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Citation: Physics of Fluids (1994-present) 27, 037101 (2015); doi: 10.1063/1.4913673
View online: http://dx.doi.org/10.1063/1.4913673
View Table of Contents: http://scitation.aip.org/content/aip/journal/pof2/27/3?ver=pdfcov
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Study of the shock wave structure by regularized Grad’s set of equations

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(Received 1 September 2014; accepted 12 February 2015; published online 6 March 2015)

In this work, we continue to study the possibility of applying moment equations for strongly nonequilibrium flows by an example of the problem of the shock wave structure in a monatomic gas in a wide range of Mach numbers for various models of molecular interaction. The object of the study is the so-called regularized 13-moment Grad’s system (R13). First time, both linear and nonlinear versions of this system of equations were considered for the problem at such wide range of parameters. The Godunov method with increased accuracy is used as a numerical tool for solving the R13 system. The numerical results for the R13 system are analyzed by using data obtained by the Direct Simulation Monte Carlo (DSMC) method, experimental data, and analytical results. As a whole, the R13 system provides an adequate description of the shock wave structure in a wide range of Mach numbers. For Mach numbers around 2, good agreement with experimental and DSMC results is observed for both linear and nonlinear versions of the system. For high Mach numbers, the result strongly depends on the molecular interaction model used: shock wave structure predictions of the nonlinear R13 system are better for Maxwell molecules and worse for hard spheres as compared to the linear version. Particular attention in this work is paid to studying nonmonotonicity of the total temperature profile (temperature overshoot) in the structure of a strong shock wave. It is shown that the moment equations correctly predict the existence of the temperature overshoot. At the same time, the solution of the moment equations overpredicts the temperature overshoot at least two-fold for Mach number \( M = 8 \), and the nonlinear version of the R13 system yields a better result for this parameter than the linear version. © 2015 AIP Publishing LLC. [http://dx.doi.org/10.1063/1.4913673]

I. INTRODUCTION

As the degree of rarefaction of the gas flow (Knudsen number) increases, the gas distribution function starts to deviate from the equilibrium Maxwell distribution. For this reason, the continuum approach based on Navier-Stokes equations is inapplicable for strongly rarefied flows. The kinetic approach based on solving the Boltzmann equation is formally applicable for all degrees of rarefaction. However, in solving real applied problems by methods based on the kinetic approach, such as the Direct Simulation Monte Carlo (DSMC) method,1 numerical solution of the Boltzmann equation,2–4 and various model equations (BGK, ESM, Shakhov etc.,5–7), there are significant constraints associated with computational engineering capabilities. An alternative for computations of moderately rarefied flows is the use of continuum methods, which can simulate the behavior of significantly

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nonequilibrium gas flows, in contrast to Navier-Stokes equations. Here, we can mention the approach proposed in Ref. 8 Burnett equations and their modifications,\textsuperscript{9–11} gas-kinetic methods,\textsuperscript{13,14} Grad’s moment method,\textsuperscript{9,15,16} and others. The task of this work is to check whether the regularized system of one of the most successful modifications of the original Grad’s equations (R13)\textsuperscript{16} is suitable for modeling nonequilibrium flows. For this purpose, we consider the classical problem of the kinetic theory of gases in which effects associated with thermal nonequilibrium of the flow are manifested: the problem of the shock wave structure in a monatomic gas.

In the middle of the 20th century, Grad proposed an approach\textsuperscript{9,15} in which the so-called system of moment equations was derived from the kinetic Boltzmann equation. The nonequilibrium distribution function is determined by means of its expansion in the Hermite polynomials around the equilibrium Maxwell distribution function. This system is written with respect to macroparameters (moments of the distribution function) and describes the gas not only when it can be considered as continuum but also in the transitional flow regime, i.e., it takes rarefaction effects into account. In the general case, the system of moment equations is infinite. Some additional closure relations are introduced to obtain a finite system. Thus, higher-order moments that are not included into the system are expressed in terms of moments retained in the system. This approach was first implemented by Grad in Ref. 14, where he derived a system of 13 equations by using the simplest closure relations.

Later on, various systems consisting of 20, 26, and more equations were developed with Grad’s moment method.\textsuperscript{9} It turned out later, however, that Grad’s method has some drawbacks. It was shown\textsuperscript{9,17} that the series in the Hermite polynomials representing the distribution function in the shock wave does not converge in the case of a finite radius of molecular interaction. As a result, there appear unphysical jumps of gas-dynamic parameters in supersonic flows at Mach numbers greater than 1.65.\textsuperscript{18,19} Various modifications of Grad’s system of equations were constructed to avoid the unphysical nature of obtained results.

In this work, we consider a 13-moment Grad’s system with its modification proposed by Struchtrup and Torrilhon\textsuperscript{16} who called the resultant system the “regularized Grad’s system” (or R13). Regularization of Grad’s system implies that high-order moments are presented in the form of expressions containing 13 moments (density, three components of velocity, six components of the symmetric stress tensor, and three components of the heat flux) and their gradients. The solution of the resultant system of equations does not contain unphysical jumps of gas-dynamic parameters inside the shock wave front at Mach numbers greater than 1.65.\textsuperscript{19} Later on, the regularization procedure proposed by Struchtrup and Torrilhon was also applied for the 20-moment\textsuperscript{20} and 26-moment\textsuperscript{21} systems of Grad’s equations.

In this work, we study the applicability of the R13 system to nonequilibrium flows by an example of a problem of the structure of a plane shock wave. It is the classical problem of the kinetic theory of gases, which involves many specific features of nonequilibrium high-velocity flows. It is known that traditional models of continuum gas dynamics, such as Navier-Stokes equations, fail to ensure a correct description of the shock wave structure at high Mach numbers. Therefore, it is particularly interesting to consider the applicability of the R13 system to solving this problem in a wide range of Mach numbers.

One of the poorly studied specific features of this problem is the nonmonotonicity of the total temperature profile for the shock wave structure in a monatomic gas at sufficiently high Mach numbers. It was shown\textsuperscript{22} that a peak (temperature overshoot) is expected to appear in the temperature profile on the rear front of a strong shock wave. This peak appears in simulations with all molecular interaction potentials at Mach numbers $M > 3.9$\textsuperscript{23,24} and increases with further enhancement of the shock wave intensity. The first numerical results that confirm this phenomenon were obtained by solving the full\textsuperscript{23} and model\textsuperscript{9} Boltzmann equations. Later on, this peak was obtained by other researchers during the direct numerical solution of the Boltzmann equation [e.g., Ref. 25], by using the DSMC method\textsuperscript{26,27} and in solving the model kinetic equations.\textsuperscript{6,28} It was shown\textsuperscript{29} that this peak also appears in solving the R13 system. The magnitude of this temperature overshoot in the solution of the R13 equations was estimated for the first time in Ref. 27.

The applicability of the R13 system is determined in the present work through comparisons with both experimental data and DSMC results obtained by the SMILE software system.\textsuperscript{30} Particular attention is paid to the difference in results predicted by the linear and nonlinear versions of the
R13 system for different models of molecular interaction and different Mach numbers and to the ability of the R13 system to predict fine details of the shock wave structure, such as the temperature overshoot.

II. FORMULATION OF THE PROBLEM

A one-dimensional plane shock wave problem is considered. The flow direction is from left to right. In this formulation, the free-stream gas-dynamic quantities $\rho_1$, $u_1$, and $T_1$ (conditions on the left boundary) are input parameters of the problem. To impose the boundary conditions on the subsonic right boundary, the corresponding values of the gas-dynamic quantities $\rho_2$, $u_2$, and $T_2$ are calculated from the free-stream parameters $\rho_1$, $u_1$, and $T_1$ with the use of conservation equations (Rankine-Hugoniot conditions)

\[
\begin{aligned}
\rho u = \text{const}, \\
\rho u^2 + p = \text{const}, \\
u^2 + h = \text{const},
\end{aligned}
\]

where $\rho$ is the density, $u$ is the velocity, $p$ is the pressure, and $h$ is the enthalpy; for a monatomic gas, $h = \frac{5}{2}RT$, where $R = \frac{k}{m}$.

All results are further presented in the dimensionless form. The temperature and density are normalized in accordance with the formulas

\[
\overline{T} = \frac{T - T_1}{T_2 - T_1}, \quad \overline{\rho} = \frac{\rho - \rho_1}{\rho_2 - \rho_1},
\]

where $\rho_1, T_1$ are the free-stream values and $\rho_2, T_2$ are the values behind the shock wave front. With the above-given normalization, the macroparameters on the upstream and downstream boundaries have the values of 0 and 1, respectively.

III. MATHEMATICAL MODEL

The regularized 13-moment Grad’s system (R13) proposed in 2003 by Struchtrup and Torrilhon\textsuperscript{16} has the following tensor form:

\[
\begin{aligned}
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_k}{\partial x_k} &= 0, \\
\rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} + \frac{\partial p}{\partial x_i} + \frac{\partial \sigma_{ik}}{\partial x_k} &= 0, \\
3 \frac{\partial k T}{\partial t} + 3 \frac{\partial k T}{\partial x_k} + \frac{\partial q_k}{\partial x_k} + p \frac{\partial v_k}{\partial x_k} + \sigma_{ij} \frac{\partial v_i}{\partial x_j} &= 0, \\
\frac{\partial \sigma_{ij}}{\partial t} + \frac{\partial \sigma_{ij} v_k}{\partial x_k} + \frac{4}{5} \frac{\partial q_{(i)}}{\partial x_j} + 2 \frac{\partial \sigma_{(k)} v_j}{\partial x_k} + 2 \sigma_{(k)} v_j v_k \frac{\partial v_i}{\partial x_k} + \frac{\partial m_{ijk}}{\partial x_k} &= -\frac{\sigma_{ij}}{\tau},
\end{aligned}
\]

where the density $\rho$, velocity $u_i$, pressure $p$, viscous stress tensor $\sigma_{ij}$, and heat flux $q_i (i = x, y, z)$ form 13 primitive variables; the 14th variable, i.e., the temperature $T$, is related to other variables via the equation of state. Equations (2)–(4) are the classical relations of continuity and the momentum and energy conservation laws; Eqs. (5) and (6) are the relations derived by Grad in Ref. 15 for the components of the stress tensor and of the heat flux vector, respectively. Higher-order moments that
appeared in the 13-moment system of equations owing to the regularization procedure \(^{16}\) (new terms in equations as compared with Grad’s system \(^{15}\)) have the following analytical form:

\[
m_{ijk} = -2\tau \left[ \frac{k}{m} \frac{\partial \sigma_{ij}}{\partial x_k} - \frac{k}{m} T \sigma_{ij} \frac{\partial \ln \rho}{\partial x_k} + \frac{4}{5} q(i) \frac{\partial U_j}{\partial x_k} - \frac{\sigma_{ij}}{\rho} \frac{\partial \sigma_{kj}}{\partial x_i} \right],
\]

\[
R_{ij} = -\frac{24}{5} \tau \left[ \frac{k}{m} T \frac{\partial q(i)}{\partial x_j} + \frac{k}{m} q(i) \frac{\partial T}{\partial x_j} - \frac{k}{m} T q(i) \frac{\partial \ln \rho}{\partial x_j} - \frac{1}{\rho} q(i) \frac{\partial \sigma_{kj}}{\partial x_j} \right] + \frac{5}{7} \frac{k}{m} T \left( \sigma_{kj} \frac{\partial U_j}{\partial x_k} + \sigma_{kj} \frac{\partial U_k}{\partial x_j} - \frac{2}{3} \sigma_{ij} \frac{\partial u_j}{\partial x_k} \right) - \frac{5}{6} \frac{\sigma_{ij}}{\rho} \frac{\partial u_k}{\partial x_k} - \frac{5}{6} \frac{\sigma_{ij}}{\rho} \frac{\partial u_k}{\partial x_k},
\]

\[
\Delta = -12\tau \left[ \frac{k}{m} T \frac{\partial q_k}{\partial x_k} + \frac{5}{2} \frac{k}{m} q_k \frac{\partial T}{\partial x_k} - \frac{k}{m} T q_k \frac{\partial \ln \rho}{\partial x_k} + \frac{1}{\rho} q_k \frac{\partial \sigma_{jk}}{\partial x_k} + \frac{k}{m} T \sigma_{ij} \frac{\partial U_j}{\partial x_k} \right].
\]

In addition to the full R13 system, we studied the behavior of the linear version \(^{29}\) of this system. In the linear case, the calculation of high-order moments involves only terms that are responsible for the so-called gradient transport mechanism (GTM) \(^{21,31}\) for the stress tensor and heat flux. It is these terms that ensure stabilization of the original Grad’s system of equations. The remaining terms omitted in the linear case form the so-called non-gradient transport mechanism (NGTM) \(^{21,31}\).

In the linear case (GTM), higher-order moments have the following form: \(^{21,31,32}\)

\[
m_{ijk} = -2\tau \frac{k}{m} \frac{\partial \sigma_{ij}}{\partial x_k}, \quad R_{ij} = -\frac{24}{5} \tau \frac{k}{m} T \frac{\partial q(i)}{\partial x_j}, \quad \Delta = -12\tau \frac{k}{m} T \frac{\partial q_k}{\partial x_k},
\]

In all relations given above, the variable \(k\) that is not a subscript is the Boltzmann constant, \(\tau\) is the relaxation time, and \(m\) is the mass of one molecule. The broken brackets in the subscripts indicate the traceless part of the tensor. \(^{29}\) Summation is performed over repeated subscripts. This system of equations was derived for the Maxwell model of molecular interaction. At the same time, the system is used for other potentials of molecular interaction with the viscosity law obtained on the basis of these potentials. The viscosity is defined by the power law

\[
\mu = \frac{p}{\nu} = p\tau = \mu_{ref} \left( \frac{T}{T_{ref}} \right)^\omega,
\]

where \(0.5 \leq \omega \leq 1.0\). The values \(\omega = 0.5\) and \(\omega = 1.0\) correspond to the models of hard spheres and Maxwell molecules, respectively. \(^{29}\) In addition to the limiting cases of hard spheres and Maxwell molecules, we also consider the case with \(\omega = 0.72\) corresponding to viscosity of argon. \(^{33}\)

In 2006, Torrilhon \(^{32}\) proposed a divergent form of writing the R13 system for a two-dimensional case. In the two-dimensional case, the number of equations decreases to nine, and the system can be written in the form

\[
\frac{\partial U(W)}{\partial t} + \text{div} F(W) = P(W),
\]

where \(W\) is the vector of the primitive variables

\[
W = \{\rho, u_x, u_y, p, p_s, p_y, \sigma, q_x, q_y\}^T,
\]

\[p_y = \sigma_{yy}, \quad \sigma = \sigma_{xy}, \quad p = (p_x + p_y + p_z)/3.\] The vectors \(U(W), P(W),\) and \(F_x(W), F_y(W)\) are the vectors of conservative variables, relaxation terms, and fluxes, respectively. The forms of the \(U(W)\) and \(P(W)\) vectors for the two-dimensional case are (Ref. 32):
The form of $F_x(W) = (F_x(W), F_y(W))$ vector is (Ref. 32):

$$
F_x = \begin{pmatrix}
\rho u_x \\
\rho u_x v_x + p_x \\
\rho u_x v_y + \sigma \\
\rho u_x v_x^2 + 2(p_x v_x + \sigma v_y) + 3p v_x + 2q_x \\
\rho u_x v_y^2 + p_y v_x + 2\sigma v_x + \frac{2}{3}q_y + m_{xx} \\
\rho u_x v_y + 2p_x v_y + 2\sigma v_x + \frac{2}{3}q_y + m_{xy} \\
(\rho v^2 + 3p + 4p_y) v_x v_y + (7\theta + v^2) p_x + 4\sigma v_x v_y + \frac{32}{3}q_x v_y + 4 + 2p + \bar{R}_{xx} \\
(\rho v^2 + 3p + 2(p_x + p_y)) v_x v_y + (7\theta + 3v^2) \sigma + \frac{14}{3}q_x v_y + q_y v_x + \bar{R}_{xy} \\
(\rho v^2 + 3p + 4p_y) v_y^2 + (7\theta + v^2) p_y + 4\sigma v_x v_y + \frac{32}{3}q_y v_y + \frac{4}{3}q_x v_x - 2\theta p + \bar{R}_{yy}
\end{pmatrix}
$$

$\bar{F}_i = \frac{1}{A_{ij}} (\hat{F}_{i+1/2j} + \hat{F}_{i+1/2j} + \hat{F}_{i-1/2j} + \hat{F}_{ij+1/2j})$, where $\bar{F}_{i+1/2j}$ is the numerical flux through the face between the cells indicated by the subscripts $i+1, j$ and $i, j$:

$$
\bar{F}_{i+1/2j} = (\Delta y F_x - \Delta x F_y)_{i+1/2j}
$$

Here, $F_x$ and $F_y$ are the components of the vector $F$. The hyperbolic part of the flux $\bar{F}_{i+1/2j}$ (corresponding to the system of Grad’s equations) is approximated by the approximate HLL method.
of solving the Riemann problem

$$
\tilde{F}_{i+1/2j} \approx \tilde{F}^{G13} = \frac{b_R}{\Delta b} \tilde{F}^{G13}_L - \frac{b_L}{\Delta b} \tilde{F}^{G13}_R + \frac{b_R b_L}{\Delta b} (U_R - U_L).
$$

where the subscripts L and R are used to indicate the parameters “on the left” and “on the right” of the face. The quantities $b_L$ and $b_R$ are found as follows:

$$
b_L = \min(0,a_L), \quad b_R = \max(0,a_R), \quad \Delta b = b_R - b_L.
$$

The maximum velocities of propagation of disturbances to the left and right from the gas particle trajectory $a_L$ and $a_R$ are set in accordance with Ref. 31 as

$$
a_L = v_{n,L} - c_L^{\text{max}}, \quad a_R = v_{n,R} + c_R^{\text{max}},
$$

where $c^{\text{max}}$ is determined by the empirical formula

$$
c^{\text{max}}_{\theta^{1/2}} = c^{(p)}(P_2) + \left( c^{(p)}(P_1) - c^{(p)}(P_2) \right) |\bar{n} \cdot \bar{V}| + c^{(q)} \left( \frac{||\bar{q}||}{P \theta^{1/2}} \right) \bar{n} \cdot \bar{q},
$$

where $P_{1,2}$ are determined as eigenvalues of the matrix

$$
\begin{pmatrix}
\frac{p_s}{p} & \frac{\sigma}{p} \\
\frac{\sigma}{p} & \frac{p_s}{p}
\end{pmatrix},
$$

and $\tilde{V}_i$ is determined as an eigenvector corresponding to $P_1$. The expression for $c^{\text{max}}$ involves two empirical functions

$$
c^{(p)}(P) = c^{(0)}_{\text{max}}/\theta^{1/2} - 0.9 + P - 0.1P^2,
$$

$$
c^{(q)}(Q) = \left( c^{(0)}_{\text{max}}/\theta^{1/2} \right)^4 + 25Q \right)^{1/4} - c^{(0)}_{\text{max}}/\theta^{1/2}.
$$

The second order of accuracy in space on smooth solutions is reached by using essentially two-dimensional procedures of reconstruction of the primitive variables inside each computational cell. Usual central difference approximation is used for discretization of the “elliptical” part of the fluxes (diffuse terms).

Approximation in time is performed by a modified second-order explicit-implicit Runge-Kutta method

$$
U^{(1)} = U^n - \Delta t \text{div}(F^n) + \Delta t P(U^{(1)}),
$$

$$
U^{n+1} = \frac{1}{2} \left( U^n + U^{(1)} \right) + \frac{\Delta t}{2} \text{div}(F^{(1)}) + \frac{\Delta t}{2} P(U^{n+1}),
$$

i.e., the term with $\text{div}(F)$ is approximated explicitly, and the relaxation term is approximated implicitly. Therefore, a system of nonlinear equations has to be solved in each cell at each stage of the method. This fact does not make the computation too slow, because the structure of the relaxation terms allows this nonlinear system to be easily solved.

V. DSMC COMPUTATIONS

DSMC results are used as a benchmark for numerical solution of R13 system of equations. The DSMC computations were performed by SMILE software system based on the majorant frequency scheme. The parameters of the numerical method were chosen in such a way that they ensured an accurate result: the collision cell size was more than five times smaller than the local mean free path, the number of simulated particles in each cell was more than 1000, and the time step was more than three times smaller than the mean local flight time needed for the particle to pass over the collision cell. The computational domain length was usually from 60 to 150 free-stream mean free paths. At the initial time, the domain was seeded by particles in accordance with the mean values of gas-dynamic parameters, which were defined by piecewise-constant functions with a discontinuity at the center of the computational domain, and these values corresponded to conditions ahead of
and behind the shock wave front related by the Rankine-Hugoniot conditions. On the computational domain boundaries, the simulated particles were generated in accordance with equilibrium distribution functions determined by the parameters ahead of and behind the wave front. Molecular interaction was described by the Variable Hard Spheres (VHS) model, which corresponds to the model of hard spheres for $\omega = 0.5$ and to the model of pseudo-Maxwell molecules for $\omega = 1$; in the latter case, molecular scattering is isotropic, in contrast to the model of Maxwell molecules. Further in the paper, all results for Maxwell molecules were obtained by the DSMC method with the VHS model for $\omega = 1$. Note that the Variable Soft Sphere (VSS) model is widely used in the DSMC method. In this model, scattering is not isotropic, and it is more suitable for modeling gas mixtures than the VHS model because it describes diffusion processes more accurately. However, results of DSMC computations of the shock-wave structure in a one-component gas with the VHS and VSS models have been compared before and no significant difference in macroparameters’ profiles has been observed (see Ref. 39). Therefore, the simpler VHS model is employed for the present study.

**VI. RESULTS AND DISCUSSION**

A typical flow structure in the shock wave front for argon ($\omega = 0.72$) is demonstrated in Fig. 1, which shows the DSMC results and the results of solving the R13 equations (linear version). The coordinate hereinafter is normalized to the free-stream mean free path: $x = X/\lambda$, where $\lambda$ is the mean free path of VHS molecules with the density and temperature corresponding to the incoming flow

$$\lambda = \left(\frac{\sqrt{2\pi d_{\text{ref}}^2 \rho \left(\frac{T_{\text{ref}}}{T}\right)^{\omega-1/2}}}{m}\right)^{-1}.$$

We assumed that the reference diameter $d_{\text{ref}}$ at the temperature $T_{\text{ref}}$ used in the DSMC computations can be determined based on the value of the viscosity coefficient $\mu_{\text{ref}}$ at the same temperature by using the expression from Ref. 1 for VSS molecules (Eq. (4.62) on page 92), which has the following form in the VHS case:

$$d_{\text{ref}} = \left[\frac{15\sqrt{m k T_{\text{ref}} / \pi}}{2 (5 - 2\omega) (7 - 2\omega) \mu_{\text{ref}}}\right]^{1/2}.$$

This expression reduces to the first-approximation Chapman-Enskog expression for hard sphere molecules. The expression of Pekeris and Alterman is preferable for hard spheres. However, application of this expression would lead only to scaling of R13 macroparameter profiles along the x coordinate by a factor of $1.016 \, 034$, which is hardly noticeable. As this effect is extremely weak, the standard VHS expression is used for all models of molecular interaction in the paper for consistency.

![FIG. 1. Density and temperature profiles in the shock wave front, $M = 2.05$, argon.](image)
The flow direction is from left to right. The origin of the coordinate system is fitted to the wave center (to the point where the density value is 0.5). The accuracy of the numerical solution of the R13 system presented in this paper is considered in detail below.

A. Accuracy of the numerical solution

The temperature profiles for the Mach number $M = 8.0$ with the Maxwell model of molecular interaction, which were obtained by solving the R13 system with the use of computational grids with 1.25, 2.50, 5.00, 10.00, and 20.00 cells per mean free path in the incoming flow $\lambda$ are compared in Fig. 2. Figure 2(a) shows the entire temperature profile, and Fig. 2(b) shows the zoomed region of the overshoot in the total temperature distribution. The analysis of these results reveals that the solution converges in this numerical method. It turned out that a grid with ten computational cells per mean free path is sufficient to obtain the solution with desired accuracy.

B. Comparison with Yen’s relation

In the problem of the shock wave structure, the temperature component along the flow $T_x$ is called the streamwise temperature, and $T_\perp = \frac{1}{2}(T_y + T_z)$ is the transverse temperature. In these notations, we have

$$T = \frac{1}{3}(T_x + 2T_\perp).$$  \hspace{1cm} (24)

Yen was the first researcher who obtained an analytical dependence (Yen’s relation) that related the streamwise temperature to the dimensionless density in a one-dimensional steady flow

$$\frac{T_x}{T_1}(\rho) = \frac{1}{3}\left[(5M_1^2 + 3)\left(\frac{\rho}{\rho_1}\right)^{-1} - 5M_1^2\left(\frac{\rho}{\rho_1}\right)^{-2}\right],$$  \hspace{1cm} (25)

where $M_1$, $T_1$, and $\rho_1$ are the Mach number, temperature, and number density, respectively (the subscript of unity corresponds to free-stream values of these parameters). Yen’s relation yields an exact analytical dependence of streamwise temperature on density and directly follows from the laws of conservation of mass and momentum. Numerical results obtained by the DSMC method and by solving the R13 system (the linear version of the equations) are tested by means of comparisons with Yen’s relation. The calculated results for the hard-sphere model are compared with Yen’s relation for the dependence of the streamwise temperature on density in Fig. 3. The DSMC profile

![FIG. 2. Convergence of the numerical solution on the grid for the temperature distribution in the entire front (a) and in the region of the temperature overshoot (b) for the R13 system.](image-url)
of the streamwise temperature is in excellent agreement with Yen's relation obtained from the DSMC density profile. Similar agreement between the streamwise temperature and Yen's relation is observed for the solution of the R13 equations. This agreement demonstrates that the conservation laws are satisfied with high accuracy when the R13 equations are solved.

C. Comparison with experimental data

Numerical results are compared in Fig. 4 with experimental data\textsuperscript{33} on the density profile inside the shock wave front at Mach numbers 2.05 and 8 for argon ($\omega = 0.72$). For the Mach number $M = 2.05$, both the DSMC results and the results of solving the R13 system are in excellent agreement with the experimental data. For small Mach numbers, there is no noticeable nonequilibrium in the shock wave front; for this reason, the R13 equations ensure an adequate description of the internal structure of the shock wave (both linear and nonlinear versions) without noticeable differences from the experimental data and DSMC solution. For the Mach number $M = 8$, the DSMC results are in excellent agreement with the experiments, whereas the R13 results are slightly different from the experimental data. The linear version of the R13 system, which is indicated in the figures by $\text{lin}$, predicts higher values of density (more than 20%) in the leading front of the shock wave ($-4 < x < -1$) than the experimental data. The nonlinear version, which is indicated by $\text{nonlin}$, ensures a smaller difference from the experimental data, but the density profile has a qualitative specific feature, namely, a noticeable inflection at the point $x \sim -1$, which makes the profile essentially asymmetric with respect to the wave center. In the experimental and DSMC density profiles, this inflection is observed approximately at the wave center ($x \sim 0$), and the profiles are approximately symmetric.

FIG. 3. Streamwise temperature for $M = 2.0$ (a) and $M = 8.0$ (b). Comparison of numerical results with Yen’s relation.\textsuperscript{41}

FIG. 4. Density for $M = 2.05$ (a) and $M = 8.0$ (b). Comparison of numerical results obtained by different methods with experimental data.
FIG. 5. Comparison of the shock wave structures for hard sphere molecules and $M = 2.0$ predicted by the linear (a) and nonlinear (b) versions of the R13 system with DSMC results. Density and temperature.

with respect to the wave center. However, as a whole, we can state that both versions of the R13 system accurately predict the internal structure of the shock wave in argon even at high Mach numbers.

The kinetic theory of gases traditionally deals with two limiting cases of molecular interaction: molecules are considered as hard spheres ($\omega = 0.5$) or as Maxwell molecules ($\omega = 1$). It should be noted that $\omega$ usually takes intermediate values between these two limits for most gases. The two limiting cases are considered in more detail below. The main attention is paid to cases with Mach numbers 2 and 8, which correspond to situations with weak and strong deviation from the equilibrium state, respectively.

D. Shock wave structure, $M = 2$

Results of numerical simulations for the Mach number $M = 2.0$ are presented below. Figures 5 and 6 show the profiles of macroparameters for the hard sphere model. The DSMC results are compared with the solution of the linear (left) and nonlinear (right) versions of the R13 system. It is seen that the linear version yields a solution that perfectly coincides with the DSMC solution, in terms of both density and all components of temperature. It is surprising that the nonlinear version yields results that are somewhat different from the DSMC solution, in particular, underpredictions of the streamwise temperature at $-7 < X < -3$ are observed. For instance, at $X = -5$, the streamwise temperature predicted by the nonlinear version is twice lower than the corresponding DSMC value. As a whole, however, we can say that both versions of the R13 system ensure fairly good agreement

FIG. 6. Comparison of the shock wave structures for hard sphere molecules and $M = 2.0$ predicted by the linear (a) and nonlinear (b) versions of the R13 system with DSMC results. Different components of temperature.
with the benchmark DSMC solution. The above-mentioned asymmetry of the density profile with respect to the shock wave center should also be noted; it is especially well visible in the nonlinear version.

Figures 7 and 8 show similar results for Maxwell molecules. As in the case of hard spheres, the results predicted by solving the R13 equations agree very well with the results of DSMC simulations. However, in contrast to the case of hard sphere molecules, the nonlinear version of the R13 system ensures a better result than the linear version of the system. This is particularly well seen in Fig. 8, which shows different components of temperature. The linear version of R13 overpredicts both the total temperature and its components in the leading front of the shock wave, i.e., at \( X < -2 \). For example, this excess reaches 50\% for the parallel temperature. For the nonlinear version, such a difference from DSMC results is not observed.

The differences in the results for different models of molecular interaction is explained first of all by the fact that the R13 equations used in the present study were originally derived under the assumption of interaction according to the model of Maxwell molecules.\(^{19}\) The linear version is obtained from the original nonlinear version by eliminating some terms (21 and 29). It is seen that the error associated with elimination of these terms leads to a worse result in the case where Maxwell molecules are simulated. However, if the R13 equations are used for modeling molecules as hard spheres (the dynamic viscosity is proportional to the square root of temperature), there appears an error induced by the fact that the equations were derived under the assumption of another interaction potential, and the results predicted by the nonlinear version of the R13 system differ from the DSMC solution. In the linear version with the hard sphere model, the result is possibly improved owing to mutual annihilation of two errors mentioned above. Below, we consider the case with a high
E. Shock wave structure, $M = 8$

Figures 9 and 10 show the results of flow modeling for the Mach number $M = 8.0$ with the hard sphere model. The difference from the DSMC computations is noticeably greater than for the low Mach number. Nevertheless, the linear version of the R13 system predicts the internal structure of the shock wave fairly well, whereas the difference of the results obtained within the framework of the nonlinear version from the DSMC predictions is appreciably greater. In particular, the temperature profile is substantially wider, and the density profile is strongly asymmetric with respect to the shock wave center. The temperature profiles for the nonlinear case have singularities that are not observed in the DSMC solution. In particular, there are inflections in the profiles of the transverse and total temperatures close to the rear part of the wave front (for values of parameters appreciably greater than 0.5), whereas the DSMC profiles are smooth and have no clearly expressed inflection points.

In the case of Maxwell molecules (the results for this case are illustrated in Figs. 11 and 12), the difference of the results predicted by solving the R13 system from the DSMC results is even greater. As in the case of hard spheres, there are typical inflections in the profiles in the nonlinear case. The main differences from the DSMC solution are observed in the narrow zone of the shock wave front; the temperature starts to grow later and more drastically. As a whole, the nonlinear version of the R13 system better predicts the shock wave structure than the linear version for Maxwell molecules.
FIG. 11. Comparison of the shock wave structures for Maxwell molecules and $M = 8.0$ predicted by the linear (a) and nonlinear (b) versions of the R13 system with DSMC results. Density and temperature.

In the nonlinear case, the slope of the temperature profiles in the leading front of the shock wave is smaller, and the result is in better agreement with the DSMC predictions.

As a whole, the results for the Mach number $M = 8.0$ are consistent with those for $M = 2.0$. Again, the best results for Maxwell molecules are provided by the nonlinear version, whereas the opposite situation is observed for the linear case, which is apparently explained by the effect of summation of two different errors. Thus, if the R13 system is used with a viscosity law that differs from the Maxwell model, then elimination of non-gradient transport terms in expressions for high-order moments may paradoxically make the result approach the solution of the Boltzmann equation. The greatest difference of the nonlinear result from the DSMC data is observed on the leading front of the shock wave. Below, we consider how the R13 equations describe the find structure of the shock wave, in particular, much attention is given to the presence of the total temperature peak in the wave front.

F. Temperature overshoot inside the shock wave

An interesting object to be studied within the problem of the shock wave structure is the peak in the total temperature distribution on the rear front of the wave. This nonmonotonicity (overshoot) in the total temperature profile for a monatomic gas was observed in previous studies. For instance, Shakhov\(^6\) assumed that one of the possible reasons for the total temperature peak in the case with the S-model was the failure of the numerical solution to reach a steady state. In the same year, Elliott and Baganoff demonstrated\(^22\) that the nature of this peak is not numerical. Later on, it was found

FIG. 12. Comparison of the shock wave structures for Maxwell molecules and $M = 8.0$ predicted by the linear (a) and nonlinear (b) versions of the R13 system with DSMC results. Different components of temperature.
that this peak also appears in solving the Boltzmann kinetic Equation (23), model equations (e.g., Ref. 28), and in DSMC computations (e.g., Refs. 24 and 26). Yen\textsuperscript{23} noted that the temperature peak emerges in the shock wave structure of a monatomic gas at the Mach number $M = 4.0$ regardless of the choice of the molecular interaction model. Erofeev and Friedlander\textsuperscript{24} refined the value of the Mach number at which the temperature overshoot appears ($M = 3.9$). The overshoot magnitude increases with increasing Mach number. Struchtrup\textsuperscript{29} demonstrated that this phenomenon is also modeled in solving the R13 system of equations. The ability of the linear and nonlinear versions of the R13 system to correctly predict the magnitude of this peak for different models of molecular interaction is analyzed below.

Figure 13 shows the numerical results for the total temperature profile in the zoomed region of the rear front of the wave for two versions of the R13 system; these results are compared with the DSMC solution for two models of molecular interaction: hard spheres (a) and Maxwell molecules (b). It is seen from the figures that the temperature profiles predicted by the linear and nonlinear versions of the R13 system for the Mach number $M = 2.0$ almost coincide with the DSMC data for both models of molecular interaction. The temperature distributions are monotonic, i.e., no overshoot is observed. However, in the case of a strong shock wave with the Mach number $M = 8.0$, the peak in the temperature profile is clearly observed for all solutions considered here. The magnitude of the peak predicted by the DSMC method for hard spheres (approximately 0.9%) is slightly greater than that for Maxwell molecules (about 0.7%). The overshoot values predicted by the R13 system are substantially higher than the DSMC values (approximately 3% for the linear version and 2% for the nonlinear version) regardless of the molecular interaction model used. Thus, the nonlinear version of the R13 system provides a better prediction of this fine effect.

An analysis shows that the presence of a peak in the total temperature profile is connected to the fact that the function $T_\perp \rho$ nonlinearly depends on the normalized number density $\bar{\rho}$. In particular, if this dependence is linear (e.g., for Mott-Smith’s solution\textsuperscript{42}), it can be demonstrated that the peak on the total temperature curve does not occur. Indeed, let

$$\frac{T_\perp}{T_1} \rho(\bar{\rho}) = A \bar{\rho} + B.$$  \hspace{1cm} (26)

Then, after determining the constants $A, B$ from the Rankine-Hugoniot conditions for a monatomic gas, we have

$$\frac{T_\perp}{T_1}(\rho) = \frac{1}{12} \left[ 5(3 + M_1^2) - (5M_1^2 + 3) \left( \frac{\rho}{\rho_1} \right)^{-1} \right].$$  \hspace{1cm} (27)

Further, using the form of total temperature (24) and Yen’s relation (25), we obtain

$$\frac{T}{T_1}(\rho) = \frac{1}{18} \left[ 5(3 + M_1^2) + (5M_1^2 + 3) \left( \frac{\rho}{\rho_1} \right)^{-1} - 10M_1^2 \left( \frac{\rho}{\rho_1} \right)^{-2} \right].$$  \hspace{1cm} (28)
The derivative of the total temperature has the form

$$\frac{d(T/T_1)}{d(\rho/\rho_1)} = \frac{1}{18} \left[ 20M_1^2 \left( \frac{\rho}{\rho_1} \right)^{-3} - (5M_1^2 + 3) \left( \frac{\rho}{\rho_1} \right)^{-2} \right] ,$$

whence it follows the condition of existence of the peak

$$1 \leq \frac{\rho}{\rho_1} = \frac{20M_1^2}{5M_1^2 + 3} \leq \frac{\rho_2}{\rho_1} ,$$

which is invalid because the Rankine-Hugoniot conditions yield

$$\frac{\rho_2}{\rho_1} = \frac{4M_1^2}{M_1^2 + 3} \leq \frac{20M_1^2}{5M_1^2 + 3} .$$

Therefore, this peak can exist only if $T_{\perp}(\rho)$ deviates from a linear function.

In Figs. 14 and 15, the function $T_{\perp}(\rho)$ deviates from its free-stream value. For the Mach number $M = 2.0$ (Fig. 14), this function behaves almost linearly in all cases, which agrees with the absence of the peak in the total temperature profile at low Mach numbers. At high Mach numbers, however, significant deviations from linearity are observed for all cases ($M = 8.0$, Fig. 15). This fact is consistent with the existence of the temperature overshoot in all solutions in the high Mach number case for all models of molecular interaction. The greatest convexity of the function $T_{\perp}(\rho)$ is observed in the solution provided by the linear version of the R13 system, which is significantly greater than the convexity of the DSMC data. The convexity predicted by the nonlinear version of the R13 system is closer to that in the DSMC computations. Such a behavior of the temperature profiles is typical for all interaction potentials. The greatest deviation of this function from the linear
dependent predicted by the linear version of the R13 system agrees with the maximum value of the temperature overshoot (Fig. 13).

VII. CONCLUSIONS

The internal structure of a plane shock wave in a monatomic gas is studied by two methods: Grad’s regularized 13-moment system of equations (nonlinear and linear versions of the R13 system) and the DSMC method. The shock wave structure is analyzed by these two methods for low (\(M = 2\)) and high (\(M = 8\)) Mach numbers and for different models of molecular interaction. A comparison of the streamwise temperature distributions obtained by both methods with Yen’s relation\(^{41}\) shows that the conservation laws are perfectly satisfied in these methods. Macroparameters of the gas in the internal structure of the shock wave are analyzed. The density profiles predicted by the linear and nonlinear versions of the R13 system agree well with DSMC data and experimental results in the entire examined range of parameters. At the same time, it is more difficult to obtain a correct temperature distribution in the shock wave structure. A comparison of the distributions of temperature and its directed components calculated by solving the R13 system with DSMC results reveals a noticeable difference with increasing shock wave intensity. The greatest difference of the results of solving the moment equations from the DSMC reference data is observed on the leading front of the shock wave (in the supersonic flow region).

It is interesting that the linear version of the R13 system yields better results than the nonlinear version if the hard sphere approximation is used. On the contrary, the nonlinear version provides more adequate results for the Maxwell interaction potential. Apparently, this observation can be explained by the fact that the system of equation was derived for the Maxwell potential of molecular interaction (see Ref. 16); therefore, if another interaction potential is used, the associated error can mitigate the error associated with the simplified linear presentation of high-order moments in these equations.

A total temperature overshoot is observed on the rear front of the shock wave at high Mach number both in the solution of the moment equations and in the solution of the Boltzmann kinetic equation. The magnitude of this temperature peak predicted by the R13 system is appreciably greater than the value of this peak in the reference kinetic solution obtained by the DSMC method. The nonlinear version of the R13 system predicts the magnitude of this overshoot more correctly for all potentials of molecular interaction.

The version of the R13 system obtained for the hard sphere model\(^{43,44}\) is of considerable interest for further research.

ACKNOWLEDGMENTS

This work was supported by the Russian Government under the grant “Measures to Attract Leading Scientists to Russian Educational Institutions” (Contract No. 14.Z50.31.0019) and by the Russian Foundation for Basic Research (Project Nos. 14-02-31079, 14-08-01252, and 15-58-52044). The authors would like to thank the reviewers for providing valuable comments and suggestions.


