

A General Discrete Velocity Model Including Internal Degrees of Freedom

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Abstract. This paper deals with the problem of describing spatially inhomogeneous gases by applying model Boltzmann equations. A plane discrete velocity model is presented, capable of describing a gas of particles with internal degrees of freedom. The number of particle speeds is variable. All possible collisions, both elastic and inelastic, are calculated. The corresponding equation system for $2L+1$ speeds is given explicitly, where L is a nonnegative integer. For the case $L = 1$ solutions in the form of shock waves are found numerically.

1. Introduction

Modern gas kinetics cannot be confined to spatially homogeneous gases. Typical problems such as the investigation of shockwaves require the investigation of anisotropic and inhomogeneous cases. Since the corresponding equations have a complicated mathematical structure, they are hard to work out. Therefore, simplified models have become relevant in the study of relaxation processes. Numerous methods, analytical as well as numerical, have been developed for examining inhomogeneous gases. For numerical solutions, Monte Carlo methods and lattice gas automata are popular. Most activities in the field of analytical solutions focus either on developing nonlinear perturbation methods or on solving equations by using Lie groups. Moreover, the discrete kinetic theory offers an alternative method for treating such problems. The reason for the growing interest in the study of discrete velocity models (DVMs) is the hope of gaining new insight into kinetic theory and fluid dynamics. Broadwell [1] presented his famous model in 1964, since then many other models have been proposed. A survey on the results of the discrete kinetic theory can be found, for example, in [2, 3].

At present, there is a trend to extend the DVM to gas mixtures [4, 5] as well as accounting for removal and source terms [6]. Not much is known about including inelastic interactions [7] or chemical reactions [8].

The aim of this paper is to present a general DVM which is suitable for describing a gas consisting of particles with internal degrees of freedom. Contrary to other models, the number of particle speeds is variable. The corresponding equation system is valid in the range of three up to $2L + 1$ speeds with $L \in \mathbb{N}$. Therefore the model is useful for analytical as well as numerical investigations, depending on the chosen value of L . With increasing L , the discrete model approaches a continuum description, but the velocity directions remain discrete. Such a model can be interpreted as an extension of the multigroup method [9] to spatially inhomogeneous gases. Furthermore, the problem of the ill temperature definition [10] can be overcome. The main benefit of our model is in its simple way of considering inelastic collisions without any additional assumptions or restrictions.

This paper is organized as follows. In section 2, the requirements that must be considered in our model are defined. A general model, taking into account these specifications, is presented. Its properties, in particular all possible elastic collisions, are presented. For practical application, the model has to be restricted, which is done in section 3, where the values of particle speeds are confined to a special set. All remaining elastic as well as all possible inelastic collisions are shown. The corresponding equation system for $2L + 1$ speeds is given in an explicit form. In section 4, the equation system is solved numerically for binary elastic collisions and by allowing two different velocity moduli. At infinity, the shock wave profiles obtained reach exactly the Maxwell densities, which follow alternatively from the Rankine Hugoniot equations.

2. The general model

We consider a gas, consisting of particles of identical mass m which possess translational and internal degrees of freedom. These particles are free of external forces. Particles with different internal quantum states α establish different species. A change of internal energy E_α results from inelastic collisions. The probability density for a collision process

$$(\mathbf{v}_1, \mathbf{v}_2)_{\alpha, \beta} \rightarrow (\mathbf{v}_3, \mathbf{v}_4)^{\gamma, \delta}, \quad (1)$$

where two particles, one being in state α with a velocity \mathbf{v}_1 and the other being in state β with a velocity \mathbf{v}_2 , collide and change to states γ and δ with velocities \mathbf{v}_3 and \mathbf{v}_4 , is denoted by $(W_{\alpha, \beta}^{\gamma, \delta})_{\mathbf{v}_1, \mathbf{v}_2}^{\mathbf{v}_3, \mathbf{v}_4}$. As is the case for continuum gas kinetics, the probability density should obey two fundamental symmetries [11], the interaction symmetry:

$$(W_{\alpha, \beta}^{\gamma, \delta})_{\mathbf{v}_1, \mathbf{v}_2}^{\mathbf{v}_3, \mathbf{v}_4} = (W_{\beta, \alpha}^{\delta, \gamma})_{\mathbf{v}_2, \mathbf{v}_1}^{\mathbf{v}_4, \mathbf{v}_3} \quad (2)$$

and microscopic reversibility:

$$(W_{\alpha, \beta}^{\gamma, \delta})_{\mathbf{v}_1, \mathbf{v}_2}^{\mathbf{v}_3, \mathbf{v}_4} = (W_{\gamma, \delta}^{\alpha, \beta})_{\mathbf{v}_3, \mathbf{v}_4}^{\mathbf{v}_1, \mathbf{v}_2}. \quad (3)$$

The principle of microscopic reversibility is only valid in this form for gases consisting of particles with nondegenerate internal quantum states (which is assumed here). For a binary collision as in equation (1), momentum and energy conservation reads:

$$\mathbf{v}_1 + \mathbf{v}_2 = \mathbf{v}_3 + \mathbf{v}_4 \tag{4}$$

and

$$v_1^2 + v_2^2 = v_3^2 + v_4^2 - 2q_{\alpha,\beta}^{\gamma,\delta}. \tag{5}$$

Furthermore, in a DVM, all particle velocities are restricted to a set M :

$$\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3, \mathbf{v}_4 \in M. \tag{6}$$

The difference in internal energy before and after the collision is given by:

$$mq_{\alpha,\beta}^{\gamma,\delta} = Q_{\alpha,\beta}^{\gamma,\delta} = (E_\alpha + E_\beta) - (E_\gamma + E_\delta). \tag{7}$$

To be suitable for describing a realistic gas, we expect our model to meet the following conditions.

- C1. Existence of inelastic collisions ($q_{\alpha,\beta}^{\gamma,\delta} \neq 0$), that is, collisions that comply with momentum but not with energy conservation.
- C2. The particle velocities of all species belong to the same set M .
- C3. Existence of mixing speed (MS) collisions, that is, collisions where at least one of the postcollisional speeds v_3 or v_4 differs from both precollisional speeds v_1 and v_2 .
- C4. Proceeding from an initial state where all particles have the same speed, but different flight directions, all other permitted velocities should be attainable in a sequence of elastic collisions.

Condition C1 serves to include the energy exchange between internal and translational degrees of freedom in our model. Conditions C2 and C3 provide for a realistic model. In connection with the existence of different particle speeds, condition C3 allows a nontrivial description of the temperature of the system. For instance, in systems with only two velocity moduli, there is no exchange of energy between the “hot” subsystem, composed of particles with faster speed and the “cold” subsystem of particles with slower speed. The energy of hot and cold particles is separately conserved. By applying condition C4, particles of all speeds can indirectly interact with each other by means other than trivial collisions such as $(\mathbf{v}_1, \mathbf{v}_2)_{\alpha,\beta} \rightarrow (\mathbf{v}_1, \mathbf{v}_2)^{\alpha,\beta}$. Otherwise particles with certain velocities could exist, so that the particle densities are completely independent of the value of all other particle densities. Since those particles do not participate in the dynamical behavior of the system, they are undesirable.

In this paper, we confine ourselves to a plane model with eight velocity directions. On the one hand this limits the size of the DVM equation system, on the other hand it allows a variety of different collisions.

The set M of permitted velocities is the union of L disjoint subsets M^i and the zero velocity:

$$M := \left(\bigcup_{i=1, \dots, L} M^i \right) \cup \{\mathbf{0}\}. \quad (8)$$

Every set M^i consists of eight velocities:

$$M^i := \left\{ \mathbf{v}_{i,m} \mid \mathbf{v}_{i,m} = \begin{pmatrix} 0 \\ A_i \end{pmatrix}, \begin{pmatrix} A_i \\ A_i \end{pmatrix}, \begin{pmatrix} A_i \\ 0 \end{pmatrix}, \begin{pmatrix} A_i \\ -A_i \end{pmatrix}, \right. \\ \left. \begin{pmatrix} 0 \\ -A_i \end{pmatrix}, \begin{pmatrix} -A_i \\ -A_i \end{pmatrix}, \begin{pmatrix} -A_i \\ 0 \end{pmatrix}, \begin{pmatrix} -A_i \\ A_i \end{pmatrix} \right\}.$$

Note that

$$m = 1, 3, 5, 7 \text{ for } |\mathbf{v}_{i,m}| = A_i, \quad m = 2, 4, 6, 8 \text{ for } |\mathbf{v}_{i,m}| = \sqrt{2}A_i \quad (9)$$

with $A_i \in \mathbb{R}^+ \setminus \{0\}$. The zero velocity is defined by:

$$\mathbf{0} = \mathbf{v}_{0,m} := \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \quad (10)$$

Thus the speed and direction of a particle velocity can be easily identified by the two subscripts of the velocities $\mathbf{v}_{i,m}$. The second subscript m is related to the directions as shown in Figure 1. The density of particles with velocity $\mathbf{v}_{i,m}$ and internal state α is denoted by $N_{i,m}^\alpha(\mathbf{r}, t)$ and for particles at rest by $R^\alpha(\mathbf{r}, t)$.

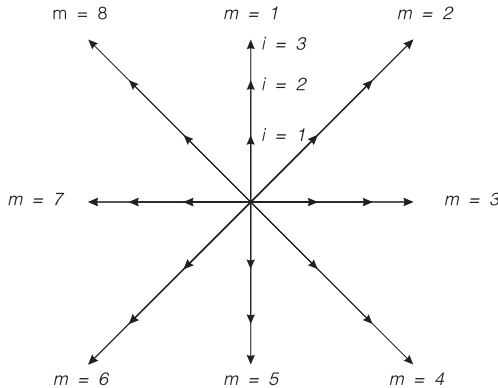


Figure 1: Relation between the subscript m for the velocity $v_{i,m}$ and the velocity direction.

Table 1: Elastic collision types.

Number	Collision type	
[1]	$\begin{pmatrix} A_i \\ 0 \end{pmatrix} + \begin{pmatrix} -A_i \\ 0 \end{pmatrix} \leftrightarrow \begin{pmatrix} 0 \\ A_i \end{pmatrix} + \begin{pmatrix} 0 \\ -A_i \end{pmatrix}$	SS
[2]	$\begin{pmatrix} A_i \\ A_i \end{pmatrix} + \begin{pmatrix} -A_i \\ -A_i \end{pmatrix} \leftrightarrow \begin{pmatrix} A_i \\ -A_i \end{pmatrix} + \begin{pmatrix} -A_i \\ A_i \end{pmatrix}$	SS
[3]	$\begin{pmatrix} A_i \\ A_i \end{pmatrix} + \begin{pmatrix} -A_i \\ 0 \end{pmatrix} \leftrightarrow \begin{pmatrix} A_i \\ 0 \end{pmatrix} + \begin{pmatrix} -A_i \\ A_i \end{pmatrix}$	DS
[4]	$\begin{pmatrix} A_i \\ A_i \end{pmatrix} + \begin{pmatrix} -2A_i \\ 0 \end{pmatrix} \leftrightarrow \begin{pmatrix} 0 \\ 2A_i \end{pmatrix} + \begin{pmatrix} -A_i \\ -A_i \end{pmatrix}$	DS
[5]	$\begin{pmatrix} 0 \\ 2A_i \end{pmatrix} + \begin{pmatrix} 2A_j \\ 0 \end{pmatrix} \leftrightarrow \begin{pmatrix} A_i+A_j \\ A_i+A_j \end{pmatrix} + \begin{pmatrix} A_j-A_i \\ -A_j+A_i \end{pmatrix}$	MS
[6]	$\begin{pmatrix} A_i \\ -A_i \end{pmatrix} + \begin{pmatrix} -A_i \\ A_i \end{pmatrix} \leftrightarrow \begin{pmatrix} \sqrt{2}A_i \\ 0 \end{pmatrix} + \begin{pmatrix} -\sqrt{2}A_i \\ 0 \end{pmatrix}$	SS
[7]	$\begin{pmatrix} A_i \\ A_i \end{pmatrix} + \begin{pmatrix} -A_i(2+\sqrt{2}) \\ 0 \end{pmatrix} \leftrightarrow \begin{pmatrix} 0 \\ -\sqrt{2}A_i \end{pmatrix} + \begin{pmatrix} -A_i(1+\sqrt{2}) \\ A_i(1+\sqrt{2}) \end{pmatrix}$	DS
[8]	$\begin{pmatrix} A_i \\ A_i \end{pmatrix} + \begin{pmatrix} -A_i(2-\sqrt{2}) \\ 0 \end{pmatrix} \leftrightarrow \begin{pmatrix} 0 \\ \sqrt{2}A_i \end{pmatrix} + \begin{pmatrix} -A_i(1-\sqrt{2}) \\ A_i(1-\sqrt{2}) \end{pmatrix}$	DS
[9]	$\begin{pmatrix} 2A_i \\ 0 \end{pmatrix} + \begin{pmatrix} A_i(\sqrt{5}-3) \\ 0 \end{pmatrix} \leftrightarrow \begin{pmatrix} 0 \\ -A_i(\sqrt{5}-1) \end{pmatrix} + \begin{pmatrix} A_i(\sqrt{5}-1) \\ A_i(\sqrt{5}-1) \end{pmatrix}$	MS
[10]	$\begin{pmatrix} 2A_i \\ 0 \end{pmatrix} + \begin{pmatrix} -A_i(\sqrt{5}+3) \\ 0 \end{pmatrix} \leftrightarrow \begin{pmatrix} 0 \\ A_i(\sqrt{5}+1) \end{pmatrix} + \begin{pmatrix} -A_i(\sqrt{5}+1) \\ -A_i(\sqrt{5}+1) \end{pmatrix}$	MS
[11]	$\begin{pmatrix} 2A_i \\ 2A_i \end{pmatrix} + \begin{pmatrix} -4A_i \\ 0 \end{pmatrix} \leftrightarrow \begin{pmatrix} A_i(\sqrt{5}-1) \\ -A_i(\sqrt{5}-1) \end{pmatrix} + \begin{pmatrix} -A_i(\sqrt{5}+1) \\ A_i(\sqrt{5}+1) \end{pmatrix}$	MS

The results of a systematic calculation of all possible elastic collisions in this model are shown in Table 1. As can be seen, the general model permits 11 different types of collisions. Only one example of each type is displayed in Table 1. All others can be found by applying the following symmetry operations.

- S1. Exchange x and y components for all velocities involved in the collision.
- S2. Reflect the collision on the X -axis.
- S3. Reflect the collision on the Y -axis.

In the last column we distinguished between a mixing speed (MS), a dual speed (DS), and a single speed (SS) collision. SS collision means that all particles involved in the collision have the same speed before as well as after the collision. Correspondingly, two different speeds occur in a DS collision. We are not able to calculate the very general set of velocities of our model that can be attained in accordance to condition C4. But we can show, at least in the following collision sequence, that all velocities occurring in Table 1 are part of this general set. We cite only one of the precollision and one of the postcollision partners according to Table 1 with the collision type and symmetry operations labeled:

$$\left. \begin{array}{c} \binom{A_i}{0} \xrightarrow{[5]} \binom{A_i}{A_i} \xrightarrow{[6],(S3)} \binom{\sqrt{2}A_i}{0} \xrightarrow{[5]} \binom{\sqrt{2}A_i}{\sqrt{2}A_i} \\ \binom{A_i}{0} \xrightarrow{[5]} \binom{2A_i}{0} \end{array} \right\} \xrightarrow{[5]} \binom{(2\pm\sqrt{2})A_i}{0} \xrightarrow{[7],[8]} \binom{(1\pm\sqrt{2})A_i}{(1\pm\sqrt{2})A_i}$$

$$\left. \begin{array}{c} \binom{2A_i}{2A_i} \\ \binom{4A_i}{0} \end{array} \right\} \xrightarrow{[11]} \left. \begin{array}{c} \binom{(\sqrt{5}\pm 1)A_i}{(\sqrt{5}\pm 1)A_i} \\ \binom{(\sqrt{5}\pm 1)A_i}{0} \end{array} \right\} \xrightarrow{[9],[10]} \binom{(\sqrt{5}\pm 3)A_i}{0}.$$

This sequence also shows an iterative way of finding the complete set of velocities attained in accordance to condition C4. Instead of A_i , all velocity components found in the collision sequence can be inserted in the first velocity of the sequence. With these new initial values the next generation of velocities according to condition C4 can be calculated.

3. The restricted model

The multitude of different collisions as represented in Table 1 is only possible in a model where the velocity components A_i can take arbitrary values. For two reasons a restriction of this scope is necessary for every model used to find practical solutions. On the one hand, it is necessary to limit the size of the DVM equation system as it depends strongly on the number of different collisions taken into account. On the other hand, we have to confine the permitted set of particle velocities to a known set of velocities according to condition C4. Of the several different ways to confine the set, we examine four different possibilities for qualification. In all four cases we define $A_1 = 1$.

1. A velocity set M with velocity components $A_i = \sqrt{i}$, $i \in \mathbb{N}$ shows equidistant kinetic energy values. This offers the advantage that in every collision which meets energy conservation, all velocities automatically adhere to the given set M . Unfortunately, we cannot prove that the required velocities form a set of velocities according to condition C4.
2. In contrast, we can show that all velocities with components $A_i = i$, $i \in \mathbb{N}$ establish a set M of velocities in accordance to condition C4. This can be proved easily, by a sequence of type [5] collisions:

$$\begin{array}{ccc}
 \binom{n}{n} + \binom{1}{-1} & \longrightarrow & \binom{n+1}{0} + \binom{0}{n-1} \\
 \uparrow & & \downarrow \\
 \binom{0}{0} + \binom{n+1}{n+1} & \longleftarrow & \binom{0}{n+1} + \binom{n+1}{0}.
 \end{array}$$

It must be considered that only collisions of type [1], [2], [3], [4], and [5] are possible for this set M . Furthermore, collision type [5] in the form

$$\begin{pmatrix} 0 \\ i \end{pmatrix} + \begin{pmatrix} j \\ 0 \end{pmatrix} \longrightarrow \begin{pmatrix} \frac{i+j}{2} \\ \frac{i+j}{2} \end{pmatrix} + \begin{pmatrix} \frac{j-i}{2} \\ -\frac{j-i}{2} \end{pmatrix} \tag{11}$$

has to be restricted in such a manner that

$$\begin{aligned} i = \text{even} &\iff j = \text{even} \\ i = \text{odd} &\iff j = \text{odd} \end{aligned}$$

is valid. For the inverse collision no such restrictions apply. Conditions C1 through C5 are valid.

3. With velocity components $A_i = i^2$, $i \in \mathbf{N}$ no set of velocities according to condition C4 can be found.
4. The velocities with components $A_i = 2^i$, $i \in \mathbf{N}$ form in combination with the zero velocity a set M of velocities according to condition C4. In this case, collision types [1], [2], [3], and [4] remain without any restriction. Collision type [5] is possible only when $A_i = A_j$ or $A_j = 0$:

$$\begin{aligned} \text{[5a]} \quad \begin{pmatrix} A_i \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ A_i \end{pmatrix} &\leftrightarrow \begin{pmatrix} A_i \\ A_i \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \end{pmatrix} \\ \text{[5b]} \quad \begin{pmatrix} A_i \\ A_i \end{pmatrix} + \begin{pmatrix} -A_i \\ A_i \end{pmatrix} &\leftrightarrow \begin{pmatrix} 0 \\ 2A_i \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \end{aligned}$$

Conditions C1 through C5 are valid and easily proven.

For the following investigations we confine ourselves to case 4. Therefore only collision types [1] through [4], [5a], and [5b] must be taken into account.

The next question that we have to answer is which inelastic collision types are relevant under the restrictions of case 4. A systematic calculation results in three different types as shown in Table 2.

Table 2: Inelastic collision types.

Number	Collision type	$ g_{\gamma,\delta}^{\alpha,\beta} $	
[1]	$\begin{pmatrix} A_i \\ 0 \end{pmatrix} + \begin{pmatrix} -A_i \\ 0 \end{pmatrix} \leftrightarrow \begin{pmatrix} A_k \\ 0 \end{pmatrix} + \begin{pmatrix} -A_k \\ 0 \end{pmatrix}$	$2^{2i+1}(2^{2(k-i)} - 1)$	for $i < k$
[2]	$\begin{pmatrix} A_i \\ A_i \end{pmatrix} + \begin{pmatrix} -A_i \\ -A_i \end{pmatrix} \leftrightarrow \begin{pmatrix} A_k \\ A_k \end{pmatrix} + \begin{pmatrix} -A_k \\ -A_k \end{pmatrix}$	$2^{2i+2}(2^{2(k-i)} - 1)$	for $i < k$
[3a]	$\begin{pmatrix} A_i \\ 0 \end{pmatrix} + \begin{pmatrix} -A_i \\ 0 \end{pmatrix} \leftrightarrow \begin{pmatrix} A_k \\ A_k \end{pmatrix} + \begin{pmatrix} -A_k \\ -A_k \end{pmatrix}$	$2^{2i+1}(2^{2(k-i)+1} - 1)$	for $i \leq k$
[3b]		$2^{2k+1}(2^{2(i-k)} - 2)$	for $i > k$

Based on physical grounds, we have omitted all collisions where the relative particle speed either before or after the collision is zero. Table 2 also displays the possible values of internal energy $q_{\alpha,\beta}^{\gamma,\delta}$ that can be achieved with the corresponding collision type. As expected in a DVM, only a limited number of discrete values for $q_{\alpha,\beta}^{\gamma,\delta}$ are possible. Another difference to the continuum model is the fact that for a given value of $q_{\alpha,\beta}^{\gamma,\delta}$, only one collision (and of course its symmetric partners) exists and leads to this value. This is because the difference in particle speed between adjacent sets of velocities M_i and M_{i+1} is larger than that between the lower set M_i and the zero vector. This fact can only be met by examining another model. None of the four cases mentioned previously is promising, as case 1 seems to be impossible and case 2 shows the same problem but for other reasons.

The equation system for the restricted discrete model in continuous space has the general form:

$$\frac{\partial}{\partial t} N_{i,m}^\alpha(\mathbf{r}, t) + \mathbf{v}_{i,m} \cdot \nabla N_{i,m}^\alpha(\mathbf{r}, t) = T_{i,m}^\alpha(\mathbf{r}, t) \tag{12}$$

with

$$T_{i,m}^\alpha = \sum_{\beta,\gamma,\delta} \sum_{(j,n),(k,o),(l,p)} \left(W_{\gamma,\delta}^{\alpha,\beta} \right)_{(i,m)(j,n)}^{(k,o),(l,p)} (N_{k,o}^\gamma N_{l,p}^\delta - N_{i,m}^\alpha N_{j,n}^\beta).$$

The probability density $(W_{\gamma,\delta}^{\alpha,\beta})$ was defined in section 2. We wrote (i, m) for $\mathbf{v}_{i,m}$ and analogously for the other subscripts.

We need values of $W_{\gamma,\delta}^{\alpha,\beta}$ that are realistic, simple, and meet the symmetries S2 and S3. This occurs if we set:

$$\left(W_{\gamma,\delta}^{\alpha,\beta} \right)_{(i,m)(j,n)}^{(k,o),(l,p)} = \begin{cases} p_e & \text{for elastic collisions} \\ p_i & \text{for inelastic collisions} \\ 0 & \text{for all other cases.} \end{cases} \tag{13}$$

Here, all elastic collisions have the same probability regardless of the initial and final states of the colliding particles. The same applies for inelastic collisions.

Due to the limited number of different collision types, we can write the right-hand side of equation (12), $T_{i,m}^\alpha$, in a more explicit form. This form should be useful especially for numerical evaluations.

We split the scattering term $T_{i,m}^\alpha$ into separate terms for SS, DS, MS, and inelastic collisions. Inclusion of SS and/or DS collisions in the equation system is optional. With the definition

$$[n] = \begin{cases} n & \text{for } n \leq 4 \\ n - 4 & \text{for } n > 4 \end{cases} \tag{14}$$

and the abbreviation:

$$\sum_\beta S^{(\alpha,\beta)}(\underline{\alpha,\beta}) = \sum_\beta \left(S^{(\alpha,\beta)}(\alpha,\beta) + S^{(\alpha,\beta)}(\beta,\alpha) \right) \tag{15}$$

we find the following for each type of collision.

SS collisions

$$T_{i,m}^\alpha \Big|_{SS} = p_e \begin{cases} \sum_{\beta} S_{i,[2m]}^{(\alpha,\beta)(\alpha,\beta)} & \text{for } m = 2, 4, 6, 8 \\ \sum_{\beta} S_{i,[2m-1]}^{(\alpha,\beta)(\alpha,\beta)} & \text{for } m = 1, 3, 5, 7 \end{cases} \quad (16)$$

with the abbreviations:

$$\begin{aligned} S_{i,1}^{(\alpha,\beta)(\alpha,\beta)} &:= N_{i,3}^\alpha N_{i,7}^\beta - N_{i,1}^\alpha N_{i,5}^\beta & S_{i,2}^{(\alpha,\beta)(\alpha,\beta)} &:= N_{i,4}^\alpha N_{i,8}^\beta - N_{i,2}^\alpha N_{i,6}^\beta \\ S_{i,3}^{(\alpha,\beta)(\alpha,\beta)} &:= N_{i,1}^\alpha N_{i,5}^\beta - N_{i,3}^\alpha N_{i,7}^\beta & S_{i,4}^{(\alpha,\beta)(\alpha,\beta)} &:= N_{i,2}^\alpha N_{i,6}^\beta - N_{i,4}^\alpha N_{i,8}^\beta. \end{aligned} \quad (17)$$

DS collisions

$$T_{i,m}^\alpha \Big|_{DS} = p_e \begin{cases} \sum_{\beta} \left(D_{i,m}^{(\alpha,\beta)(\alpha,\beta)} - D_{i,[m+3]}^{(\beta,\alpha)(\alpha,\beta)} + D_{i,[m+2]+4}^{(\alpha,\beta)(\beta,\alpha)} - D_{i,m+4}^{(\beta,\alpha)(\alpha,\beta)} \right) & \text{for } m = 2, 4, 6, 8 \\ \sum_{\beta} \left(D_{i,m+2}^{(\alpha,\beta)(\beta,\alpha)} - D_{i,[m]}^{(\alpha,\beta)(\alpha,\beta)} - D_{i-1,[m+1]+4}^{(\alpha,\beta)(\alpha,\beta)} + D_{i-1,m+4}^{(\alpha,\beta)(\alpha,\beta)} \right) & \text{for } m = 1, 3, 5, 7 \end{cases} \quad (18)$$

with the abbreviations:

$$\begin{aligned} D_{i,1}^{(\alpha,\beta)(\alpha,\beta)} &:= N_{i,1}^\alpha N_{i,4}^\beta - N_{i,2}^\alpha N_{i,5}^\beta & D_{i,5}^{(\alpha,\beta)(\alpha,\beta)} &:= N_{i+1,7}^\alpha N_{i,2}^\beta - N_{i+1,1}^\alpha N_{i,6}^\beta \\ D_{i,2}^{(\alpha,\beta)(\alpha,\beta)} &:= N_{i,3}^\alpha N_{i,6}^\beta - N_{i,4}^\alpha N_{i,7}^\beta & D_{i,6}^{(\alpha,\beta)(\alpha,\beta)} &:= N_{i+1,1}^\alpha N_{i,4}^\beta - N_{i+1,3}^\alpha N_{i,8}^\beta \\ D_{i,3}^{(\alpha,\beta)(\alpha,\beta)} &:= N_{i,5}^\alpha N_{i,8}^\beta - N_{i,6}^\alpha N_{i,1}^\beta & D_{i,7}^{(\alpha,\beta)(\alpha,\beta)} &:= N_{i+1,3}^\alpha N_{i,6}^\beta - N_{i+1,5}^\alpha N_{i,2}^\beta \\ D_{i,4}^{(\alpha,\beta)(\alpha,\beta)} &:= N_{i,7}^\alpha N_{i,2}^\beta - N_{i,8}^\alpha N_{i,3}^\beta & D_{i,8}^{(\alpha,\beta)(\alpha,\beta)} &:= N_{i+1,5}^\alpha N_{i,8}^\beta - N_{i+1,7}^\alpha N_{i,4}^\beta. \end{aligned} \quad (19)$$

MS collisions

$$\begin{aligned} T_{i,m}^\alpha \Big|_{MS} &= p_e \begin{cases} \sum_{\beta} \left(M_{i,2m}^{(\alpha,\beta)(\alpha,\beta)} - M_{i,2m-1}^{(\beta,\alpha)(\alpha,\beta)} - M_{i,2[m+1]-1}^{(\alpha,\beta)(\alpha,\beta)} \right) & \text{for } m = 2, 4, 6, 8 \\ \sum_{\beta} \left(M_{i-1,2m-1}^{(\alpha,\beta)(\alpha,\beta)} - M_{i,2m}^{(\alpha,\beta)(\alpha,\beta)} - M_{i,2[m+3]}^{(\beta,\alpha)(\alpha,\beta)} \right) & \text{for } m = 1, 3, 5, 7 \end{cases} \quad (20) \\ T_{0,m}^\alpha \Big|_{MS} &= p_e \sum_{\beta} \sum_i \sum_{m=1}^8 M_{i,m}^{(\alpha,\beta)(\beta,\alpha)} \quad (21) \end{aligned}$$

with the abbreviations:

$$\begin{aligned}
M_{i,1}^{(\alpha,\beta)(\alpha,\beta)} &:= N_{i,8}^\alpha N_{i,2}^\beta - N_{i+1,1}^\alpha R^\beta & M_{i,2}^{(\alpha,\beta)(\alpha,\beta)} &:= N_{i,1}^\alpha N_{i,3}^\beta - N_{i,2}^\alpha R^\beta \\
M_{i,3}^{(\alpha,\beta)(\alpha,\beta)} &:= N_{i,2}^\alpha N_{i,4}^\beta - N_{i+1,3}^\alpha R^\beta & M_{i,4}^{(\alpha,\beta)(\alpha,\beta)} &:= N_{i,3}^\alpha N_{i,5}^\beta - N_{i,4}^\alpha R^\beta \\
M_{i,5}^{(\alpha,\beta)(\alpha,\beta)} &:= N_{i,4}^\alpha N_{i,6}^\beta - N_{i+1,5}^\alpha R^\beta & M_{i,6}^{(\alpha,\beta)(\alpha,\beta)} &:= N_{i,5}^\alpha N_{i,7}^\beta - N_{i,6}^\alpha R^\beta \\
M_{i,7}^{(\alpha,\beta)(\alpha,\beta)} &:= N_{i,6}^\alpha N_{i,8}^\beta - N_{i+1,7}^\alpha R^\beta & M_{i,8}^{(\alpha,\beta)(\alpha,\beta)} &:= N_{i,7}^\alpha N_{i,1}^\beta - N_{i,8}^\alpha R^\beta.
\end{aligned} \tag{22}$$

Inelastic collisions

In the restricted model, all inelastic collisions have the form

$$\left((i, m)(i, n) \right)_{\alpha,\beta} \rightarrow \left((k, o)(k, p) \right)^{\gamma,\delta}.$$

For every given and realizable $q_{\gamma,\delta}^{\alpha,\beta}$, one can easily find the corresponding values \hat{i}, \hat{k} for the subscripts i, k . Inelastic collisions will therefore occur only in the scattering terms for particle densities $N_{i,m}^\alpha$ and $N_{k,m}^\alpha$. Moreover, it has to be considered that for a given state α there might be several combinations of β, γ, δ which lead to the same value of $q_{\gamma,\delta}^{\alpha,\beta}$, depending on the structure of the internal energy states. We did not make a regulation here. Taking this fact into account, we define the summation $\sum_{\gamma,\delta}^*$ as the summation over all combinations of β, γ, δ that result in identical values for $q_{\gamma,\delta}^{\alpha,\beta}$. If no such combination exists, the summation vanishes. With the definition

$$\langle n \rangle = \begin{cases} 1 & \text{for } n \leq 2 \\ 0 & \text{for } n > 2 \end{cases} \tag{23}$$

the scattering term for the inelastic collision types [3a] and [3b] according to Table 2 reads:

$$T_{i,m}^\alpha \Big|_{IN} = p_i \begin{cases} \delta(\hat{k} - i) \sum_{\gamma,\delta}^* \left(I_{i,\hat{k},m}^{(\gamma,\delta)(\alpha,\beta)} + I_{i,\hat{k},[m+2]}^{(\gamma,\delta)(\beta,\alpha)} \right) & \text{for } m = 2, 4, 6, 8 \\ \delta(\hat{i} - i) \sum_{\gamma,\delta}^* \left(I_{i,\hat{k},[2m-1+\langle m \rangle]}^{(\alpha,\beta)(\gamma,\delta)} + I_{i,\hat{k},[2m-\langle m \rangle]}^{(\beta,\alpha)(\gamma,\delta)} \right) & \text{for } m = 1, 3, 5, 7 \end{cases} \tag{24}$$

with the abbreviations:

$$\begin{aligned}
I_{i,\hat{k},1}^{(\alpha,\beta)(\gamma,\delta)} &:= N_{i,1}^\beta N_{i,5}^\alpha - N_{\hat{k},2}^\gamma N_{\hat{k},6}^\delta & I_{i,\hat{k},2}^{(\alpha,\beta)(\gamma,\delta)} &:= N_{i,1}^\alpha N_{i,5}^\beta - N_{\hat{k},4}^\gamma N_{\hat{k},8}^\delta \\
I_{i,\hat{k},3}^{(\alpha,\beta)(\delta,\gamma)} &:= N_{i,3}^\beta N_{i,7}^\alpha - N_{\hat{k},2}^\delta N_{\hat{k},6}^\gamma & I_{i,\hat{k},4}^{(\alpha,\beta)(\delta,\gamma)} &:= N_{i,3}^\alpha N_{i,7}^\beta - N_{\hat{k},4}^\delta N_{\hat{k},8}^\gamma.
\end{aligned} \tag{25}$$

4. Application

In the case of binary elastic scattering and allowing only two velocity moduli, but eight directions, we found numerical solutions in the form of shock waves. It turned out that the values of these density profiles at $\pm\infty$ are in exact agreement with those obtained from the Rankine Hugoniot equations (RHEs).

From now on, we will only consider a one component gas with the velocity moduli $|\mathbf{v}_{1,m}| = A_1 = v$ for $m = 1, 3, 5, 7$, and $|\mathbf{v}_{1,m}| = \sqrt{2}A_1 = \sqrt{2}v$ for $m = 2, 4, 6, 8$ (Figure 1 for $i = 1$). The particles interact by collisions of types [1], [2], and [3] (Table 1 including symmetry operations S1, S2, and S3):

$$\begin{aligned}
 v \begin{pmatrix} 1 \\ -1 \end{pmatrix} + v \begin{pmatrix} -1 \\ 0 \end{pmatrix} &\leftrightarrow v \begin{pmatrix} 1 \\ 0 \end{pmatrix} + v \begin{pmatrix} -1 \\ -1 \end{pmatrix} \\
 v \begin{pmatrix} -1 \\ 1 \end{pmatrix} + v \begin{pmatrix} 0 \\ -1 \end{pmatrix} &\leftrightarrow v \begin{pmatrix} 0 \\ 1 \end{pmatrix} + v \begin{pmatrix} -1 \\ -1 \end{pmatrix} \\
 v \begin{pmatrix} 1 \\ 1 \end{pmatrix} + v \begin{pmatrix} 0 \\ -1 \end{pmatrix} &\leftrightarrow v \begin{pmatrix} 0 \\ 1 \end{pmatrix} + v \begin{pmatrix} 1 \\ -1 \end{pmatrix}.
 \end{aligned}
 \tag{26}$$

The probability density $W_{\mathbf{v}_i, \mathbf{v}_j}^{\mathbf{v}_h, \mathbf{v}_k}$ for the collisions $(\mathbf{v}_i, \mathbf{v}_j) \leftrightarrow (\mathbf{v}_h, \mathbf{v}_k)$ is related to the corresponding transition probability density $w_{\mathbf{v}_i, \mathbf{v}_j}^{\mathbf{v}_h, \mathbf{v}_k}$ through the relation

$$W_{\mathbf{v}_i, \mathbf{v}_j}^{\mathbf{v}_h, \mathbf{v}_k} = S |\mathbf{v}_i - \mathbf{v}_j| w_{\mathbf{v}_i, \mathbf{v}_j}^{\mathbf{v}_h, \mathbf{v}_k},
 \tag{27}$$

where $\sum_{h,k=1}^8 w_{\mathbf{v}_i, \mathbf{v}_j}^{\mathbf{v}_h, \mathbf{v}_k} = 1$ for all $i, j = 1, \dots, 8$ and S denotes the cross-sectional area. If all q admissible outputs referred to the input $(\mathbf{v}_i, \mathbf{v}_j)$ are assumed to be equally probable, then

$$w_{\mathbf{v}_i, \mathbf{v}_j}^{\mathbf{v}_h, \mathbf{v}_k} = \begin{cases} \frac{1}{q} & \text{for admissible collisions} \\ 0 & \text{otherwise.} \end{cases}
 \tag{28}$$

In our case, $q = 2$ corresponding to equation (26). The case of simple exchange of velocities between the two particles is included in this number. The discrete Boltzmann equations resulting from this model read as:

$$\begin{aligned}
 \frac{\partial}{\partial t} N_1 + v \frac{\partial}{\partial y} N_1 &= R_1, & \frac{\partial}{\partial t} N_2 + v \left(\frac{\partial}{\partial x} + \frac{\partial}{\partial y} \right) N_2 &= R_2 \\
 \frac{\partial}{\partial t} N_3 + v \frac{\partial}{\partial x} N_3 &= R_3, & \frac{\partial}{\partial t} N_4 + v \left(\frac{\partial}{\partial x} - \frac{\partial}{\partial y} \right) N_4 &= R_4 \\
 \frac{\partial}{\partial t} N_5 - v \frac{\partial}{\partial y} N_5 &= R_5, & \frac{\partial}{\partial t} N_6 - v \left(\frac{\partial}{\partial x} + \frac{\partial}{\partial y} \right) N_6 &= R_6 \\
 \frac{\partial}{\partial t} N_7 - v \frac{\partial}{\partial x} N_7 &= R_7, & \frac{\partial}{\partial t} N_8 - v \left(\frac{\partial}{\partial x} - \frac{\partial}{\partial y} \right) N_8 &= R_8
 \end{aligned}
 \tag{29}$$

with

$$\begin{aligned}
 R_1 &= Sv[(N_3N_7 - N_1N_5) + \frac{\sqrt{5}}{2}(N_8N_5 - N_6N_1) + \frac{\sqrt{5}}{2}(N_2N_5 - N_1N_4)] \\
 R_2 &= Sv[\sqrt{2}(N_4N_8 - N_2N_6) + \frac{\sqrt{5}}{2}(N_1N_4 - N_2N_5) + \frac{\sqrt{5}}{2}(N_8N_3 - N_7N_2)] \\
 R_3 &= Sv[(N_1N_5 - N_3N_7) + \frac{\sqrt{5}}{2}(N_7N_2 - N_8N_3) + \frac{\sqrt{5}}{2}(N_4N_7 - N_3N_6)] \\
 R_4 &= Sv[\sqrt{2}(N_2N_6 - N_4N_8) + \frac{\sqrt{5}}{2}(N_3N_6 - N_4N_7) + \frac{\sqrt{5}}{2}(N_2N_5 - N_1N_4)] \\
 R_5 &= Sv[(N_3N_7 - N_1N_5) + \frac{\sqrt{5}}{2}(N_1N_4 - N_2N_5) + \frac{\sqrt{5}}{2}(N_6N_1 - N_5N_8)] \\
 R_6 &= Sv[\sqrt{2}(N_4N_8 - N_2N_6) + \frac{\sqrt{5}}{2}(N_5N_8 - N_6N_1) + \frac{\sqrt{5}}{2}(N_4N_7 - N_3N_6)] \\
 R_7 &= Sv[(N_1N_5 - N_3N_7) + \frac{\sqrt{5}}{2}(N_3N_6 - N_4N_7) + \frac{\sqrt{5}}{2}(N_8N_3 - N_7N_2)] \\
 R_8 &= Sv[\sqrt{2}(N_2N_6 - N_4N_8) + \frac{\sqrt{5}}{2}(N_7N_2 - N_8N_3) + \frac{\sqrt{5}}{2}(N_6N_1 - N_5N_8)].
 \end{aligned} \tag{30}$$

The corresponding collisional invariants [12]

$$\begin{aligned}
 \psi^1 &= (1, 1, 1, 1, 1, 1, 1) \\
 \psi^2 &= \frac{1}{v}(0, v, v, v, 0, -v, -v, -v) \\
 \psi^3 &= \frac{1}{v}(v, v, 0, -v, -v, -v, 0, v) \\
 \psi^4 &= \frac{1}{v^2}(v^2, 2v^2, v^2, 2v^2, v^2, 2v^2, v^2, 2v^2)
 \end{aligned} \tag{31}$$

satisfying the relations

$$\begin{aligned}
 -\psi_1 & & +\psi_3 & & -\psi_5 & & +\psi_7 & & = 0 \\
 & \psi_2 & & -\psi_4 & & +\psi_6 & & -\psi_8 & = 0 \\
 & \psi_2 & -\psi_3 & & +\psi_5 & & +\psi_7 & -\psi_8 & = 0 \\
 -\psi_1 & & & & +\psi_5 & -\psi_6 & & +\psi_8 & = 0 \\
 & & -\psi_3 & +\psi_4 & & -\psi_6 & +\psi_7 & & = 0 \\
 \psi_1 & -\psi_2 & & +\psi_4 & -\psi_5 & & & & = 0
 \end{aligned} \tag{32}$$

have the physical meaning of conservation of mass, conservation of the x - and y -component of momentum, and conservation of energy. The vectors

$$\begin{aligned}
 \phi^1 &= (1, 1, 1, 1, 1, 1, 1, 1) \\
 \phi^2 &= (0, 1, 1, 1, 0, -1, -1, -1) \\
 \phi^3 &= (1, 1, 0, -1, -1, -1, 0, 1) \\
 \phi^4 &= (1, 2, 1, 2, 1, 2, 1, 2)
 \end{aligned} \tag{33}$$

represent a basis in the space F of collisional invariants with $\dim F = 4$. Since $\log \hat{N}$ is a collisional invariant [12], the maxwellian densities, which are responsible for the vanishing of the collision term in the Boltzmann equation, can be calculated by the relation

$$\hat{N} = \exp \sum_{i=1}^4 h_i \phi^i, \tag{34}$$

and have the explicit form

$$\begin{aligned}
 \hat{N}_1 &= Ae^{h_3+h_4} & \hat{N}_5 &= Ae^{-h_3+h_4} \\
 \hat{N}_2 &= Ae^{h_2+h_3+2h_4} & \hat{N}_6 &= Ae^{-h_2-h_3+2h_4} \\
 \hat{N}_3 &= Ae^{h_2+h_4} & \hat{N}_7 &= Ae^{-h_2+h_4} \\
 \hat{N}_4 &= Ae^{h_2-h_3+2h_4} & \hat{N}_8 &= Ae^{-h_2+h_3+2h_4}
 \end{aligned}
 \tag{35}$$

where $A = e^{h_1}$. Next, we assume that N_i does not depend on the y -coordinate and $N_1 = N_5$, $N_2 = N_4$, and $N_6 = N_8$. Because of this simplification $h_3 = 0$ in equation (35) (the maxwellians), and equation (29) (the Boltzmann equations) simplify to

$$\begin{aligned}
 \frac{\partial}{\partial t} N_1 &= Sv(N_3N_7 - N_1^2) \\
 \frac{\partial}{\partial t} N_2 + v \frac{\partial}{\partial x} N_2 &= Sv \frac{\sqrt{5}}{2} (N_6N_3 - N_7N_2) \\
 \frac{\partial}{\partial t} N_3 + v \frac{\partial}{\partial x} N_3 &= Sv[(N_1^2 - N_3N_7) + \sqrt{5}(N_7N_2 - N_6N_3)] \\
 \frac{\partial}{\partial t} N_6 - v \frac{\partial}{\partial x} N_6 &= Sv \frac{\sqrt{5}}{2} (N_7N_2 - N_6N_3) \\
 \frac{\partial}{\partial t} N_7 - v \frac{\partial}{\partial x} N_7 &= Sv[(N_1^2 - N_3N_7) + \sqrt{5}(N_6N_3 - N_7N_2)].
 \end{aligned}
 \tag{36}$$

This system of nonlinear partial differential equations can be transformed by the substitution

$$z = x + \xi t$$

into a system of nonlinear ordinary differential equations. In other words, from a physical point of view, we are looking for shock wave solutions, where ξ is the speed of the shock wave. With the abbreviation $\beta = \xi/v$ (speed of the shock wave in terms of the particle speed v) the following system of ordinary differential equations is obtained:

$$\begin{aligned}
 \frac{dN_1}{dz} &= \frac{S}{\beta} (N_3N_7 - N_1^2) \\
 \frac{dN_2}{dz} &= \frac{S}{\beta+1} \frac{\sqrt{5}}{2} (N_6N_3 - N_7N_2) \\
 \frac{dN_3}{dz} &= \frac{S}{\beta+1} [(N_1^2 - N_3N_7) + \sqrt{5}(N_7N_2 - N_6N_3)] \\
 \frac{dN_6}{dz} &= \frac{S}{\beta-1} \frac{\sqrt{5}}{2} (N_7N_2 - N_6N_3) \\
 \frac{dN_7}{dz} &= \frac{S}{\beta-1} [(N_1^2 - N_3N_7) + \sqrt{5}(N_6N_3 - N_7N_2)].
 \end{aligned}
 \tag{37}$$

The transformation

$$\begin{aligned}
 z &\rightarrow y = \frac{e^z - 1}{e^z + 1} \\
 z \in [-\infty, \infty] &\rightarrow y \in [-1, 1]
 \end{aligned}
 \tag{38}$$

on a finite interval [4] yields, from the mathematical point of view, an alternative system of differential equations in order to look for solitonic solutions:

$$\begin{aligned}
 \frac{dN_1}{dy} (1 - y^2) &= \frac{2S}{\beta} (N_3N_7 - N_1^2) \\
 \frac{dN_2}{dy} (1 - y^2) &= \frac{S}{\beta+1} \sqrt{5} (N_6N_3 - N_7N_2) \\
 \frac{dN_3}{dy} (1 - y^2) &= \frac{2S}{\beta+1} [(N_1^2 - N_3N_7) + \sqrt{5}(N_7N_2 - N_6N_3)] \\
 \frac{dN_6}{dy} (1 - y^2) &= \frac{S}{\beta-1} \sqrt{5} (N_7N_2 - N_6N_3) \\
 \frac{dN_7}{dy} (1 - y^2) &= \frac{2S}{\beta-1} [(N_1^2 - N_3N_7) + \sqrt{5}(N_6N_3 - N_7N_2)].
 \end{aligned}
 \tag{39}$$

The system of equation (39) is now defined over a finite interval, which is an advantage for solving this system numerically. We expect, of course, that the retransformed solution of equation (39) agrees with the solution of equation (37).

With the aid of the basis vectors (equation (33)) of the space F of collision invariants, the conservation equations are obtained by projecting the left-hand side of the Boltzmann equations (equation (36)) on these vectors:

$$\begin{aligned} \frac{\partial}{\partial t}(2N_1 + 2N_2 + N_3 + 2N_6 + N_7) + v \frac{\partial}{\partial x}(2N_2 + N_3 - 2N_6 - N_7) &= 0 \\ \frac{\partial}{\partial t}(2N_2 + N_3 - 2N_6 - N_7) + v \frac{\partial}{\partial x}(2N_2 + N_3 + 2N_4 + 2N_6 + N_7) &= 0 \\ \frac{\partial}{\partial t}(2N_1 + 4N_2 + N_3 + 4N_6 + N_7) + v \frac{\partial}{\partial x}(4N_2 + N_3 - 4N_6 - N_7) &= 0. \end{aligned} \quad (40)$$

Introducing again the variable $z = x + \xi t$ and the dimensionless speed of the shock wave $\beta = \xi/v$ in equation (40) and integrating them over $z \in [-\infty, \infty]$, one yields the RHEs

$$\begin{aligned} 2\beta N_1^+ + 2(\beta + 1)N_2^+ + (\beta + 1)N_3^+ + 2(\beta - 1)N_6^+ + (\beta - 1)N_7^+ &= \alpha \\ 2(\beta + 1)N_2^+ + (\beta + 1)N_3^+ - 2(\beta - 1)N_6^+ - (\beta - 1)N_7^+ &= \eta \\ 2\beta N_1^+ + 4(\beta + 1)N_2^+ + (\beta + 1)N_3^+ + 4(\beta - 1)N_6^+ + (\beta - 1)N_7^+ &= \gamma \end{aligned} \quad (41)$$

with the abbreviations

$$\begin{aligned} \alpha &:= 2\beta N_1^- + 2(\beta + 1)N_2^- + (\beta + 1)N_3^- + 2(\beta - 1)N_6^- + (\beta - 1)N_7^- \\ \eta &:= 2(\beta + 1)N_2^- + (\beta + 1)N_3^- - 2(\beta - 1)N_6^- - (\beta - 1)N_7^- \\ \gamma &:= 2\beta N_1^- + 4(\beta + 1)N_2^- + (\beta + 1)N_3^- + 4(\beta - 1)N_6^- + (\beta - 1)N_7^- \end{aligned} \quad (42)$$

The densities at $\pm\infty$, $N_i^- = N_i(z = -\infty)$, and $N_i^+ = N_i(z = +\infty)$, are not independent; they are coupled over the RHEs. By assuming equilibrium densities for N_i^- and N_1^+ with $h_3 = 0$ and $g_3 = 0$, respectively,

$$\begin{aligned} \hat{N}_1^- &= Ae^{h_4} & \hat{N}_1^+ &= Ge^{g_4} \\ \hat{N}_2^- &= Ae^{h_2+2h_4} & \hat{N}_2^+ &= Ge^{g_2+2g_4} \\ \hat{N}_3^- &= Ae^{h_2+h_4} & \hat{N}_3^+ &= Ge^{g_2+g_4} \\ \hat{N}_6^- &= Ae^{-h_2+2h_4} & \hat{N}_6^+ &= Ge^{-g_2+2g_4} \\ \hat{N}_7^- &= Ae^{-h_2+h_4} & \hat{N}_7^+ &= Ge^{-g_2+g_4} \end{aligned} \quad (43)$$

with $A = e^{h_1}$ and $G = e^{g_1}$, we obtain from equations (41) and (42) a system of three transcendental equations relating the equilibrium constants $(h_1, h_2, h_4; g_1, g_2, g_4)$ and the speed of the shock wave β :

$$\begin{aligned} \alpha &= 2\beta Ge^{g_4} + 2G(2e^{g_4} + 1)e^{g_4}[\beta \cosh g_2 + \sinh g_2] \\ \eta &= 2G(2e^{g_4} + 1)e^{g_4}[\beta \sinh g_2 + \cosh g_2] \\ \gamma &= 2G\beta e^{g_4} + 2Ge^{g_4}(4e^{g_4} + 1)[\beta \cosh g_2 + \sinh g_2] \end{aligned} \quad (44)$$

Table 3: Given values for the Maxwell exponents $h_1, h_2,$ and h_4 at $z = -\infty$ and g_2 at $z = +\infty$; calculated values of the Maxwell exponents g_2 and g_4 at $z = +\infty$, and the shock wave velocity β from the RHEs for three examples.

Example	$h_1, h_2, h_4, g_1, g_2, g_4, \beta$	N_i^-	N_i^+
1	$h_1=0.8, h_2=0.7, h_4=0.6$	$N_1^- = 4.055199966845$	$N_1^+ = 2.975243914392$
	$g_1=0.941281314301$	$N_2^- = 14.879731724873$	$N_2^+ = 3.453439645391$
	$g_2=0$	$N_3^- = 8.166169912568$	$N_3^+ = 2.975243914392$
	$g_4=0.149044709367$	$N_6^- = 3.669296667619$	$N_6^+ = 3.453439645391$
	$\beta_1 = -0.962918011040$	$N_7^- = 2.013752707470$	$N_7^+ = 2.975243914392$
	2	$h_1=0.8, h_2=0.7, h_4=0.6$	$N_1^- = 4.055199966845$
$g_1=0.891508496163$		$N_2^- = 14.879731724873$	$N_2^+ = 7.961651918351$
$g_2=0.4$		$N_3^- = 8.166169912568$	$N_3^+ = 5.382066999080$
$g_4=0.391564004797$		$N_6^- = 3.669296667619$	$N_6^+ = 3.577400809135$
$\beta_2 = -0.973781404422$		$N_7^- = 2.013752707470$	$N_7^+ = 2.418318589506$
3		$h_1=1, h_2=2, h_4=2$	$N_1^- = 20.085536923188$
	$g_1=1.930718354165$	$N_2^- = 1096.633158428459$	$N_2^+ = 27.273067358466$
	$g_2=0.2$	$N_3^- = 148.413159102577$	$N_3^+ = 15.154674206889$
	$g_4=0.587590658713$	$N_6^- = 20.085536923188$	$N_6^+ = 18.281683767260$
	$\beta_3 = -0.996631975589$	$N_7^- = 2.718281828459$	$N_7^+ = 10.158481912017$

with the abbreviations

$$\begin{aligned}
 \alpha &= 2\beta A e^{h_4} + 2A(2e^{h_4} + 1)e^{h_4}[\beta \cosh h_2 + \sinh h_2] \\
 \eta &= 2A(2e^{h_4} + 1)e^{h_4}[\beta \sinh h_2 + \cosh h_2] \\
 \gamma &= 2A\beta e^{h_4} + 2Ae^{h_4}(4e^{h_4} + 1)[\beta \cosh h_2 + \sinh h_2].
 \end{aligned}
 \tag{45}$$

At first, we assume the exponents $h_1, h_2,$ and h_4 of the maxwellians at $z = -\infty$ and g_2 at $z = +\infty$ as given quantities and solve the RHEs in equation (44) for the unknowns $g_1, g_4,$ and β numerically by means of the Newton–Raphson method. This is done both in the case of vanishing and nonvanishing drift velocity at $z = +\infty$. Drift equal to zero means that the gas is at rest, the drift velocity $\mathbf{U} = \frac{1}{n} \sum_{i=1}^8 N_i \mathbf{v}_i, n = \sum_{i=1}^8 N_i,$ vanishes. The assumed values for $h_1, h_2, h_4,$ and g_2 and the calculated values $g_1, g_4,$ and β for three examples are shown in Table 3. The Maxwell densities at $z = -\infty$ and at $z = +\infty$ are obtained with equation (43).

In the next step the systems of differential equations (equations (37) and (39)) are solved for $S = 1$ by two integration algorithms, namely the Runge–Kutta method (rkqs) [13] and semi-implicit Euler discretization with h -extrapolation (eulsim).¹ Now the maxwellian exponents $h_1, h_2, h_4,$ and the

¹The integrator eulsim was written by P. Deuffhard, U. Nowak, and U. Poehle of Konrad-Zuse-Zentrum für Informationstechnik Berlin (ZIB), Numerical Software Development.

Table 4: Comparison between the densities obtained from the RHEs and from the integration of the Boltzmann equations (equations (37) and (39)). The system in equation (37) is always solved with rkqs. The system in equation (39) is solved in the first example with eulsim and in the second example with rkqs.

Example	Densities from the solution of the RHE	Solution of equation (37) $N_i(z)$	Solution of equation (39) $N_i(z)$
1	$N_1^+ = 2.975243914392$ $N_2^+ = 3.453439645391$ $N_3^+ = 2.975243914392$ $N_6^+ = 3.453439645391$ $N_7^+ = 2.975243914392$	$N_1^+ = 2.975243914391$ $N_2^+ = 3.453439645425$ $N_3^+ = 2.975243914304$ $N_6^+ = 3.453439645391$ $N_7^+ = 2.975243914391$	$N_1^+ = 2.975243914341$ $N_2^+ = 3.453439645356$ $N_3^+ = 2.975243914367$ $N_6^+ = 3.453439645356$ $N_7^+ = 2.975243914381$
2	$N_1^+ = 3.607707398590$ $N_2^+ = 7.961651918351$ $N_3^+ = 5.382066999080$ $N_6^+ = 3.577400809135$ $N_7^+ = 2.418318589506$	$N_1^+ = 3.607707398591$ $N_2^+ = 7.961651918379$ $N_3^+ = 5.382066999006$ $N_6^+ = 3.577400809134$ $N_7^+ = 2.418318589507$	$N_1^+ = 3.607707398591$ $N_2^+ = 7.961651918400$ $N_3^+ = 5.382066998950$ $N_6^+ = 3.577400809134$ $N_7^+ = 2.418318589506$
3	$N_1^+ = 12.407597826058$ $N_2^+ = 27.273067358466$ $N_3^+ = 15.154674206889$ $N_6^+ = 18.281683767260$ $N_7^+ = 10.158481912017$	$N_1^+ = 12.407597826057$ $N_2^+ = 27.273067358858$ $N_3^+ = 15.154674206018$ $N_6^+ = 18.281683767261$ $N_7^+ = 10.158481912016$	

shock wave velocity β are assumed as given quantities (Table 3). The solutions $N_i(y)$ found by integrating the system in equation (39) are transformed into solutions $N_i(z)$ by applying the inverse transformation of equation (38). The Maxwellian densities at $z = +\infty$ obtained by solving the system of differential equations (equations (37) and (39)) and the solutions N_i^+ of the RHE are compared in Table 4. We would like to emphasize that the densities N_i^+ of the initial value problem (equations (37) and (39), respectively), at $z = +\infty$ coincide with the solutions N_i^+ of the RHE in the order of 10^{-8} .

The density profiles resulting from the integration of the system in equation (39) with eulsim (Table 3, Example 1) are shown in Figure 2. By integrating the corresponding system in equation (37) with rkqs we obtained identical density profiles. The profiles obtained by integrating the system in equation (37) with rkqs (Table 3, Examples 2 and 3) are shown in Figures 3, 4, and 5. The profiles obtained by integrating the system in equation (39) with rkqs in Example 2 coincide with the density profiles in Figure 3. For special values of the Maxwell exponents h_1 , h_2 , h_4 and the shock wave velocity β (Example 3), we obtained some overshooting for the density N_3 as can be seen in Figure 4. In Figure 5 a detail from Figure 4 is shown with a higher resolution.

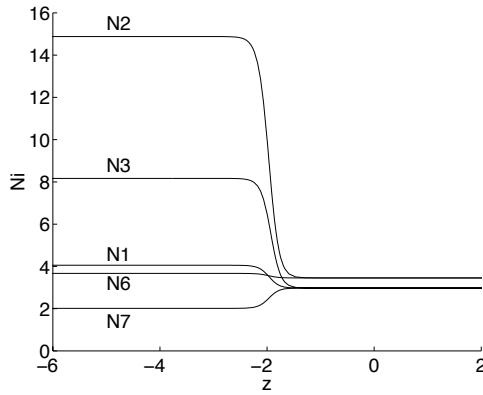


Figure 2: Density profiles $N_i(z)$, obtained by integrating the system in equation (39) with the eulsim algorithm (Example 1 in Tables 3 and 4).

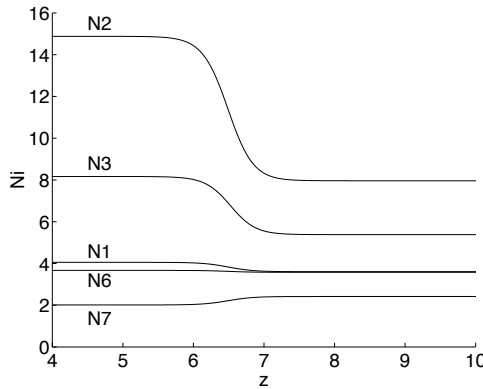


Figure 3: Density profiles $N_i(z)$, obtained by integrating the system in equation (39) with the rkqs algorithm (Example 2 in Tables 3 and 4).

5. Conclusion

It is well known that the Boltzmann equation for spatially inhomogeneous gases is too complex for finding analytical solutions in general. A promising way to overcome this problem is to find discrete models that are on the one hand easier to describe, and on the other hand keep the most important features of the real gases. A plane discrete velocity model with a variable number of particle speeds has been presented. The particles can interact elastically as well as inelastically. For the case of particles which have the velocity moduli v and $\sqrt{2}v$ and which can interact by binary elastic collisions, we found density profiles in the form of shock waves numerically. The values

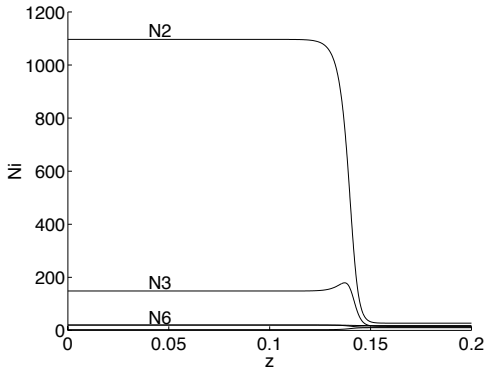


Figure 4: Density profiles $N_i(z)$, obtained by integrating the system in equation (37) with the rkqs algorithm (Example 3 in Tables 3 and 4).

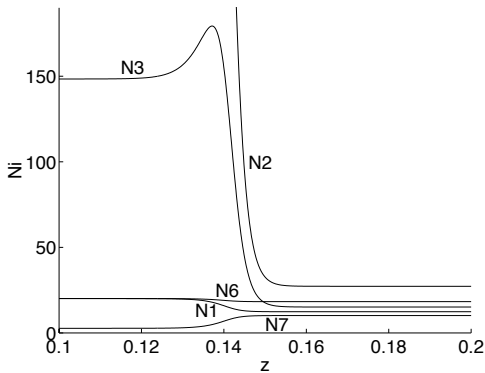


Figure 5: Density profiles $N_i(z)$ (detail from Figure 4 in higher resolution) obtained by integrating the system in equation (37) with the rkqs algorithm (Example 3 in Tables 3 and 4).

of these solutions at $\pm\infty$ are in good agreement with the equilibrium values resulting from the Rankine Hugoniot equations. Further work on these topics is encouraged.

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