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The Analysis of Different Variants of R13 Equations Applied to the Shock-Wave Structure

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Abstract. This paper studies the applicability of various versions of the regularized 13-moment system (R13) as applied to the problem of the shock wave structure in a monatomic Maxwell gas in a wide range of Mach numbers ($1.0<M<8.0$). Over time, several versions of the R13 equations were presented, which differ in non-linear contributions for high-order moments. The challenge of this study is to determine the range of applicability of each variant of the moment equations as applied to non-equilibrium supersonic flows, depending on the Mach number and local Knudsen number. Numerical results obtained for the R13 system are compared to DSMC data computed by the SMILE++ software system.

INTRODUCTION

Macroscopic equations for rarefied flows can be derived as approximations to the Boltzmann equation, with the goal to have faster numerical calculations, or even exact solutions, while allowing for some inaccuracy due to the approximation. The Navier-Stokes and Fourier equations of classical hydrodynamics serve this purpose well only for sufficiently small Knudsen numbers Kn. For processes in the transition regime, successful extensions of the hydrodynamic equations are based on Grad's moment method [1], and in the following we consider the regularized 13 moment (R13) equations, which correct Grad's celebrated 13 moment system by accounting for the influence of higher moments [2]. The R13 equations were shown to give a good description of all relevant rarefactions effects, such as jump and slip, transpiration flow, Knudsen layers, thermal stresses, non-Fourier heat flux, shock structures, etc.

Over the years, due to refinement of the derivation of the equations, there appeared a number of different variants of the R13 equations, with differences particularly in the non-linear contributions to higher moments. All variants agree in the sense that their Chapman-Enskog expansion [3] to super-Burnett order, i.e., third order in Kn, yields the same result. Moreover, the R13 equations show great success for microflows, for which the non-linear terms play only a minor role, and can often be ignored. However, the full non-linear equations differ, and hence show different behavior for flows in which non-linarites play a marked role. The goal of the present study is to examine the different variants for their ability to describe shock structures in good agreement to solutions of the Boltzmann equation, which here are produced by DSMC simulations.

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FORMULATION OF THE PROBLEM

A one-dimensional plane shock wave problem is considered (flow from left to right), where the free-stream gas-dynamic variables ρ_1, v_{x1}, and T_1 (on the left) are input parameters. To impose the boundary conditions on the subsonic right boundary, the corresponding values ρ_2, v_{x2}, and T_2 are calculated from the free-stream parameters ρ_1, u_1, and T_1 with the use of conservation equations (Rankine-Hugoniot conditions)

$$\rho v_x = const,\ \rho v_x^2 + p = const,\ \frac{v_x^2}{2} + h = const. \tag{1}$$

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

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

$$\bar{T} = \frac{T - T_1}{T_2 - T_1}, \qquad \bar{\rho} = \frac{\rho - \rho_1}{\rho_2 - \rho_1},$$

With this, the macroparameters on the upstream and downstream boundaries have the values of 0 and 1, respectively.

R13 VARIANTS

Regularization of the Grad's original 13-moment system [1] was derived in 2003 [2] by Chapman-Enskog expansion [3] of higher moment equations only, based on the artificial assumption of faster relaxation times for higher moments. The tensor form of the regularized 13-moment system (R13) can be written as

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho \upsilon_k}{\partial x_k} = 0, \tag{2}$$

$$\rho \frac{\partial \upsilon_i}{\partial t} + \rho \upsilon_k \frac{\partial \upsilon_i}{\partial x_k} + \frac{\partial p}{\partial x_i} + \frac{\partial \sigma_{ik}}{\partial x_k} = 0, \tag{3}$$

$$\frac{3}{2}\rho \frac{\partial \theta}{\partial t} + \frac{3}{2}\rho \upsilon_k \frac{\partial \theta}{\partial x_k} + \frac{\partial q_k}{\partial x_k} + p\frac{\partial \upsilon_k}{\partial x_k} + \sigma_{ij}\frac{\partial \upsilon_i}{\partial x_j} = 0, \tag{4}$$

$$\frac{\partial \sigma_{ij}}{\partial t} + \frac{\partial \sigma_{ij}\upsilon_k}{\partial x_k} + \frac{4}{5}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + 2p\frac{\partial \upsilon_{\langle i}}{\partial x_{j\rangle}} + 2\sigma_{k\langle i}\frac{\partial \upsilon_{j\rangle}}{\partial x_k} + \frac{\partial m_{ijk}}{\partial x_k} = -\frac{\sigma_{ij}}{\tau}, \tag{5}$$

$$\begin{aligned} &\frac{\partial q_i}{\partial t} + \frac{\partial q_i \upsilon_k}{\partial x_k} + \frac{5}{2}p\frac{\partial \theta}{\partial x_i} + \frac{5}{2}\sigma_{ik}\frac{\partial \theta}{\partial x_k} + \theta\frac{\partial \sigma_{ik}}{\partial x_k} - \sigma_{ik}\theta\frac{\partial \rho}{\partial x_k} - \frac{\sigma_{ij}}{\rho}\frac{\partial \sigma_{jk}}{\partial x_k} \\ &+\frac{7}{5}q_k\frac{\partial \upsilon_i}{\partial x_k} + \frac{2}{5}q_k\frac{\partial \upsilon_k}{\partial x_i} + \frac{2}{5}q_i\frac{\partial \upsilon_k}{\partial x_k} + \frac{1}{2}\frac{\partial R_{ik}}{\partial x_k} + \frac{1}{6}\frac{\partial \Delta}{\partial x_i} + m_{ijk}\frac{\partial \upsilon_j}{\partial x_k} = -\frac{2}{3}\frac{q_i}{\tau}, \end{aligned} \tag{6}$$

where the density ρ, velocity υ_i, temperature in energy units $\theta = \frac{k}{m}T$ (k is the Boltzmann constant), viscous stress tensor σ_{ij}, and heat flux $q_i\,(i = x, y, z)$ form 13 primitive variables; the 14$^{\text{th}}$ variable is the pressure $p = \rho\theta$, where $\tau = \mu / p$ is the relaxation time, and μ is the viscosity coefficient. The angular brackets in the subscripts indicate the trace-free and symmetric part of the tensor. Equations (2) – (4) are the conservation laws for mass, momentum and energy; equations (5) and (6) are the moment equations for stress tensor and heat flux vector, respectively. These 13 equations must be closed by constitutive relations for the higher moments R_{ij}, Δ, m_{ijk}, and these differ based on the method of (regularizing) closure, as discussed next. For Grad's original 13 moment equations [1], $R_{ij} = \Delta = m_{ijk} = 0$.

Original Variant (2003)

The original variant of the R13 system obtained by Struchtrup and Torrilhon [2] in 2003 can be written as

$$\Delta = 6\frac{\sigma_{kl}\sigma_{kl}^{NSF}}{\rho} + \frac{56}{5}\frac{q_k q_k^{NSF}}{p} - 12\mu\theta\frac{\partial}{\partial x_k}\left(\frac{q_k}{p}\right) + \underline{12\frac{\mu}{p}\frac{q_k}{\rho}\frac{\partial\sigma_{kl}}{\partial x_l}}, \tag{7}$$

$$\begin{aligned} R_{ij} &= \frac{24}{7}\frac{\sigma_{k\langle i}\sigma_{j\rangle k}^{NSF}}{\rho} + \frac{64}{25}\frac{q_{\langle i}q_{j\rangle}^{NSF}}{p} - \frac{24}{5}\mu\theta\frac{\partial}{\partial x_{\langle i}}\left(\frac{q_{j\rangle}}{p}\right) \\ &\quad + \underline{\frac{24}{5}\frac{\mu}{p}\frac{q_{\langle i}}{\rho}\frac{\partial\sigma_{j\rangle k}}{\partial x_k} + 4\frac{\mu\theta}{p^2}\sigma_{ij}\frac{\partial q_k}{\partial x_k} + 4\frac{\mu\theta}{p^2}\sigma_{ij}\sigma_{kl}\frac{\partial\upsilon_k}{\partial x_l}}, \end{aligned} \tag{8}$$

$$m_{ijk} = \frac{8}{15}\frac{\sigma_{\langle ij}q_{k\rangle}^{NSF}}{p} + \frac{4}{5}\frac{q_{\langle i}\sigma_{jk\rangle}^{NSF}}{p} - 2\mu\theta\frac{\partial}{\partial x_{\langle i}}\left(\frac{\partial\sigma_{jk\rangle}}{p}\right) + \underline{2\frac{\mu\theta}{p^2}\sigma_{\langle ij}\frac{\partial\sigma_{k\rangle l}}{\partial x_l}}. \tag{9}$$

Relations (7)-(9) are written in a compact form by using the equation of state for an ideal gas and the Navier-Stokes and Fourier laws, with $\sigma_{ij}^{NSF} = -2\mu\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}$, $q_i^{NSF} = -\frac{15}{4}\mu\frac{\partial\theta}{\partial x_i}$ and $p\frac{\partial}{\partial x_k}\left(\frac{1}{p}\right) = -\frac{1}{p}\frac{\partial p}{\partial x_k}$.

Linearization around equilibrium reduces the equations to

$$\Delta = -12\tau\theta\frac{\partial q_l}{\partial x_l},\ R_{ij} = -\frac{24}{5}\tau\theta\frac{\partial q_{\langle i}}{\partial x_{j\rangle}},\ m_{ijk} = -2\tau\theta\frac{\partial\sigma_{\langle ij}}{\partial x_{k\rangle}}. \tag{10}$$

These terms provide the main gradient transport mechanisms (GTM) [4] for the stress tensor and heat flux. The terms omitted in the linear case form the so-called non-gradient transport mechanisms (NGTM) [5]. The linear variant (10) and the original nonlinear variant (7)-(9) were studied for shock structures in [6-8].

The underlined terms of Eqs. (7)-(9) are terms of the 4th order in Knudsen number, which do not contribute to the super-Burnett order. It should be noted that full balance laws for Δ, R_{ij}, and m_{ijk} should be used to reach the rigorous equations at 4th order.

Order of Magnitude Closure (2005)

Struchtrup [6] proposed a new variant of relations for high-order moments, based on a careful examination of the order of magnitude in Knudsen number of all terms in the equations. Here, and in all variants discussed further, the fourth-order terms with respect to the Knudsen number are removed. Additional nonlinear terms appear in the relations for $\{\Delta, R_{ij}\}$, as compared to Eqs. (7)-(9), which were ignored in the original derivation, where only linear production terms for Maxwell molecules were used. Their omission in the original equations is the reason why there were discrepancies in the super-Burnett coefficients [9]. The resulting system reads

$$\Delta = -\frac{\sigma_{kl}\sigma_{kl}}{\rho} + 6\frac{\sigma_{kl}\sigma_{kl}^{NSF}}{\rho} + \frac{56}{5}\frac{q_k q_k^{NSF}}{p} - 12\mu\theta\frac{\partial}{\partial x_k}\left(\frac{q_k}{p}\right), \tag{11}$$

$$R_{ij} = -\frac{4}{7}\frac{\sigma_{k\langle i}\sigma_{j\rangle k}}{\rho} + \frac{24}{7}\frac{\sigma_{k\langle i}\sigma_{j\rangle k}^{NSF}}{\rho} + \frac{64}{25}\frac{q_{\langle i}q_{j\rangle}^{NSF}}{p} - \frac{24}{5}\mu\theta\frac{\partial}{\partial x_{\langle i}}\left(\frac{q_{j\rangle}}{p}\right), \tag{12}$$

$$m_{ijk} = \frac{8}{15}\frac{\sigma_{\langle ij}q_{k\rangle}^{NSF}}{p} + \frac{4}{5}\frac{q_{\langle i}\sigma_{jk\rangle}^{NSF}}{p} - 2\mu\theta\frac{\partial}{\partial x_{\langle i}}\left(\frac{\partial\sigma_{jk\rangle}}{p}\right). \tag{13}$$

The First Modification for Boundary Conditions (2008)

This modification appeared in the course of solving the problem of a steady gas flow in a channel in the transitional regime with essentially subsonic velocities. The question of formulating proper boundary conditions for the R13 equations is under ongoing investigation [10]. Torrilhon and Struchtrup [11] proposed a system of boundary conditions for simulating gas interaction with the solid wall at a given temperature for obtaining a simpler variant of analytical expressions for Δ, R_{ij}, and m_{ijk} than those described above. This variant is based on several simplifications. First of all, the nonlinear terms that appeared in Eqs. (11) and (12) are omitted. The second significant simplification is setting the pressure derivatives to zero, which is fairly applicable for the particular problems considered in [11]. Thus, Eqs. (11)-(13) reduce to

$$\Delta = 6\frac{\sigma_{kl}\sigma_{kl}^{NSF}}{\rho} + \frac{56}{5}\frac{q_k q_k^{NSF}}{p} - 12\frac{\mu}{p}\frac{\partial q_k}{\partial x_k} \tag{14}$$

$$R_{ij} = \frac{24}{7}\frac{\sigma_{k\langle i}\sigma_{j\rangle k}^{NSF}}{\rho} + \frac{64}{25}\frac{q_{\langle i}q_{j\rangle}^{NSF}}{p} - \frac{24}{5}\frac{\mu}{p}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} \tag{15}$$

$$m_{ijk} = \frac{8}{15}\frac{\sigma_{\langle ij}q_{k\rangle}^{NSF}}{p} + \frac{4}{5}\frac{q_{\langle i}\sigma_{jk\rangle}^{NSF}}{p} - 2\frac{\mu}{p}\frac{\partial \sigma_{\langle ij}}{\partial x_{k\rangle}} \tag{16}$$

The next step in simplifications is the replacement of $\left\{\sigma_{ij}^{NSF}, q_i^{NSF}\right\}$ by $\left\{\sigma_{ij}, q_i\right\}$ in Eqs. (14)-(16), which does not change the order of magnitude of these equations, i.e., they still yield the correct super-Burnett equations. However, it alters the mathematical properties of the equations such that linear and non-linear equations require the same number of boundary conditions. This nonlinear variant of the R13 equations is the roughest one because of the above-mentioned simplifications, in particular the assumption of constant pressure, which, however, was justified for the processes simulated in [11]. On the other hand, it is obvious that this modification is problematic for studying nonlinear problems such as shock structures. Nevertheless, we decided to check the area of applicability of this variant and the variant with replacement of $\left\{\sigma_{ij}^{NSF}, q_i^{NSF}\right\}$ by $\left\{\sigma_{ij}, q_i\right\}$.

Modified Order of Magnitude Closure (2013)

The most recent variant of the R13 equations is based on the variant of 2005 (11)-(13), only that $\left\{\sigma_{ij}^{NSF}, q_i^{NSF}\right\}$ is again replaced by $\left\{\sigma_{ij}, q_i\right\}$ in order to preserve the order of accuracy of the equations. With this, linear and non-linear equations require the same number of boundary conditions. Compared to the equations in the previous section, the pressure is not restricted. This variant was successfully applied for the first time for simulating a slow steady transitional flow in a cavity [12]:

$$\Delta = 5\frac{\sigma_{kl}\sigma_{kl}}{\rho} + \frac{56}{5}\frac{q_k q_k}{p} - 12\mu\theta\frac{\partial}{\partial x_k}\left(\frac{q_k}{p}\right) \tag{17}$$

$$R_{ij} = \frac{20}{7}\frac{\sigma_{k\langle i}\sigma_{j\rangle k}}{\rho} + \frac{64}{25}\frac{q_{\langle i}q_{j\rangle}}{p} - \frac{24}{5}\mu\theta\frac{\partial}{\partial x_{\langle i}}\left(\frac{q_{j\rangle}}{p}\right) \tag{18}$$

$$m_{ijk} = \frac{4}{3}\frac{\sigma_{\langle ij}q_{k\rangle}}{p} - 2\mu\theta\frac{\partial}{\partial x_{\langle i}}\left(\frac{\sigma_{jk\rangle}}{p}\right) \tag{19}$$

NUMERICAL SCHEME

The numerical method used for solving the various variants of the R13 system in this work was described in detail in [8]. A high-order Godunov scheme is used for computing the internal spatial cells. The viscosity coefficient in calculated by the power-law formula

$$\mu = \mu_0\left(\frac{T}{T_0}\right)^{\omega} \tag{20}$$

where $0.5 \le \omega \le 1.0$. The values $\omega = 0.5$ and $\omega = 1.0$ correspond to the models of hard spheres and Maxwell molecules, respectively [6]. The convergence of numerical scheme of R13 has been demonstrated in [8]. All computations described in this paper were performed for Maxwell molecules.

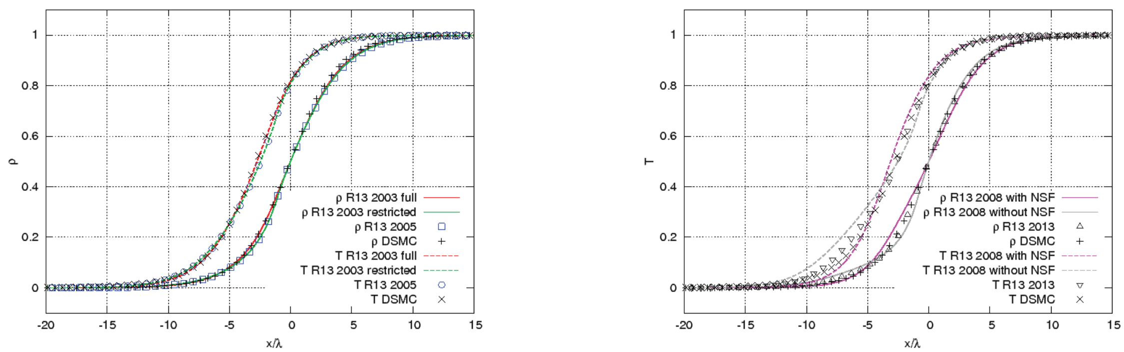
The DSMC computations were performed by the SMILE++ software system [13,14] based on the majorant frequency scheme [15]. Molecular interaction was described by the Variable Hard Sphere (VHS) model [16], which corresponds to the model of hard spheres for $\omega = 0.5$ and to the model of pseudo-Maxwell 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 $\omega = 1$. The parameters of the numerical method in the DSMC computations (the collision cell size, the number of simulated particles, the time step) were chosen in such a way that they ensured an accurate result and were similar to [8].

RESULTS AND DICUSSION

Previously, only the linear variant of the R13 system (10) [6,17] and the nonlinear variant (7)-(9) were used for supersonic flows in general, and for the problem of the shock wave structure in particular, whereas the fourth-order terms with respect to the Knudsen numbers were neglected [7, 8]. Numerical results for the R13 system and DSMC computations were obtained in a wide range of Mach numbers (1.0<M<8.0). In this section, we report the results that could be obtained for all nonlinear variants of the R13 system discussed above. These results are compared with reference data computed by the DSMC method.

M=2.0

For weak shock waves, the results were obtained for all variants described above. The density and temperature profiles obtained by solving the R13 system are compared in Fig. 1 with the reference DSMC data for the Mach number M=2.0. It is seen that all R13 versions work well in this regime. It should be noted that the roughest modification (14)-(16) with replacement of $\left\{\sigma_{ij}^{NSF}, q_i^{NSF}\right\}$ by $\left\{\sigma_{ij}, q_i\right\}$, which was used in [11] for steady gas flows in microchannels, ensures good agreement with the DSMC results for this Mach number. A similar pattern is also observed for other macroparameters, including the streamwise heat flux and components of the viscous stress tensor.



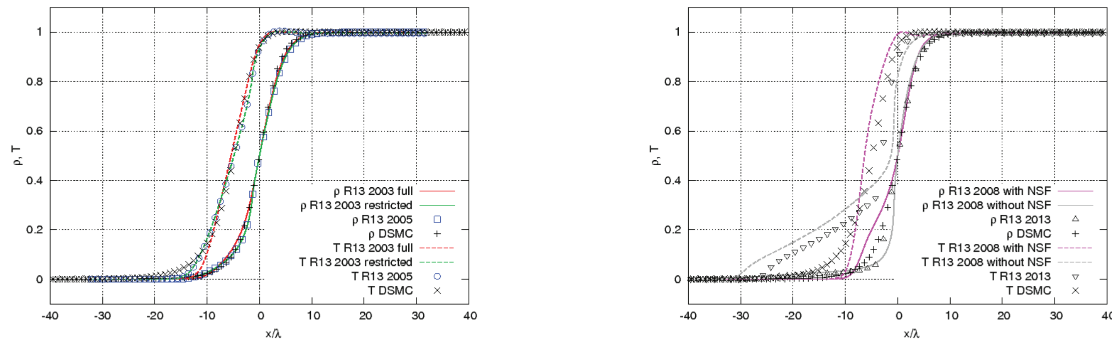
(a) (b)

FIGURE 1. Comparison of R13 density and temperature profiles with DSMC data for M=2.0: (a) Original variant (2003 full), the same variant without 4th order corrections (2003 restricted), and order of magnitude closure modification (2005). (b) Boundary condition modification (2008 with NSF), the same with $\left\{\sigma_{ij}^{NSF}, q_i^{NSF}\right\} = \left\{\sigma_{ij}, q_i\right\}$ (2008 without NSF), and modified order of magnitude closure variant (2013).

M=4.0

The same comparison is performed in Fig. 2 for Mach number M=4.0. As the shock wave becomes stronger, nonlinear terms contribute more, and the pattern becomes appreciably different. As could be expected, the worst result is provided by the roughest variant, which is the modification of the R13 system applied to subsonic flows in microchannels in [11]. Replacement of $\left\{\sigma_{ij}^{NSF}, q_i^{NSF}\right\}$ by $\left\{\sigma_{ij}, q_i\right\}$, which is also used in the variant of 2013, yields significantly deteriorated results for the temperature profile. Concerning the earlier R13 variant, the original variant with allowance for the fourth-order terms with respect to the Knudsen number provides the best results, as could be expected.

It is of interest that the emergence of the additional nonlinear terms $\left\{-\frac{\sigma_{ij}\sigma_{ij}}{\rho}, -\frac{4}{7}\frac{\sigma_{k\langle j}\sigma_{j\rangle k}}{\rho}\right\}$ in Eqs. (11)-(13) does not exert any significant influence. It should be noted that a tendency of emerging of a point with a drastic change in the derivatives of both temperature and density in the middle of the shock wave is observed for this Mach number. The same behavior can be seen in the comparison of heat flux profiles for M=4.0 in Fig 3(a).

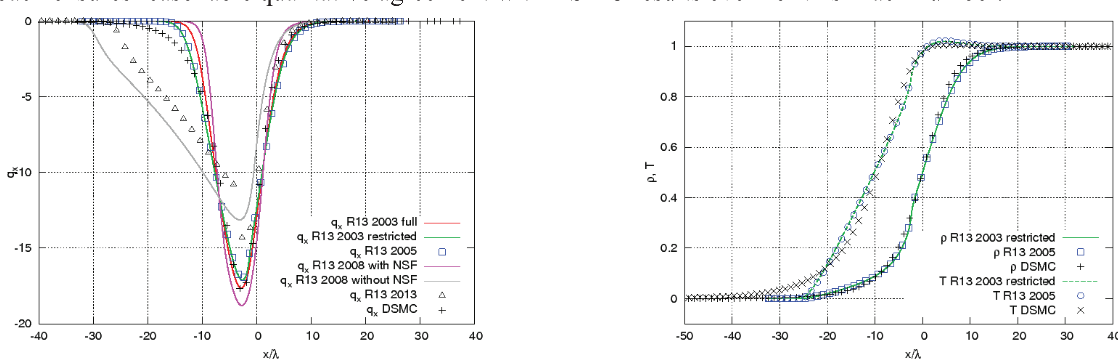


(a) (b)

FIGURE 2. Comparison of R13 density and temperature profiles with DSMC data for M=4.0: (a) Original variant (2003 full), the same variant without 4th order corrections (2003 restricted), and order of magnitude closure modification (2005). (b) Boundary condition modification (2008 with NSF), the same with $\left\{\sigma_{ij}^{NSF}, q_i^{NSF}\right\} = \left\{\sigma_{ij}, q_i\right\}$ (2008 without NSF), and modified order of magnitude closure variant (2013).

M=8.0

For Mach numbers M>4.0, the numerical solution could not be obtained by using the original variant of 2003 with allowance for the fourth-order terms. It is still not clear whether the reason is the chosen numerical scheme or the mathematical properties of the equations. Concerning other variants, the simplified versions of 2008 and 2013, which were already problematic for M=4.0, yield even worse results for M=8.0. The results of the earlier modifications of 2003 and 2005 can be hardly distinguished (Fig. 3(b)), similar to the situation for M=4.0. The difference between the R13 and DSMC becomes more significant. The point of the drastic change in the temperature and density derivatives at the center of the shock wave becomes even more noticeable. Nevertheless, the moment approach ensures reasonable qualitative agreement with DSMC results even for this Mach number.



(a) (b)

FIGURE 3. (a) Comparison of R13 heat flux profiles with DSMC data for M=4.0 (b): M=8.0. Density and temperature. Comparison of the original variant without 4th order corrections (2003 restricted) and order of magnitude closure modification (2005).

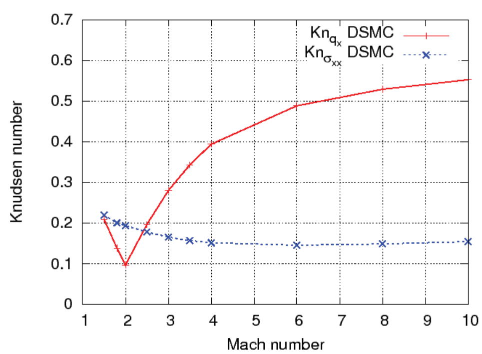
Distribution of local Knudsen number as a function of Mach number

The Knudsen number, which is the ratio of the mean free path of molecules to the reference linear scale of the considered problem, is one of the basic measures of gas rarefaction. It is also convenient to use this similarity parameter for estimating the degree of flow nonequilibrium. The difficulty in applying the classical definition of the Knudsen number in the problem of the shock wave structure is the absence of an obvious reference length scale. An alternative for the classical definition is the use of the *local* Knudsen number $Kn = \frac{\lambda}{Q}\left|\frac{dQ}{dl}\right|$, where λ is the mean free path, Q stands for a macroparameter of interest (density, temperature, etc.), and l is the spatial direction with the greatest growth of this parameter. Density is most often used as the parameter Q in studying the shock wave structure. Based on the density gradient, the inverse thickness of the shock wave is obtained, which is an analogy of the maximum Knudsen number Kn_ρ in the shock wave [6, 18]. The value of Kn_ρ does not exceed 0.2 for the Maxwell gas, e.g., it is smaller than 0.3 for argon [6, 18]. Some publications describe Kn_T calculations on the basis of temperature profiles [19]. The value of Kn_T is significantly different from Kn_ρ. For this reason, it is of interest to evaluate the local Knudsen number on the basis of other macroparameters of the flow.

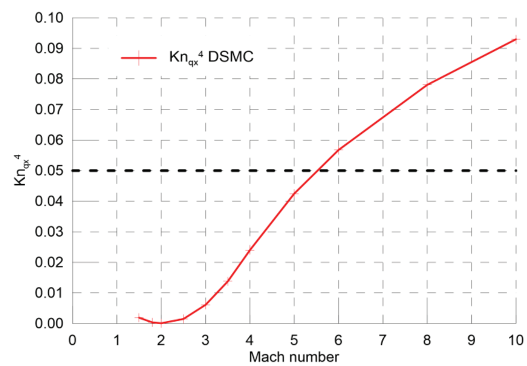
Here we use the idea of estimating the Knudsen number on the basis of the streamwise heat flux q_x and the viscous stress tensor component σ_{xx}, which was proposed by Lockerby et al. [20]:

$$Kn_{\sigma_{xx}} = \frac{\left|\sigma_{xx} - \sigma_{xx}^{NSF}\right|}{\max\left(\sigma_{xx}^{NSF}\right)},\ \sigma_{xx}^{NSF} = -\frac{4}{3}\mu\frac{\partial v_x}{\partial x},\ Kn_{q_x} = \frac{\left|q_x - q_x^{NSF}\right|}{\max\left(\left|q_x^{NSF}\right|\right)},\ q_x^{NSF} = -\frac{15}{4}\mu\frac{\partial\theta}{\partial x}. \tag{21}$$

This definition is the normalized deviation of the considered parameter from the same parameter calculated by the Navier-Stokes-Fourier relations. Figure 4 (a) shows the distribution of the maximum values of $Kn_{\sigma_{xx}}$ and Kn_{q_x} as functions of the shock wave Mach number, which were calculated on the basis of DSMC data. As is seen from Fig. 4 (a), the value of $Kn_{\sigma_{xx}}$ does not experience significant changes with shock wave enhancement; like Kn_ρ, it remains smaller than 0.2 in the examined range of Mach numbers. The behavior of Kn_{q_x} is more interesting. On the one hand, a clear minimum is observed at M=2.0; on the other hand, Kn_{q_x} monotonically increases in the considered range of Mach numbers at M>2.0.



(a)



(b)

FIGURE 4. Distribution of the maximum local Knudsen number Kn_{q_x} and $Kn_{\sigma_{xx}}$ as functions of the Mach number (a) and distribution of the maximum value of $Kn_{q_x}^4$ (b). The results are based on DSMC computations.

The R13 moment equations are third-order equations with respect to the Knudsen number. Thus, the value of Kn^4 has to be a small for the modeled flow if this moment approach is used. Figure 4 (b) shows the distribution of $Kn_{q_x}^4$ over Mach number. The horizontal dashed line marks the value $Kn_{q_x}^4 = 0.05$, which can be considered as being sufficiently small; this corresponds to a Knudsen number just below 0.5. Based on these considerations, we can conclude that the formal upper boundary of the area of applicability of the R13 system for supersonic flows is $M \approx 5.5$. As a whole, this conclusion is confirmed by comparisons of the macroparameter profiles given above. On the other hand, the full nonlinear variant of the R13 system offers a possibility of obtaining good qualitative agreement with DSMC data for stronger shock waves as well.

CONCLUSIONS

We summarize our findings on the applicability of the R13 variants to shock waves. Firstly, all nonlinear variants of the R13 system considered in this paper are applicable for simulations of weak shock waves, since the various modifications exert only minor effect on results for M=2.0. However, the pattern becomes significantly different toward the range of hypersonic velocities. If the influence of the fourth-order terms with respect to the Knudsen number is not considered, the original variant of the R13 system (2003) is preferable for supersonic flow simulations. The nonlinear terms $\left\{-\frac{\sigma_{ij}\sigma_{ij}}{\rho}, -\frac{4}{7}\frac{\sigma_{k\langle j}\sigma_{j\rangle k}}{\rho}\right\}$ proposed in 2005 [6], which allow obtaining correct coefficients for the super-Burnett equations, do not exert noticeable effects in the entire range of Mach numbers considered.

Since the modifications proposed after 2005 were driven by the desire to use the same boundary conditions for linear and non-linear equations, the unsatisfactory results for strong shock waves calculated with these modifications indicate the necessity to revise the formulation of the boundary conditions of the R13 system on the solid wall for strongly supersonic flows.

Concerning the fourth-order corrections with respect to the Knudsen numbers included into the high-order relations in Eqs. (7)-(9), they ensure significant improvement of results for $\mathrm{M} \le 4.0$. At the same time, the numerical solution for the shock wave structure for $\mathrm{M} > 4.0$ could not be obtained by the method used in this study. A mathematical explanation of this observation is yet to be found.

In the study, we obtained the Knudsen number distributions based on σ_{xx} and q_x as functions of the Mach number. These data allow us to argue that there is a formal upper boundary of the mathematical model of the R13 equations. This formal boundary is confirmed by comparisons of the shock wave macroparameter profiles calculated with the use of the original R13 system with DSMC data for chosen Mach numbers. On the other hand, even beyond this upper boundary at $M \approx 5.5$, the original variant of the R13 system can be used for qualitative simulation of supersonic flows if there is no need for obtaining a detailed description of the internal structure of the shock wave.

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