Journal of Statistical Physics, Vol. 97, Nos. 3/4, 1999

Discrete Velocity Models Without Nonphysical Invariants

Alexander V. Bobylev[1] **and Carlo Cercignani**[2]

Received April 22, 1999

Models for mixtures of discrete velocity gases have been recently introduced by the authors and have produced unexpected results, particularly with regard to the possible existence of nonphysical collision invariants. Here we discuss a method to construct models without spurious invariants. The method can be extended to very general models, including polyatomic gases, chemical reactions, etc.

KEY WORDS: Discrete velocity models; Boltzmann equation; kinetic theory.

1. INTRODUCTION

The aim of the present paper is to clarify and generalize some aspects of our recent publications,[1,2] where Discrete Velocity Models (DVMs) for gas mixtures in a wide context were introduced. In particular, a general method to construct such models was proposed, a proof that the models approximate the Boltzmann equation was sketched, two specific simple models were described, a definition of the temperature for DVMs was briefly discussed. However, an important question, i.e., the possible existence of non-physical collision invariants, was not discussed. As a matter of fact, the two examples turned out to possess such spurious invariant as remarked by some of our Colleagues[3,4] and an anonymous referee of ref. 2 (see also ref. 5). Therefore the present paper fills the gap of refs. 1 and 2 and discusses a method of constructing models without spurious invariants. The method can be used for very general models, including polyatomic gases, chemical reactions, etc. As we shall see below, a key idea

[1] Keldysh Institute of Applied Mathematics, Moscow, Russia.
[2] Dipartimento di Matematica, Politecnico di Milano, Milan, Italy.

0022-4715/99/1100-0677$16.00/0

of our approach is contained in Fig. 4 of ref. 1, where a hierarchy of models for simple gases is shown. The same scheme can be used in the general case. We describe how to generalize it in Section 2, where we also prove a quite elementary Lemma, showing that our scheme does not lead to non-physical invariants. In contrast with our first examples of simple DVMs in refs. 1 and 2, these models depend strongly on the mass ratio.

In this paper we are mainly interested in DVMs which are symmetric with respect to an exchange of any pair of coordinate axes. On the other hand, this property is not very relevant for certain specific problems (axially symmetric flows). An interesting class of non-symmetric DVMs without additional invariants was recently considered by H. Cornille and one of the authors.[5] Moreover, the exact shock wave solutions were constructed and investigated in ref. 5 for the simplest non-symmetric DVMs for binary mixtures. We present a brief discussion of non-symmetric DVMs at the end of the paper and show how the models[5] can be derived on the basis of our general scheme. The scheme confirms that the simplest reasonable DVM for a mixture (the normal semi-symmetric DVM, in our terminology) contains 11 velocities for arbitrary mass ratio.[5] As to symmetric models, the best result (17 velocity model being already found in ref. 5) corresponds to $M=2$, where M is the mass ratio. A similar result (18 velocities) is obtained in Section 3 for $M=3$.

The scheme described in Section 2 and applied to mixtures in Section 3 allows to construct symmetric DVMs without non-physical invariants for binary mixtures with arbitrary rational mass ratio. It is remarkable that this can be done almost without calculations by using simple geometric considerations. Therefore the paper contans no complicated formulae; we use mainly some graphic illustrations (Figs. 1–4).

2. THE GENERAL SCHEME

In order to explain the idea of our method, we first consider an abstract countable Discrete Model (DM) of a gas assuming that

$$X=\{x_1, x_2,..., x_n,...\} \tag{2.1}$$

characterizes a set of discrete states of each particle. In applications, the vector $x \in \mathfrak{R}^m$ includes all $m \geqslant 1$ discrete phase coordinates, such as velocity, internal energy, etc. We note that the position of a particle is not included in X since it varies continuously with time for the usual DVMs. For a given set X defined as in (2.1), we can simply denote the states by the integers $\{1, 2,...\}$.

Particles may change their states by pair reactions

$$(i)+(j)\to(k)+(l) \tag{2.2}$$

with probabilities $\Gamma_{ij}^{kl}\geqslant 0$. These coefficients satisfy the following restriction:

(A) $\Gamma_{ij}^{kl}=0$ unless $p\geqslant 1$ conservation laws

$$\psi_\alpha(x_i)+\psi_\alpha(x_j)=\psi_\alpha(x_k)+\psi_\alpha(x_l), \qquad \alpha=1,..., p \tag{2.3}$$

are fulfilled for a given set of linearly independent functions $\psi_1,..., \psi_p$.

Of course, condition (A) does not mean that $\Gamma_{ij}^{kl}\neq 0$ in *all* cases satisfying (2.3). The functions $\psi_1,..., \psi_p$ are called the physical collision invariants. For brevity, we consider only pair reactions (2.2) preserving the number of particles, though various generalizations to other reactions are also possible.

Usually we consider finite DMs, defined for a finite subset X_N of the set X defined in (2.1). With a change of numeration (if required), we can always assume that

$$X_N=\{x_1, x_2,..., x_N\}\cong\{1, 2,..., N\} \tag{2.4}$$

Then the above defined coefficients Γ_{ij}^{kl} describe K possible reactions (3.2) inside the model, where K is the number of different combinations $(i, j\mid k, l)$, $1\leqslant i, j, k, l\leqslant N$, such that $\Gamma_{ij}^{kl}\neq 0$. We introduce the following

Definition. The finite DM described above is called a *normal* DM if any nontrivial solution $\phi(x)$ of the K equations

$$\phi(x_i)+\phi(x_j)=\phi(x_k)+\phi(x_l)$$
$$\text{for}\quad 1\leqslant i, j, k, l\leqslant N \qquad \text{such that} \qquad \Gamma_{ij}^{kl}>0 \tag{2.5}$$

is a linear combination of the p physical collision invariants $\psi_1,..., \psi_p$.

This definition was introduced for usual discrete velocity models for a simple gas by one of the authors.[6]

Sometimes one can easily guess the simplest normal DM such as, for example, the modified Broadwell model for a simple gas (see below, Section 3). Then the following procedure helps to "breed" such models: we begin with some given normal DM (2.4) and construct its extended version. The latter is defined by a new set of states

$$X_{N+s}=\{x_1, x_2,..., x_N, x_{N+1},..., x_{N+s}\}, \qquad s\geqslant 1 \tag{2.6}$$

where all new states $\{N+1,..., N+s\}$ satisfy the following conditions: for any $1 \leqslant r \leqslant s$ there exist three numbers $1 \leqslant i, j, k \leqslant N$ such that $\Gamma_{ij}^{kN+r} > 0$. In other words, each new state $(N+r)$ is a product of a certain reaction

$$(i)+(j) \to (k)+(N+r) \tag{2.7}$$

which includes three states $\{i, j, k\}$ being already present in the initial DM (2.4).

Then the following statement is rather obvious:

Lemma. If the initial DM is normal, then the same is true for the extended DM.

Proof. It is enough to prove the statement for $s=1$. All we need to show is that a combined system of K equations (2.5) and one more equation

$$\phi(x_{i_1})+\phi(x_{j_1})=\phi(x_{k_1})+\phi(x_{N+1}) \tag{2.8}$$

related to the reaction (2.7) for $s=1$ has no new solutions. To this goal we note that any solution of (2.5), (2.8) reads as

$$\phi(x)=\sum_{\alpha=1}^{p} c_\alpha \psi_\alpha(x)+u(x) \tag{2.9}$$

for some constants c_α ($\alpha=1,..., p$) and a function $u(x)$ linearly independent of the ψ_α ($\alpha=1,..., p$).

The function (2.9) satisfies (2.5), and therefore $u(x_1)=u(x_2)= \cdots = u(x_N)=0.$ because of the assumptions of the Lemma. Substituting (2.9) into (2.8), we then conclude that $u(x_{N+1})=0$. Hence u vanishes at all points of our set and the lemma is proved.

In the next section we describe some applications of our Lemma.

3. APPLICATIONS

3.1. Simple Gas

The simplest application of the lemma concerns a usual DVM for identical particles with integer velocities ($x \in Z^d$, $d \geqslant 2$). In addition, we assume that all (elastic) collisions with the scattering angle $\theta=\pi/2$ are allowed. Then we have $d+2$ conservation laws (mass, energy and momentum). The simplest Broadwell model with $N=2d$ velocities is not (formally) normal since it has only $d+1$ conservation laws. Therefore we transform it to a normal DVM by adding only one more velocity $v_0=0$ (Fig. 1a). This

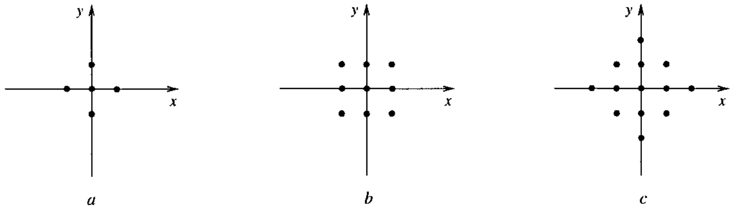

Fig. 1. The basic model for a single gas and its first extensions.

DVM satisfies the assumptions of the Lemma and can be used as a starting point for infinitely many normal DVMs obtained by successive extensions.

In particular, its first extensions correspond to the DVMs shown in Fig. 1 for $d = 2$ (see also Fig. 4 of our previous paper[1]). One can easily prove that all cubic (quadratic) models used in numerical experiments are normal if the scattering cross section is positive for a scattering angle $\theta = \pi/2$. This generalizes a related result,[7] which was proved in a more complicated and lengthy way.

Sometimes it is convenient to use normal symmetric DVMs without zero components of velocities. To construct such models one can begin with an asymmetric model shown in Fig. 2a for the plane case (the Broadwell model with four velocities $(\pm 1, \pm 1)$ plus one more velocity $(2, 0)$). Then we make its successive symmetric extensions; the first extension is shown in Fig. 2b.

3.2. Mixtures

Let us now apply the same scheme to mixtures. We consider a binary mixture of gases with integer molecular masses m_1 (light particles) and m_2

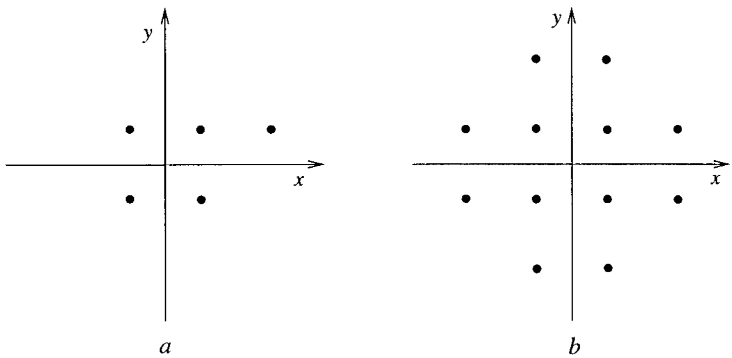

Fig. 2. An asymmetric model can be used as a starting point to construct a symmetric model.

(heavy particles) such that $1 \leqslant m_1 < m_2$. In order to find a starting point for successive extensions, we first fix an arbitrary normal DVM for light particles with integer (vector) velocities $v_1, v_2,..., v_N \in Z^d$. The model has $d+2$ conservation laws, whereas any *DVM* for a binary mixture has $d+3$ such laws, because the mass of each species is preserved. Therefore we add only one velocity $w_0 = 0$ for the heavy particles and obtain a (trivial) model for the mixture with $N+1$ integer velocities $\{v_1, v_2,..., v_N; w_0\}$. Here and below we denote by $v \in Z^d$ ($w \in Z^d$) the velocities of light (heavy) particles. This trivial model, however, has exactly $d+3$ conservation laws and satisfies the assumptions of the Lemma. Therefore we choose it as a starting point and proceed to successive extensions. Thus we need to have at least one kind of collision between particles of different masses which reads as follows:

$$(v_i) + (w_0) \to (v_k) + (w_1), \qquad (w_0 = 0) \tag{3.1}$$

for some values $i, k \leqslant N$ and $w_1 \in Z^d$. The simplest collision of this type corresponds to the following values:[1, 2]

$$v_i = (m_1 + m_2,...), \qquad v_k = -(m_2 - m_2,...), \qquad w_1 = (2m_1,...) \tag{3.2}$$

where the dots denote zero components of d-dimensional vectors. First we consider symmetric models only. Assuming that the initial DVM for light particles is symmetric with respect to all coordinate axes, we need to have at least $4d$ velocities with directions along any axis and projections $\pm(m_1 \pm m_2)$ onto the axis. By using the above extension scheme, we obtain a $(N+2d+1)$-velocity model, which includes now $2d$ new velocities $\{w_1, w_2,..., w_{2d}\}$ for the heavy particles, having a speed $|w| = 2m_1$. We note that the above constructed $(2d+1)$ velocity DVM for heavy particles coincides with the simplest normal symmetric DVM shown in Fig. 1a for $d=2$. If we do not add more velocities of heavy particles, then the combined model for two species is split into two independent normal DVMs in the limit of non-interacting species since the DVM for light particles is normal by assumption. In order to construct symmetric normal DVMs with a minimal number of velocities we fix this simplest model for heavy particles and consider the initial DVM for light particles. It is obvious that such minimal DVMs correspond to the plane case $d=2$. Therefore, from now on, we consider the plane case only.

The final step is to choose the initial DVM in such a way that the model contains 8 velocities $v = \pm(m_1 \pm m_2, 0)$ and $v = \pm(0, m_1 \pm m_2)$. We note that

$$0 \leqslant \frac{m_2 - m_1}{m_2 + m_1} = \frac{a}{b} < 1 \tag{3.3}$$

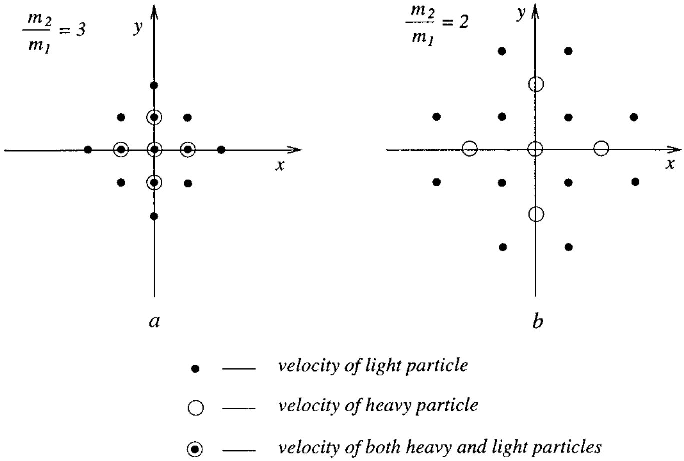

Fig. 3. The simplest symmetric models for mixtures with $m_2/m_1 = 2$ and $m_2/m_1 = 3$.

where a/b is an irreducible fraction. Thus the denominator is an integer $b \geqslant 2$ defining the maximal values of $|v_x|$, $|v_y|$ in the minimal (with respect to the number of velocities) model. Hence, in the best case, $b = 2$; this occurs for $m_2 = 3m_1$ and the combined DVM satisfying all reasonable restrictions contains $13 + 5 = 18$ velocities (Fig. 3a).

Thus in the above class of DVMs for binary mixtures we obtain the following results:

(a) The minimal number of velocities of heavy particles equals 5, provided the model for heavy particles is in turn normal. If, in addition, we demand that all velocities must participate in collisions of identical particles ($w_0 = 0$ does not satisfies this condition in the above model), then we need to add at least 4 more velocities ($\pm 2m_1$, $\pm 2m_1$) to the set of velocities of heavy particles. Such a model for a simple gas is shown in Fig. 1b.

(b) The minimal number of velocities of light particles depends on the denominator b of the fraction (3.3) and increases with b. In particular the minimal DVM for light particles contains 13 velocities for $b = 2$ ($m_2 = 3m_1$) and 16 velocities for $b = 3$ ($m_2 = 2m_1$).

On the other hand, a simple generalization of the reaction (3.1), (3.2) leads to values

$$v_i = (m_2 + m_1, y), \qquad v_k = (m_1 - m_2, y), \qquad w_1 = (2m_1, 0) \tag{3.4}$$

in Eq. (3.1) with arbitrary y (note that Eq. (3.2) corresponds to $y=0$). Another way to construct symmetric DVMs is to choose $y=m_2-m_1$. One can easily verify that such a collision yields the best result in the case $m_2=2m_1$ ($12+5=17$ velocities, Fig. 3b). We note that this minimal symmetric model was first found in ref. 5. To prove that the models shown in Fig. 3 are normal it is enough to verify this property only for light particles. The verification is obvious since the two DVMs (Fig. 3a,b) are respectively the second extension of the minimal symmetric DVM (Fig. 1c) and the first symmetric extension of the minimal asymmetric DVM (Fig. 2b).

3.3. Nonsymmetric DVMs

Finally we consider some non-symmetric models.[5] In applications we are often interested in axially symmetric problems. Then one can use DVMs which are not necessarily symmetric with respect to an exchange of the coordinate axes. Therefore we consider *semi-symmetric* models which are invariant only under reflections with respect to both x and y axes. Such DVMs for mixtures were first proposed and studied in ref. 5. As we shall see below, the models[5] can be easily derived and generalized on the basis of the above described general scheme. First we note that the simplest semi-symmetric normal DVMs for a simple gas contain 5 or 6 velocities (Fig. 4). The models are obtained from non-symmetric Broadwell models in a way similar to that used for the symmetric models as shown in Figs. 1, 2. Thus we can fix, for example, the model described in Fig. 4b for heavy particles and try to find an appropriate model for light particles. It is easy to check that it is impossible to combine two five velocity models for both species. Therefore a minimal number of velocities of light particles equals 6 (Fig. 4c). The last step is to find velocities w_k, $k=0,\dots,4$, in the model of heavy particles (Fig. 4b) and the velocities v_j, $j=1,\dots,6$, in the model of light particles (Fig. 4c). In order to do this we demand that the collision

$$(v_2)+(w_0)\to(v_4)+(w_1) \tag{3.5}$$

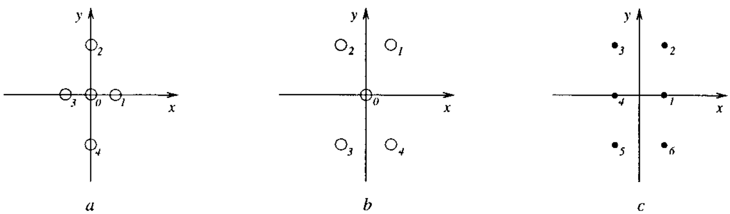

Fig. 4. The simplest non-symmetric models for a single gas. They can be used as building blocks of non-symmetric models for a mixture.

satisfies all conservation laws

$$m_1 v_2 = m_2 w_1 + m_1 v_4, \qquad m_1 v_2^2 = m_2 w_1^2 + m_1 v_4^2 \tag{3.6}$$

We assume without a loss of generality that $v_4 = (-1, 0)$ and denote $v_2 = (1, y)$, $w_1 = (x, z)$. The conservation laws lead to equalities

$$y = 2(M-1)^{-1/2}, \qquad x = 2/M, \qquad z = (2/M)(M-1)^{-1/2} \tag{3.7}$$

where $M = m_2/m_1$.

Thus, we have derived the 11 velocity model first published in ref. 5 as the simplest possible normal semi-symmetric DVM for binary mixtures. It is remarkable that this model has the same structure for any mass ratio. Moreover it is valid for irrational values of M. One can construct another version of this model by using the scheme shown in Fig. 4b for velocities of heavy particles.

Apparently the idea of reconstructing such a universal *symmetric* normal DVM for binary mixtures with arbitrary mass ratio cannot be realized with the above procedure. This may be a partial explanation of the circumstance that our previous attempt in ref. 1 produced non-physical invariants. On the other hand, the above described scheme allows to construct normal symmetric DVMs for any given rational mass ratio.

ACKNOWLEDGMENTS

Support from the Gruppo Nazionale di Fisica Matematica of the Italian Research Council (CNR) is gratefully acknowledged by both authors. A. V. Bobylev also acknowledges support by the Russian Basic Research Foundation (grant "Boltzmann") and thanks V. V. Vedenyapin for his contribution to the proof of normality of DVMs for a simple gas.

REFERENCES

1. A. V. Bobylev and C. Cercignani, Discrete velocity models for mixtures, *Jour. Stat. Phys.* **91**:327-342 (1998).
2. C. Cercignani and A. V. Bobylev, Discrete velocity models: the case of mixtures, *Transp. Th. Stat. Phys.* (to appear, 1999).
3. H. Cornille, private communication (1998).
4. V. V. Vedenyapin and Yu. N. Orlov, Polynomial invariants for quantum Hamiltoniants and for discrete velocity models of the Boltzmann equation, Preprint (in Russian), Keldysh Institute of Applied Mathematics (December, 1998).

5. H. Cornille and C. Cercignani, Shock waves for a discrete velocity gas mixture, submitted to *J. Stat. Phys.*
6. C. Cercignani, Sur des critères d'existence globale en théorie cinétique discrète, *C.R. Acad. Sc. Paris* **301**, Série I, No. 3, **89** (1985).
7. F. Rogier and J. Schneider, A direct method for solving the Boltzmann equation, *Transp. Th. Stat. Phys.* **23**:313–338 (1994).