + \bar{\lambda}e^{\gamma z}$. From (6.4) $X_k(N_1, N_7, a_3, a_5, a_6)$ are quadratic in (N_1, N_7) , D^{-1} and $l_i \sim D^{-2} - D^{-1}$. We get six relations between $n_{0i}, n_i, \gamma, \Theta$ and define $\alpha = n_{07}/n_{01}$, $\lambda_i = a_i/n_{01}$, $N_{i,0} = n_{0i} + n_i/(1 + \bar{\lambda})$. With α , λ_6 , λ , β , two $N_{i,0}$ we deduce all $N_i(z)$ (and macroscopic quantities) and we can choose $\bar{n}_7 < 0$:

$$\begin{aligned}
\gamma/n_1 &= 1 + d_*^2/\lambda(2 + \lambda) - 4d_*^2(2 + \lambda)\bar{n}_7^2/\lambda = 2d_*\Theta/\lambda(2 + \lambda) \\
\rightarrow 2d_*\bar{n}_7(2 + \lambda) &= \pm\sqrt{\lambda(2 + \lambda) + d_*^2 - 2d_*\Theta} \geq 0.
\end{aligned} \tag{6.5}$$

6.2.2. Wall at $z = 0$

We retain the emerging densities $N_{w,j}$, $j = 3, 6$, write $J = X_i = 0$ (wall), deduce $N_{w,i}$, $i = 1, 5, 7$ and $M_w, E_w, E_{I,w}, P_w$.

6.2.3. Numerical calculations

$d = \lambda = 2$: pressure, Figs. 3(b) and 3(c)

Fig.	$n_{3,0}$	$n_{6,0}$	α	λ_6	\bar{n}_7	θ	β	P nonmonotonic
3(b)	1.026	0.5286	0.273	13	-0.2262	0.2863	$3.71 < \beta < 3.81$	$3.728 < \beta < 3.797$
3(c)	0.122	0.863	0.165	1.6	-0.3616	0.3161	$2.899 < 2.903$	$2.8997 < 2.90216$

with β varying in nonmonotonic- P domains, including $P_\infty = P_0$ (monotonic outside) and $P_w < \inf(P_0, P_\infty)$. With $J = -2.69$ (0.9) and $M(z)$ increasing (decreasing), we have evaporation (condensation) from the state at ∞ .

Internal energy, Fig. 3(d). The parameters are the same as in Fig. 3(b) (evaporation from ∞), except $1.375 < \beta < 1.495$. We still have a domain E_I nonmonotonic, including $E_{I,\infty} = E_{I,0}$ (monotonic outside). For the wall, we have $E_{I,w} > \sup(E_{I,0}, E_{I,\infty})$ and a strict inversion for $\beta > 1.438$.

7. A class of DVMs with six independent densities $N_i(z)$, Fig. 4

In Fig. 4(a), $d = 2$, $\bar{v}_i(x, z)$ (adding $x \rightleftharpoons y$ for $d = 3$, $(8d_* + 2)$ velocities \bar{v}_i), the x coordinates are $\pm\alpha$, $\pm 2\alpha, 0$ and ± 1 , $\pm\sqrt{(4\alpha^2 + 1)}$ for z . With scaling, we restrict the study to $\alpha = \sqrt{2}$, write \bar{v}_i , $i = 1, 3, 5, 7$, giving v_{i+1} with $x, z \rightarrow -x, z$:

$$d = 2: \quad \bar{v}_1 = (2\sqrt{2}, 1) = -\bar{v}_3, \quad \bar{v}_5 = (\sqrt{2}, 1) = -\bar{v}_7, \quad \bar{v}_9 = (0, 3) = -\bar{v}_{10}. \tag{7.1}$$

We write three collisions, the l_i for N_i and the three conservation laws:

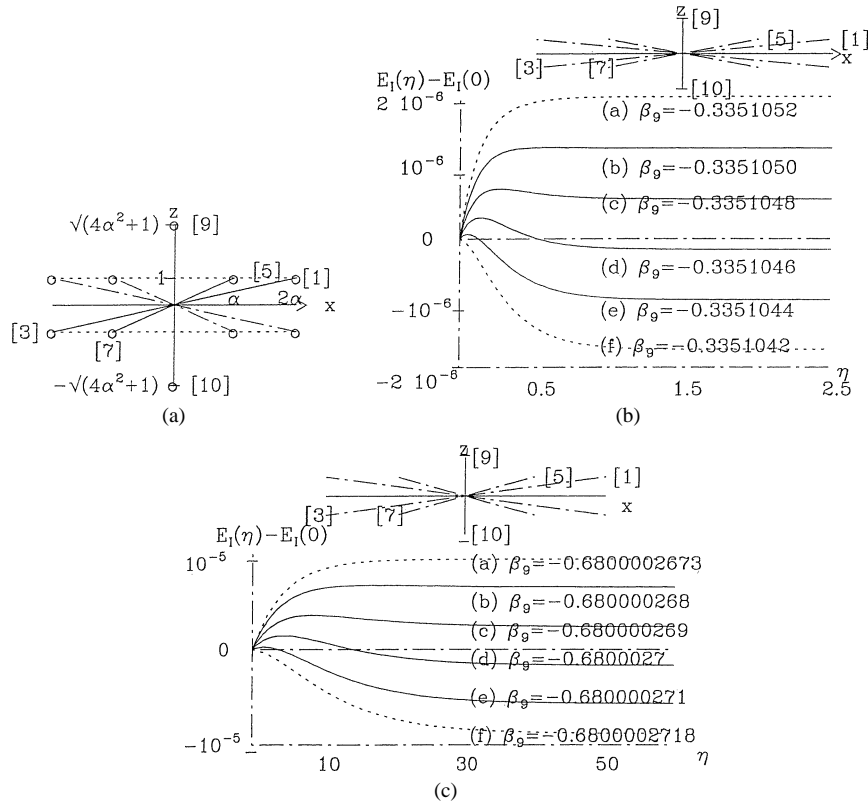


Fig. 4. (a) $d = 2$; model: six independent N_i , $i = 1, 3, 5, 7, 9, 10$, ten v_i , two along z , $N_{i+1} = N_i$, $i = 1, 3, 5, 7$, $\alpha = \sqrt{2}$. (b) $d = 2$; model with six independent N_i , internal energy E_I . (b)–(e) Transition monotonic and nonmonotonic; (a)–(f) monotonic; (b)–(c)–(d)–(e) non-monotonic. Wall: $E_{I,w} > \sup(E_{I,\infty}, E_{I,0})$; gas: $\beta_9 (<, >, =) -0.3350465 \rightarrow E_{I,0} (>, <, =) E_{I,\infty}$. (c) $d = 3$; model with six independent N_i , internal energy E_I . (b)–(e) Transition monotonic and nonmonotonic; (a)–(f) monotonic; (b)–(c)–(d)–(e) nonmonotonic. Wall: $E_{I,w} > \sup(E_{I,\infty}, E_{I,0})$; gas: $\beta_9 (<, >, =) -0.6800002693 \rightarrow E_{I,0} (>, <, =) E_{I,\infty}$.

$$X_1 = N_9 N_{10} - N_1 N_3, \quad X_2 = N_3 N_5 - N_1 N_7, \quad X_4 = N_1 N_5 - N_9 N_7, \quad (7.2)$$

$$l_i = N'_i, \quad i = 1, 5, \quad = -N'_i, \quad i = 3, 7, \quad l_9 = 3N'_9, \quad l_{10} = -3N'_{10}.$$

$$l_1 = \theta_1 X_1 + \theta_2 X_2 - X_4, \quad l_3 = \theta_1 X_1 - \theta_2 X_2, \quad l_5 = -\theta_2 X_2 - X_4, \quad l_7 = \theta_2 X_2 + X_4,$$

$$l_9 = 2d_*(-\theta_1 X_1 + X_4), \quad l_{10} = -2d_* X_1 \quad (\text{collision rates } \theta_i > 0) \quad (7.3)$$

$$2d_*(l_{1,3}^+ + l_{5,7}^+) + l_{9,10}^+ = 6d_*(3l_{1,3}^+ + l_{5,7}^+) + 9l_{9,10}^+ = 2d_*(l_{1,3}^- + l_{5,7}^-) + 3l_{9,10}^- = 0.$$

We deduce three l_i relations and N_i , $i = 3, 7, 10$ (with constant a_i) from $i = 1, 5, 9$:

$$\rightarrow \quad l_7 = -l_5, \quad l_{10} = 2d_* l_{1,5} + 2l_9, \quad l_3 = -(2l_1 + l_5 + 3l_9/2d_*) \rightarrow \quad N_7 = N_5 + a_7, \quad (7.4)$$

$$N_3 = 2N_1 + N_5 + 9N_9/2d_* + a_3, \quad N_{10} = -2d_* N_{1,5}/3 - 2N_9 + a_{10}.$$

We define scaled parameters and, for collisions X_i , terms $X_i^{(j)}/D(z)^j$:

$$\begin{aligned} \beta_i &= n_i/n_1, & \alpha_i &= n_{0i}/n_{01}, & \lambda_i &= a_i/n_{01}, & N_i(z) &= n_{0i} + n_i/D, & D(z) &= 1 + \bar{\lambda} e^{\gamma z}, \\ X_i(z) &= \sum_{j=0,1,2} n_1^j n_{01}^{(2-j)} X_i^{(j)}/D(z)^j. \end{aligned} \quad (7.5)$$

In Appendices D.1 and D.2 from β_5, β_9 and two $N_{i,0}$, we deduce all $N_i(z)$ and $E_b M_b < 0$ for the criterion. With $J = -2d_* a_{3,7}^+ - 3a_{10}$ and M, E we can deduce E_I, P :

$$M = 2d_*(N_{1,3}^+ + N_{5,7}^+) + N_{9,10}^+, \quad E = d_*(9N_{1,3}^+ + 3N_{5,7}^+) + 9N_{9,10}^+/2. \quad (7.6)$$

7.1. Wall

We start with the emerging densities $N_{i,0} = N_{w,i}$, $i = 1, 5, 9$, and in D3 with $J_w = 0$, $X_i = 0$ deduce: $N_{w,7} = N_{w,5}$, $N_{w,1} = N_{w,k}$, $k = 9, 3, 10$.

7.2. Numerical calculations

Figs. 4(b) and 4(c): with $J < 0$, $M(z) \leq M(\infty)$ (evaporation from ∞), $E_{I,w} > \sup(E_{I,0}, E_{I,\infty})$, and β_9 varying, we present domains with E_I nonmonotonic, including $E_{I,0} = E_{I,\infty}$ (E_I monotonic outside):

d	$N_{1,0} = N_{9,0}$	β_5	θ_i , $i = 1, 2$	E_I nonmonotonic
2	200	0.005	8×10^{-6} , 2.6	$-0.3351056 \leq \beta_9 \leq -0.3351044$
3	0.02	0.02	5×10^{-8} , 3.1	$-0.680000271 \leq \beta_9 \leq -0.680000268$

8. Concluding remarks

We recall that, in this paper, for a semi-infinite expanse of a gas bounded by its own condensed phase located at $z = 0$, z being the coordinate of the axis perpendicular to the interface, *our goal was to present criteria for the prediction of overshoots or inversion of the macroscopic quantities of the gas flow* Y (internal energy E_I or pressure P). They have jumps on the interface $z = 0$ as it is shown by the differences between their values Y_w in the condensed phase and Y_0, Y_∞ in the gas. On the contrary, far from the interface the state of the gas flow tends asymptotically to a Maxwellian state. The convergence of the Y to the Y_∞ of the Maxwellian state at infinity is not possible for any arbitrary choice of the variables Y_w . We must not have negative densities, *this was done with exact solutions*. In the *Euler equations* (Sections 4 and 5), we compute all the macroscopic variables of the flow at the interface and obtain the relations linking them to the macroscopic variables at infinity.

We recall [1–6] that there is evaporation (condensation) when the density of the vapor near the interface is lower (higher) than the saturation density. As the flux of matter (here J) is negative (positive), the vapor flows from the hot (cold) to the cold (hot) interface. Here, this means that we have *evaporation (condensation)* from the $+\infty$ interface if $J < 0$ (or > 0) and $M(z)$ decreases (increases) from M_∞ . Then, in Figs. 1(b)–1(d), 2(b), 2(c), 3(b), 4(b) and 4(c) (Fig. 3(c)), we have evaporation (condensation) from the interface at $+\infty$.

We were interested in *domains* where $Y(z)$, for the gas, could be *nonmonotonic (first study for the pressure)*. We have presented different variables $z, \eta = \text{const.}$, z for the coordinate perpendicular to the wall and either $Y(z)/Y_w$ or $Y(z) - Y_0$, but we observe similar patterns. Besides, the features in $d = 2$ or 3 , are also similar. We find a small subdomain with nonmonotonic $Y(z)$ (including for the gas the transition curve $Y(z)$ with $Y_0 = Y_\infty$, so separating the subdomain into $Y_0 \geq Y_\infty$) surrounded by large monotonic Y domains. Concerning the locations of the wall Y_w versus the gas Y_0 or Y_∞ , we find in general (except Fig. 2(b)) that Y_w is larger or smaller than the two gas values. For our models with 4, 4, 5, (6) independent densities, depending on a parameter, λ ($3, \alpha = \sqrt{2}$) (z projection of the velocities), *we have checked whether the conditions for nonmonotonic $Y(z)$ were satisfied*. In Lemmas 1bis and 2bis, the criteria are written in terms of the momentum and of the boundary values for the mass and the energy. In our numerical examples we have verified that the limits of these criteria correspond to the limits of the subdomains where $Y(z)$ are nonmonotonic including $Y_0 = Y_\infty$, while outside $Y(z)$ are monotonic.

- *First*, we construct one solution with positive microscopic densities, mass M and momentum J macroscopic quantities. Then we use only one varying parameter, called β or α (projections of the velocities along coordinates parallel to the wall) present only into E, E_I, P for the gas and $E_w, E_{I,w}, P_w$ for the wall. We present one-dimensional curves $Y(z, \beta)$ and $Y(z, \alpha)$. As a possible generalization, we could study the curves $Y(z, \beta, \alpha)$.
- *Second*, let us now fix the values of the parameters β, α and study the nonmonotonic $Y(z)$ domains when one of the $N_{i,0}$ parameters is varying. Now the microscopic densities, M, J as well as E, E_I, P are different. We give examples in Figs. 1(d) and 2(c) with only $N_{7,0}, N_{6,0}$ varying but find for the $Y(z, N_{i,0})$ curves the same structures as previously.
- *Third*, for systems of Riccati equations (not scalar integrable), there exists [19,20] also nonmonotonic microscopic $N_i(z)$, and we could complete a study of nonmonotonic macroscopic quantities.
- *Fourth*, we mention that in DVMs a great restriction of the models occurs, due to the acceptance of only “physical” models, here no more than three physical invariants and “physical models” with more than six independent $N_i(z)$ exist (see Appendix E for a eight N_i). *Complete analytical proofs with only binary collisions* for “physical models”, filling all the

integers of the plane for binary mixtures and for single gas have been given [23,24]. Here, such general models (without velocities parallel to the wall) are more difficult.

- *Fifth*, with only the conservation laws, without explicit collisions, we have obtained the criteria for nonmonotonic P , E_I .

We became aware of a recent thesis [25] on “Evaporation/condensation for DVMs in half-space and between two interfaces”. *First, the temperature and pressure criteria (and explicit overshoots) is not considered in [25].* Second, for the DVMs models, the main difference is that they have no velocities (except one called (C.1)) along the axis perpendicular to the interface. Here, this model (C.1), is given in Fig. 2(a) with $\lambda = 1$, but we prove that possible P nonmonotonic require $\lambda > 1$. Similarly, in Ref. [7] (not mentioned in this thesis), for a gas between two interfaces, it was shown, with a similar criterion (internal energy) that the effect cannot occur. *Third, in this thesis, there is a more general study of the evaporation/condensation problem, for instance including stationary but also nonstationary (not considered in the present paper) solutions.*

Appendix A

A.1. Model with four independent N_i , $d = 3$

No \vec{v}_i along z , Fig. 1(a).

$$\begin{aligned} 8d_*\vec{v}_i(x, y, z), \quad \eta_i^2 = 1, \quad (\eta_1\beta_x, \eta_2\beta_y, 1), \quad \eta_i = 1 \quad \rightarrow \quad \vec{v}_5 = -\vec{v}_7, \quad (\eta_1\alpha_x, \eta_2\alpha_y, \lambda), \quad \eta_i = 1, \\ \lambda > 1 \quad \rightarrow \quad \vec{v}_1 = -\vec{v}_3, \quad 4 \text{ independent } N_i, \quad i = 1, 3, 5, 7, \quad \alpha^2 := \alpha_x^2 + \alpha_y^2, \quad \beta^2 := \beta_x^2 + \beta_y^2, \end{aligned}$$

M, E, J, M_b, E_b are divided by d_* in (4.2)–(4.6) $\rightarrow M_b E_b < 0$ if $\beta \geq \lambda\alpha$, $\lambda \geq 1$.

A.1.1. Wall at $z = 0$, $\lambda = d = 2$

We retain the $N_{w,i}$, $i = 1, 5$, and from the vanishing collision and $J_w = 0$ deduce $N_{w,i+2} = N_{w,i}$ and $M_w, E_w, P_w, E_{I,w}$:

$$\begin{aligned} N_{w,1,3}^- + \lambda N_{w,5,7}^- = 0, \quad N_{w,7}/N_{w,5} = (N_{w,3}/N_{w,1})^\lambda \quad \rightarrow \quad (1 - N_{w,3}/N_{w,1}), \\ \left[\lambda N_{w,5} \sum_{q=0}^{\lambda-1} (N_{w,3}/N_{w,1})^q + N_{w,1} \right] = 0 \quad \rightarrow \quad N_{w,3} = N_{w,1}, \quad N_{w,7} = N_{w,5}, \quad M_w/4d_* = N_{w,1,5}^+, \\ E_w = 2d_*((\beta^2 + \lambda^2)N_{w,5} + N_{w,1}(\alpha^2 + 1)) = M_w E_{I,w}/2 = P_w/2, \quad 4d_* N_{w,1} C = (\lambda^2 + \beta^2)M_w - 2E_w, \\ 4d_* N_{w,5} C = 2E_w - (1 + \alpha^2)M_w. \end{aligned}$$

A.2. $\lambda = 2$

We obtain a Riccati equation with $N_1 = n_{01} + n_1/D(\eta)$.

$$\begin{aligned} J/2 := -a_3 + 2a_{5,7}^-, \quad F_1 := a_3(2a_5 - a_7), \quad F_0 := a_3a_5^2, \quad \eta = z/2\Theta, \quad D = 1 + \bar{\lambda}e^{\gamma\eta}, \\ N_1' = -JN_1^2/4 + F_1N_1 + F_0 = \gamma n_1(D^{-1} - 1)/D, \quad n_1 = -4\gamma/J \rightarrow n_i \text{ in (4.6),} \\ n_{03} = n_{01} + a_3, \quad n_{0j} = -n_{01}/4 + a_j, \quad j = 5, 7, \quad \bar{\lambda} + 1 = n_1/(N_{1,0} - n_{01}). \end{aligned}$$

We get N_i, M without β, α , when they vary, we observe different $E_I(z)$, $P(z)$.

Appendix B. Four densities $N_i(z)$, two velocities along z , $\lambda = 2$

It is sufficient to study the collision for N_1 (collision rate Θ , $\eta = z/2\Theta$):

$$l_1 = 2dN_1/dz = \Theta(N_3N_5^2 - N_1N_6^2) \quad \rightarrow \quad N_1 = n_{01} + n_1/D, \quad D = 1 + \bar{\lambda}e^{\gamma\eta}. \quad (\text{B.1})$$

Starting with the a_i known, we substitute the $N_i(N_1)$, (5.6) into (B.1). Then from D^{-2}, D^{-1}, D^0 we get n_{01}, n_1, γ , deduce n_i, n_{0i} with (5.6):

$$J := -4d_*a_3 + a_{5,6}^-, \quad F_1 := a_5^2 - a_6^2 - 16d_*a_5a_3, \quad F_0 := a_3a_5^2, \\ D = 1 + \bar{\lambda}e^{\gamma\eta}, \quad N'_1 = \gamma n_1(1/D^2 - 1/D) = -16d_*JN_1^2 + F_1N_1 + F_0, \quad (B.2)$$

$$16n_{01}^2Jd_* = F_1n_{01} + F_0, \quad 16d_*Jn_1 = F_1 - 32d_*Jn_{01} = -\gamma, \quad n_3 = n_1, \quad n_{03} = n_{01} + a_3, \\ n_j = -8d_*n_1, \quad n_{0j} = -8d_*n_{01} + a_j, \quad j = 5, 6, \quad (B.3) \\ C := \alpha_x^2 + \alpha_y^2 + 3, \quad M = 2d_*N_{1,3}^+ + N_{5,6}^+, \quad E = d_*(C + 1)N_{1,3}^+ + N_{5,6}^+/2,$$

and all parameters except $\bar{\lambda} = -1 + n_1/(N_{1,0} - n_{01})$ given with $N_{1,0}$.

B.1. Wall

$$0 = 2\lambda d_*N_{w,1,3}^- + N_{w,5,6}^- = N_{w,3}/N_{w,1} - (N_{w,6}/N_{w,5})^\lambda = (1 - N_{w,6}/N_{w,5}), \\ \left[2\lambda d_*N_{w,1} \sum_{q=0}^{\lambda-1} (N_{w,6}/N_{w,5})^q + N_{w,5} \right] \rightarrow N_{w,3} = N_{w,1}, \quad N_{w,6} = N_{w,5}, \quad M_w/2 = 2d_*N_{w,1} + N_{w,5}, \\ E_w = 2d_*(C + 1)N_{w,1} + N_{w,5} = E_{I,w}/2M_w = P_w/2, \quad N_{1,w}Cd_* = E_w - M_w/2, \\ N_{5,w}C = M_w(C + 1) - 2E_w. \quad (B.4)$$

Appendix C. Model with five independent $N_i(z)$ and λ arbitrary

C.1. Gas

We get (6.2) from the conservation laws and write (6.4) for N_7, N_1 :

$$2d_*(l_{1,3}^+ + l_7) + l_{5,6}^+ = 2d_*(\lambda l_3 - l_1 - (2 + \lambda)l_7) + \lambda l_6 - (2 + \lambda)l_5 \\ = 2d_*[l_1(1 + (\lambda + 1)^2) + l_3(\beta^2 + \lambda^2) + l_7(\beta^2 + (2 + \lambda)^2)] + \lambda^2 l_6 + (2 + \lambda)^2 l_5 = 0, \quad (C.1)$$

$$(2 + \lambda)\gamma n_7(1/D - 1)/D\Theta = 2d_*N_1N_7/\lambda + N_7J/\lambda + N_1d_*a_3/(2 + \lambda) - a_3a_5, \\ \gamma n_1(1 - 1/D)/D = -(1 + d_*^2/\lambda(2 + \lambda))N_1^2 + 4d_*^2(2 + \lambda)N_7^2/\lambda - 2d_*N_7(a_6 + a_5(2 + \lambda)/\lambda) \\ + N_1d_*(a_5/\lambda - (2 + \lambda)a_6) + a_5a_6, \\ N_i = n_{0i} + n_i D^{-1}(z). \quad (C.2)$$

With the D^{-2} terms and $\bar{n}_7 = n_7/n_1$, we get (6.5). With $\lambda_i = a_i/n_{01}$, $\alpha = n_{07}/n_{01}$ and the (C.2) rhs for D^0 , we get λ_i, α relations:

$$\lambda_3[d_*(2\alpha + 1/(2 + \lambda)) - \lambda_5] = -\alpha[2d_*/\lambda + \lambda_6 - (2 + \lambda)\lambda_5/\lambda], \\ \lambda_5[\lambda_6 + d_*(1 - 2\alpha(2 + \lambda))/\lambda] = 1 + d_*^2/\lambda(2 + \lambda) - 4d_*^2\alpha^2(2 + \lambda)/\lambda + d_*\lambda_6(2\alpha + 1/(2 + \lambda)). \quad (C.3)$$

The opposite D^{-2}, D^{-1} terms in (C.2) give (C.4) and a \bar{n}_7 polynomial (cubic).

$$2d_*\bar{n}_7/\lambda + (n_{01}/n_1)F_7 = 0, \quad 4\bar{n}_7^2 - 1 - d_*^2/\lambda(2 + \lambda) + (n_{01}/n_1)F_1 = 0, \quad (C.4)$$

$$F_7 = 2d_*(\alpha + \bar{n}_7)/\lambda + \bar{n}_7[\lambda_6 - (2 + \lambda)\lambda_5/\lambda + 2d_*\lambda_3] + d_*\lambda_3/(2 + \lambda), \\ F_1 = -2(1 + d_*^2/\lambda(2 + \lambda)) + 8d_*^2(2 + \lambda)\bar{n}_7\alpha/\lambda - 2\bar{n}_7d_*(\lambda_6 + (2 + \lambda)\lambda_5/\lambda) + d_*(\lambda_5/\lambda - \lambda_6/(2 + \lambda)) \quad (C.5)$$

$$F_7[1 + (d_*^2/\lambda)(1/(2 + \lambda) - 4\bar{n}_7^2(2 + \lambda))] + F_1\bar{n}_72d_*/\lambda = 0 \rightarrow \sum_{j=0}^3 c_j \bar{n}_7^j = 0,$$

$$n_{01} = [N_{7,0} - \beta N_{1,0}]/(\alpha - \beta) \rightarrow n_{01} \rightarrow n_1 \quad \text{and} \quad \bar{\lambda} + 1 = n_1/(N_{1,0} - n_{01}). \quad (C.6)$$

We start with (α, λ_6) given, deduce $\lambda_5, \lambda_3, \bar{n}_7, n_{01}/n_1$ in (C.3)–(C.5), $\Theta, \gamma/n_1$ in (6.5). Adding $N_{1,0}, N_{7,0}$, we get $n_{01}, \bar{\lambda}$ in (C.6) and all microscopic $N_i(z)$.

C.2. Wall

We start with $N_{w,3}$, $N_{w,6}$, $\lambda = d = 2$, write the vanishing collision terms, $J_w = 0$, deduce $N_{w,1} \rightarrow N_{w,5} \rightarrow N_{w,7}$ and M_w , $2E_w = P_w = E_{I,w} M_w$:

$$\begin{aligned} N_{w,5} &= N_{w,1}^2 / N_{w,6}, \quad N_{w,7} = N_{w,3} N_{w,5} / N_{w,6}, \quad 2N_{w,3,5}^- + N_{w,6,1}^- = 4N_{w,7}, \\ 2N_{w,1}^2 + N_{w,1} N_{w,6}^2 / (2N_{w,3} + N_{w,6}) &= N_{w,6}^2 \rightarrow N_{w,1} \rightarrow N_{w,5} \rightarrow N_{w,7}, \quad M_w = 2(N_{w,1,3}^+ + N_{w,7}) + N_{w,5,6}^+, \\ E_w &= 10N_{w,1} + N_{w,3}(4 + \beta^2) + N_{w,7}(16 + \beta^2) + 8N_{w,5} + 2N_{w,6}. \end{aligned}$$

Appendix D. Model with six independent $N_i(z)$, Fig. 4(a), $\alpha = \sqrt{2}$

D.1. From β_5, β_9 arbitrary (7.5), we get all $\beta_i, X_i^{(2)}, M_b, E_b$ and $\theta_k, k = 1, 2$:

$$\begin{aligned} \rightarrow \quad \beta_7 &= \beta_5, \quad \beta_3 = 2 + \beta_5 + 9\beta_9/2d_*, \quad \beta_{10} = -2d_*(1 + \beta_5)/3 - 2\beta_9, \quad X_1^{(2)} = \beta_9\beta_{10} - \beta_3, \\ X_2^{(2)} &= \beta_3\beta_5 - \beta_7, \quad X_4^{(2)} = \beta_5 - \beta_9\beta_7 3M_b/8n_1 = 3\beta_9 + 2d_*(1 + \beta_5) = E_b/12n_1 + d_*(2 + \beta_5) \rightarrow M_b E_b < 0 \\ \text{if } -2\beta_5 &\leq (2 + 3\beta_9)/d_* \leq -\beta_5. \end{aligned} \quad (\text{D.1})$$

We deduce θ_k while $\alpha_3 = 1/\alpha_9$, $\alpha_7 = \alpha_5/\alpha_9$, $\alpha_{10} = \alpha_9^{-2}$ and λ_i , with α_5, α_9 :

$$\begin{aligned} \gamma/n_1 &=: Y^{(2)} = \theta_1 X_1^{(2)} + \theta_2 X_2^{(2)} - X_4^{(2)} = -(\theta_2 X_2^{(2)} + X_4^{(2)})/\beta_5 = (2d_*/3\beta_9), \\ [-\theta_1 X_1^{(2)} + X_4^{(2)}] &\rightarrow \theta_2 = -(X_4^{(2)}/X_2^{(2)})[1 + 3\beta_9/2d_*]/[\beta_5 + 1 + 3\beta_9/2d_*], \\ \theta_1[2d_* X_1^{(2)}/3\beta_9] &= X_4^{(2)}[2d_*/3\beta_9 + 1/\beta_5] + \theta_2 X_2^{(2)}/\beta_5, \\ \lambda_7 &= \alpha_7 - \alpha_5, \quad \lambda_3 = \alpha_3 - 2 - \alpha_5 - 9\alpha_9/2d_*, \quad \lambda_{10} = \alpha_{10} + 2\alpha_9 + 2d_*(1 + \alpha_5)/3. \end{aligned} \quad (\text{D.2})$$

α_9, α_5 are deduced from the $D(z)^{-1}$ terms $X_i^{(1)}$ in l_i , $i = 1, 5, 9$:

$$\begin{aligned} -\gamma/n_{01} &=: Y^{(1)} = \theta_1 X_1^{(1)} + \theta_2 X_2^{(1)} - X_4^{(1)} = -[\theta_2 X_2^{(1)} + X_4^{(1)}]/\beta_5 = (2d_*/3\beta_9)[- \theta_1 X_1^{(1)} + X_4^{(1)}] \\ \rightarrow \quad \theta_2 X_2^{(1)}(1 + \beta_5 + 3\beta_9/2d_*) &+ X_4^{(1)}(1 + 3\beta_9/2d_*) = 0, \\ \theta_2 X_2^{(1)}(1 + \beta_5) + X_4^{(1)}(1 - \beta_5) &+ \beta_5 \theta_1 X_1^{(1)} = 0, \quad X_1^{(1)} = \beta_9 \alpha_{10} + \beta_{10} \alpha_9 - \beta_3 - \alpha_3, \\ X_j^{(1)} &= B_j \alpha_5 + C_j, \quad B_2 = \beta_3 - 1/\alpha_9, \quad C_2 \alpha_9 = \beta_5(1 - \alpha_9) = C_4, \quad B_4 = 1 - \beta_9/\alpha_9. \end{aligned}$$

We get two linear α_5 relations and a compatibility quartic in α_9 :

$$\begin{aligned} \alpha_5 &= -\bar{C}/\bar{B} = -\bar{E}/\bar{D}, \quad \bar{B} = \theta_2 B_2(1 + \beta_5 + 3\beta_9/2d_*) + B_4(1 + 3\beta_9/2d_*), \\ \bar{C} &= \theta_2 C_2(1 + \beta_5 + 3\beta_9/2d_*) + C_4(1 + 3\beta_9/2d_*), \quad \bar{D} = \theta_2 B_2(1 + 1/\beta_5) + B_4(1/\beta_5 - 1), \\ \bar{E} &= \theta_1 X_1^{(1)} + \theta_2 C_2(1 + 1/\beta_5) + C_4(1/\beta_5 - 1) \rightarrow \bar{C}\bar{D} = \bar{B}\bar{E}. \end{aligned} \quad (\text{D.3})$$

From β_5, β_9 , all $\beta_i, \alpha_i, \lambda_i$ and $-n_{01}/n_1 = Y^{(2)}/Y^{(1)}$ are known.

D.2. Starting with $N_{i,0} = n_{0i} + n_i/(1 + \bar{\lambda})$, $i = 1, 9$ we deduce all $N_i(z)$.

$$\begin{aligned} n_{01} &= [\beta_9 N_{1,0} - N_{9,0}]/(\beta_9 - \alpha_9), \quad n_1 = -n_{01} Y^{(1)}/Y^{(2)}, \quad \gamma = n_1 Y^{(2)} \geq 0 \rightarrow N_{i,\infty} = n_{0i}, n_{0i} + n_i, \\ \bar{\lambda} &= -1 + n_1/(N_{1,0} - n_{01}), \quad n_i = \beta_i n_1, \quad n_{0i} = \alpha_i n_{01}, \quad \alpha_k = \lambda_k n_{01} \end{aligned}$$

D.3. At the wall with $X_i = J_w = 0$ and $N_{w,i,j}^- = N_{w,i} - N_{w,j}^-$, we get:

$$\begin{aligned} N_{w,9,10}^- N_{w,9}^2 &= N_{w,9}^3 - N_{w,1}^3, \quad N_{w,j,j+2}^- N_{w,9} = N_{w,j} N_{w,9,1}^-, \quad j = 1, 5, \quad 0 = J_w = 2, \\ d_* (N_{w,1,3}^- + N_{w,5,7}^-) &+ 3N_{w,9,10}^-, \\ N_{w,9,1}^- (2d_* N_{w,1,5}/N_{w,9} + 3(1 + (N_{w,1}/N_{w,9})^2 + N_{w,1}/N_{w,9})) &= 0 \rightarrow N_{w,7} = N_{w,5} \quad \text{and} \quad N_{w,1} = N_{w,j}, \\ j &= 3, 9, 10. \end{aligned} \quad (\text{D.4})$$

Appendix E. Four–eight independent $N_i(z)$ and two, four \vec{v}_i along z models

We start with a physical four independent $N_i(z)$, for collisions with three densities belonging to a physical model, we add [10] the last and get five–eight independent N_i . For $d = 2, y = 0, \vec{v}_i(x, z): \vec{v}_1(2, 1) = -\vec{v}_3, \vec{v}_5(0, 1) = -\vec{v}_6, \vec{v}_7(0, 3) = -\vec{v}_8, \vec{v}_9(1, 2) = -\vec{v}_{11}, (x \rightarrow -x) \rightarrow \vec{v}_{i+1}, i = 1, 3, 9, 11$. For $d = 3, x = 0$, we add $\vec{v}_i(x, z) \rightarrow \vec{v}_i(y, z)$. *First*, with $N_i, i = 1, 3, 5, 6, (4d_* + 2)$ velocities \vec{v}_i and $X_1 = N_1N_6 - N_3N_5$, we get $l_3 = X_1 = -l_1, 2d_*X_1 = l_5 = -l_6$ and three invariants $l_{5,6} = l_{1,3} = 2d_*l_1 + l_5 = 0$ equivalent to the three conservation laws. *Second*, adding successively: $X_i: N_1^2 - N_6N_7, N_3^2 - N_5N_8, N_5N_7 - N_9^2, N_8N_6 - N_{11}^2$, we get physical models including $N_7, N_8, N_9, N_{11}, 4d_* + 3, 4, 6d_* + 4, 8d_* + 4$ velocities \vec{v}_i (four along the z -axis).

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