

B R I E F N O T E S

EXACT SOLUTIONS OF A DISCRETE VELOCITY MODEL OF A GAS WITH MOLECULES DISSOCIATION

R. M O N A C O (GENOVA) and T. P L A T K O W S K I (WARSZAWA)

We propose an elementary discrete velocity model of a gas, describing dissociation of diatomic molecules. We found exact analytical solutions to the following problems: 1) wave propagation in an unbounded domain; 2) boundary value problem with boundary conditions admitting sources on the walls.

1. INTRODUCTION

Lately interest has been devoted to the construction of discrete velocity models of the Boltzmann equation for gases subjected to chemical reactions (see, for instance, [1,2]). Such models generally have a rather cumbersome nonlinear structure so that the study of fluid dynamical problems as, for instance, shock-wave propagation or the stationary state of a gas confined in a bounded domain can be performed only by numerical computations.

On the other hand it is known [3,4] that some discrete models for inert gases admit exact solutions for the afore-mentioned problems. For this reason, in this note we propose an elementary discrete velocity model of the Carleman type for gases with dissociation of diatomic molecules, which provides exact analytical solutions for wave propagation in an unbounded domain, and for a stationary boundary value problem.

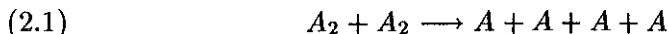
2. THE MODEL

Consider a mixture of two gases with velocities attaining on a line $x \in \mathbb{R}$: atoms A with velocities \mathbf{v}_i : $|\mathbf{v}_i| = 1$ and mass m ;

molecules A_2 with velocities \mathbf{w}_i : $|\mathbf{w}_i| = \mu$ and mass $2m$ where $i = 1, 2$ denotes particles moving, respectively, in the positive and negative directions of the x -axis.

Let $N_i(t, x)$, $M_i(t, x)$ be the distribution functions of atoms and molecules, respectively.

Atoms are treated as mass points, and therefore we assume that their collisions do not change the distribution functions N_i (Knudsen gas assumption). Collisions between molecules with incoming opposite velocities w_1, w_2 lead to chemical dissociation, i.e.



with two atoms having velocity v_1 and two velocity v_2 ; such a hypothesis assures momentum conservation throughout a collision.

Moreover, under these assumptions one can calculate the energy of the chemical link $\varepsilon > 0$; in fact energy conservation in the collision process gives

$$\varepsilon = 2m(1 - \mu^2)$$

which leads to the constraint

$$\mu < 1.$$

The above collisional scheme assures that the dissociation (2.1) is the only one which leads to changes of the particle distribution functions; moreover, it supplies the simplest possible discrete velocity model with a nonlinear collisional term which preserves momentum. Under the above assumptions, the evolution equations for the distribution functions of molecules can be written as follows:

$$(2.2) \quad \begin{aligned} \frac{\partial M_1}{\partial t} + \mu \frac{\partial M_1}{\partial x} &= -Q, \\ \frac{\partial M_2}{\partial t} - \mu \frac{\partial M_2}{\partial x} &= -Q, \end{aligned}$$

where the collisional term Q takes into account the "loss" of molecules, which is proportional to the relative velocity 2μ of the colliding particles, to the cross-sectional area S and to both distribution functions M_1 and M_2 . Thus

$$(2.3) \quad Q = 2\mu S M_1 M_2 =: \sigma M_1 M_2.$$

On the other hand, molecules which are the "loss" for chemical dissociation must appear in the evolution equations for the distribution functions of the atoms as a "gain" term. Therefore, because of mass conservation, these equations will be given by

$$(2.4) \quad \begin{aligned} \frac{\partial N_1}{\partial t} + \frac{\partial N_1}{\partial x} &= Q, \\ \frac{\partial N_2}{\partial t} - \frac{\partial N_2}{\partial x} &= Q. \end{aligned}$$

Equations (2.2) – (2.4) represent the proposed discrete velocity model; note that the equations for molecules are independent of those of atoms. Starting from this point we will search exact solutions of such equations for two classical fluid dynamical problems.

3. WAVE PROPAGATION

We look for a general solution to Eqs.(2.1) – (2.4) in the form of a soliton-type expression [3], i.e.,

$$(3.1) \quad \begin{aligned} M_i &= \frac{d_i}{1 + \exp(z_i)}, & N_i &= \frac{\tilde{d}_i}{1 + \exp(\tilde{z}_i)}, \\ z_i &= k_i t + h_i x, & \tilde{z}_i &= \tilde{k}_i t + \tilde{h}_i x, \quad i = 1, 2 \end{aligned}$$

with $d_i, \tilde{d}_i \in \mathfrak{R}_+$.

We prove the following proposition:

PROPOSITION 1. Equations (2.4) admit a non-trivial positive soliton-type solution if

$$(3.2) \quad \begin{aligned} k_1 &= -k_2 = -\tilde{k}_1 = \tilde{k}_2, & h_1 &= -h_2 = -\tilde{h}_1 = \tilde{h}_2, \\ k_1 &= \sigma(d_2 - d_1)/2, & h_1 &= \sigma(d_1 + d_2)/2, \\ \tilde{d}_1 &= \frac{2\mu d_1 d_2}{d_1(1 - \mu) + d_2(1 + \mu)}, & \tilde{d}_2 &= \frac{2\mu d_1 d_2}{d_1(1 + \mu) + d_2(1 - \mu)}, \end{aligned}$$

d_1, d_2 being two positive arbitrary constants.

P r o o f. The proof is straightforward by inserting the Eqs. (3.1) into Eqs. (2.4), and by verifying that only the relation (3.2) assures positivity of the distribution functions.

As a particular case of the solution found by Proposition 1, we discuss the following travelling wave problem. Define: $z = x + \beta t$, $z \in \mathfrak{R}$ with β being the constant propagation speed. The set of Eqs. (2.2) – (2.4) reads now

$$(3.3) \quad \begin{aligned} (\beta + \mu) \frac{dM_1}{dz} &= -Q, \\ (\beta - \mu) \frac{dM_2}{dz} &= -Q, \\ (\beta + 1) \frac{dN_1}{dz} &= Q, \\ (\beta - 1) \frac{dN_2}{dz} &= Q \end{aligned}$$

and has three first integrals,

$$(3.4) \quad \begin{aligned} (\beta + \mu)M_1 - (\beta - \mu)M_2 &= I_1, & I_1 &\in \mathfrak{R}, \\ (\beta + 1)N_1 - (\beta - 1)N_2 &= I_2, & I_2 &\in \mathfrak{R}, \\ (\beta + \mu)M_1 + (\beta + 1)N_1 &= I_3, & I_3 &\in \mathfrak{R}. \end{aligned}$$

Below we find solutions of Eqs.(3.3) with given distribution functions of atoms at $z \rightarrow -\infty$ and with limit conditions for molecules at $\pm\infty$ which correspond to the equilibrium states without dissociation ($Q = 0$). In particular, we assume

for atoms

$$(3.5)_1 \quad \begin{aligned} \lim_{z \rightarrow -\infty} N_1 &= c_1, & \lim_{z \rightarrow -\infty} N_2 &= c_2, \\ \lim_{z \rightarrow \infty} N_1 &= \gamma_1, & \lim_{z \rightarrow \infty} N_2 &= \gamma_2, \end{aligned}$$

for molecules

$$(3.5)_2 \quad \begin{aligned} \lim_{z \rightarrow -\infty} M_1 &= a, & \lim_{z \rightarrow -\infty} M_2 &= 0, \\ \lim_{z \rightarrow \infty} M_1 &= 0, & \lim_{z \rightarrow \infty} M_2 &= \alpha, \end{aligned}$$

where a, c_1, c_2 are given data, whereas $\alpha, \gamma_1, \gamma_2$ are numbers which can be determined from the first integrals (3.4) written at $\pm\infty$ (Rankine-Hugoniot conditions), i.e.

$$\begin{aligned} \alpha &= a \frac{\mu + \beta}{\mu - \beta}, \\ \gamma_1 &= c_1 + a \frac{\mu + \beta}{1 + \beta}, \\ \gamma_2 &= c_2 - a \frac{\mu + \beta}{1 - \beta}. \end{aligned}$$

In particular, the relationship for α provides the following implications:

$$\begin{aligned} i) \quad \alpha > 0 &\implies |\beta| < \mu, \\ ii) \quad \beta \in \mathfrak{R}_- &\implies \alpha < a && \text{forward propagation,} \\ iii) \quad \beta \in \mathfrak{R}_+ &\implies \alpha > a && \text{backward propagation.} \end{aligned}$$

First we solve the problem for molecules; with the help of the first integral (3.4)₁ and the limit conditions (3.5)₂ the equations (3.3)₁ are reduced to

$$\begin{aligned} \frac{dM_1}{dz} &= \frac{\sigma}{\beta - \mu} M_1(a - M_1), \\ M_2 &= \frac{\mu + \beta}{\mu - \beta} (a - M_1), \end{aligned}$$

and therefore we obtain the distribution functions for molecules, i.e.

$$(3.6) \quad \begin{aligned} M_1(z) &= \frac{a}{1 + \exp[a\sigma z/(\mu - \beta)]}, \\ M_2(z) &= \frac{\mu + \beta}{\mu - \beta} \frac{a}{1 + \exp[-a\sigma z/(\mu - \beta)]}. \end{aligned}$$

From the knowledge of M_1 and M_2 we then solve Eqs.(3.3)_{3,4} for atoms. Using the limit conditions (3.5)₁ and the first integrals (3.4)₂ and (3.4)₃, we obtain

$$(3.7) \quad \begin{aligned} N_1(z) &= c_1 + \frac{\mu + \beta}{1 - \beta} \frac{a}{1 + \exp[-a\sigma z/(\mu - \beta)]}, \\ N_2(z) &= c_2 - \frac{\mu + \beta}{1 - \beta} \frac{a}{1 + \exp[-a\sigma z/(\mu - \beta)]}. \end{aligned}$$

REMARK. Positivity of the distribution functions N_1, N_2 is provided under the conditions:

$$\begin{aligned} \text{for forward shock-waves: } & -\mu < \beta < \frac{c_2 - a\mu}{c_2 + a} < 0, \\ \text{for backward shock-waves: } & 0 < \beta < \mu < \frac{c_2 - a\mu}{c_2 + a}. \end{aligned}$$

4. A BOUNDARY VALUE PROBLEM

In this section we consider the problem of existence and uniqueness of positive stationary states of the system of dissociating molecules in a bounded interval for $x \in [-1, 1]$ with prescribed general boundary conditions on both ends of the interval. Referring only to the evolution equations for molecules, the relevant mathematical formulation reads:

$$(4.1) \quad \begin{aligned} \mu \frac{dM_1}{dx} &= -Q, \\ -\mu \frac{dM_2}{dx} &= -Q \end{aligned}$$

with the boundary conditions [4]

$$(4.2) \quad \begin{aligned} x = -1 & : M_1^- = \alpha_1 M_2^- + \delta_1, \\ x = 1 & : M_2^+ = \alpha_2 M_1^+ + \delta_2, \end{aligned}$$

where $M_i^\pm = M_i(x = \pm 1)$, $i = 1, 2$, $\alpha_i \delta_i$ are given positive parameters; note that $\alpha_1 = \alpha_2 = 1$ and $\delta_1 = \delta_2 = 0$ correspond to pure specular reflection boundary conditions without sources.

To solve the BVP (4.1), (4.2), we insert the first integral of Eq.(4.1)_{1,2}

$$(4.3) \quad M_1 + M_2 = I = \text{const} > 0$$

into Eq.(4.1)₁ and solve the resulting logistic equation for M_1 . The solution reads

$$(4.4) \quad \begin{aligned} M_1(x) &= \frac{I}{1 + (I/M_1^- - 1) \exp[\sigma' I(x + 1)]}, \\ M_2(x) &= I - M_1(x), \end{aligned}$$

where I , M_1^- are unknown constants and $\sigma' = \sigma/\mu$. Note that, in this problem, the total density $\rho = M_1 + M_2$ does not depend on x .

To find the unknown constants, we note that Eqs.(4.4) provide three relationships between the constants:

$$(4.5) \quad \begin{aligned} M_1^+ &= \frac{I}{1 + (I/M_1^- - 1) \exp(2\sigma'I)}, \\ M_1^- + M_2^- &= I, \\ M_1^+ + M_2^+ &= I. \end{aligned}$$

Together with Eqs.(4.2) we have then an algebraic system of five equations for five unknown constants which, after some manipulations, can be reduced to one nonlinear equation for I :

$$(4.6)_1 \quad \exp(2\sigma'I) = \frac{\alpha_1 I + \delta_1}{I - \delta_1} \frac{\alpha_2 I + \delta_2}{I - \delta_2}, \quad I \in \mathfrak{R}_+$$

providing that we also obtain

$$(4.6)_2 \quad M_1^- = \frac{\alpha_1 I + \delta_1}{1 + \alpha_1};$$

this ends the calculation of constants in the solutions (4.4).

In such a way the problem of existence and uniqueness of solutions of the considered BVP has been reduced to the same problem for Eq.(4.6)₁. Accordingly we can now prove the following proposition:

PROPOSITION 2.

i) In the case of boundary conditions without sources ($\delta_1 = \delta_2 = 0$) there exists a unique positive solution to the BVP (4.1), (4.2) if

$$\alpha_1 \alpha_2 > 1;$$

ii) If $\delta_1 > 0$, $\delta_2 > 0$, and $\sigma' < (1 + \alpha_1)(2\delta_1)^{-1} + (1 + \alpha_2)(2\delta_2)^{-1}$, then there exists a unique positive solution $I_0 > \max(\delta_1, \delta_2)$.

P r o o f. Let us first prove (i): Eq.(4.6)₁ provides a unique solution $I_0 > 0$ given by

$$I_0 = \frac{1}{2\sigma'} \log(\alpha_1 \alpha_2).$$

Moreover, $M_1(x)$ and $M_2(x)$ are positive, because in this case

$$\frac{I_0}{M_1^-} = \frac{1 + \alpha_1}{\alpha_1} > 1.$$

In physical terms this means that we must have production ($\alpha_1 \alpha_2 > 1$) of molecules at least at one point of the boundaries larger than adsorption at the other as a condition for the existence of a positive stationary solution. In the case of general boundary conditions (ii) the proof

is a straightforward consequence of the analytical study of the left and right hand sides of Eq.(4.6)₁. In fact the r.h.s. function has two positive poles for $I = \delta_1$, $I = \delta_2$ it is positive monotone increasing in the range $I \in]0, \min(\delta_1, \delta_2)[$, negative for $I \in]\min(\delta_1, \delta_2), \max(\delta_1, \delta_2)[$, and positive monotone decreasing for $I \in]\max(\delta_1, \delta_2), +\infty[$. Its first derivative for $I = 0$ is equal to $\frac{\alpha_1 + 1}{\delta_1} + \frac{\alpha_2 + 1}{\delta_2}$. Then if $\sigma' < \frac{\alpha_1 + 1}{2\delta_1} + \frac{\alpha_2 + 1}{2\delta_2}$, Eq. (4.6)₁ admits a unique solution in a point $I_0 > \max(\delta_1, \delta_2)$. In the opposite case Eq. (4.6)₁ has a positive solution also in the range $]0, \min(\delta_1, \delta_2)[$. \square

REMARK. In principle one can consider that either δ_1 or δ_2 can be negative numbers (sinks instead of sources). Then in the case $\delta_1\delta_2 < 0$, following the line of Proposition 2 under some "smallness" condition for the magnitude of the sink, one can still prove existence (but not uniqueness) of positive solutions to the BVP.

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DEPARTMENT OF MATHEMATICS
UNIVERSITY OF GENOVA, ITALY.

and
DEPARTMENT OF MATHEMATICS, INFORMATICS AND MECHANICS
UNIVERSITY OF WARSAWA.

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