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Supersonic Flows with Nontraditional Transport Described by Kinetic Methods

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Abstract. A new class of supersonic nonequilibrium flows is studied on the basis of solving the Boltzmann and model kinetic equations with the aim to consider new nonlinear structures in open systems and to study anomalous transfer properties in relaxation zones. The Unified Flow Solver is applied for numerical simulations. Simple gases and gases with inner degrees of freedom are considered. The experimental data related to the influence of the so-called optical lattices on the supersonic molecular beams are considered and numerical analysis of the nonequilibrium states obtained on this basis is made. The nonuniform relaxation problem with these distributions is simulated numerically and anomalous transport is confirmed. The conditions for strong changes of the temperature in the anomalous transfer zones are discussed and are realized in computations.

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Key words: The Boltzmann equation, anomalous transport, relaxation zones.

1 Introduction

The thermodynamics of nonequilibrium processes is generally used to study macroscopic transfer phenomena in gases and liquids. The classical transport equations are based on the well-known Navier-Stokes formalism. From the kinetic point of view this formalism is the limit case of the more general kinetic formalism, and if the Knudsen number is not small then the ordinary macroscopic relationships can be invalid (the irreversible thermodynamics can be invalid in this case) and for adequate description it is necessary to solve the Boltzmann equation or other kinetic equations. There are some physical effects intrinsic to the kinetic processes: thermodiffusion, thermoforesis etc (see, e.g., [1]). But

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we will consider effects differing from these phenomena based on the gradients of some quantities. In contrast to these processes the transport processes under consideration are realized because of the dissipation in the boundary and this dissipation is caused by the strong nonequilibrium. In these problems of the nonequilibrium supersonic nonuniform relaxation the boundary nonequilibrium distribution for the supersonic flow forms the gradient of the distribution function (and consequently the macroscopic parameters) downstream. Transport properties of monatomic one-component gases in the spatial nonuniform relaxation zones have been subject to research in [2,3]. The mixtures of simple gases and gases with inner degrees of freedom have been studied for these problems in [4]. The anomalous (from the traditional viewpoint) irreversible transfer of momentum and energy in the scale of the mean free path has been obtained. Namely, in 1D flow the signs of the velocity gradient and the appropriate component of the nonequilibrium stress tensor are the same as well as the signs of the temperature gradient and the heat flux. The special method of expanding in the powers of a small parameter permits to derive the closed form of the transport equations with the mentioned anomalous properties. It is important to note that for supersonic flows the known approach of expansion in powers of inverse Mach numbers $1/M$ does not provide this effect which is due to taking into account the differences of expansion for each molecular velocity.

Numerical results are obtained with the Unified Flow Solver (UFS) [5] for the Boltzmann equation and for some model kinetic equations (of the BGK-type) describing, in particular, molecular (with inner energy) one-component and multi-component gases. The approach applied in the present papers is the direct methods for solving the Boltzmann equation and model kinetic relaxation equations (details are given in [4]). We can also notice the other approaches for solving kinetic equations. The most popular approach is DSMC method which has been elaborated by Bird and the other authors (see [6]). We developed the approach of the direct numerical solving the Boltzmann equation and from our point of view it provides reliable results for the problems under consideration. This approach and the DSMC method possess advantages and disadvantages in kinetic theory (see, e.g., in [2]). We can only mention the approximated approaches, such as kinetic models with small numbers of discrete velocities (Broadwell etc). The very popular Lattice Boltzmann Method (LBM) can be applied, strictly speaking, to slow near equilibrium flows.

The formulation of the nonuniform relaxation problem for 2D case is similar to one for the supersonic free jet but with nonequilibrium boundary conditions in the orifice. The obtained anomalous terms induce the search for the non-traditional transport in numerical calculations. In the present paper we pay the attention to the possibility of experimental testing the effects. For this purpose the numerical simulation for nonequilibrium distributions obtained after modelling the electrical forces of the optical lattice are performed. For goal of the experimental physical measurement it is important to have large changes of macroparameters in the zone of the anomalous transport. Calculations on the basis of the Boltzmann equation with strong nonequilibrium boundary dissipation and large changes of mentioned values are also performed.

2 The main equations and formulation of the problem

We start from the Boltzmann kinetic equation which governs the advection and collisions of particles in a rarefied gas and which is written in the form (without external force)

$$\frac{\partial f}{\partial t}+\nabla_r(\xi f)=I(f,f), \tag{2.1}$$

where x is physical coordinate, $\xi(\xi_x,\xi_y,\xi_z)$ is the vector of molecular velocity, the collision integral (with the traditional notations):

$$I(f,f)=\int\left[f(\xi_1')f(\xi')-f(\xi)f(\xi_1)\right]|\mathbf{g}|bdbd\varepsilon d\xi_1=-\nu f+G.$$

All macroscopic parameters are treated as appropriate moments of the distribution function, e.g., density, mean velocity, stress tensor components, pressure, nonequilibrium stress tensor components, temperature, heat flux, nonequilibrium entropy and entropy flux respectively are the following expressions:

$$\begin{aligned}
&n=\int fd\xi, && \mathbf{u}=\frac{1}{n}\int f\xi d\xi, && P_{ij}=\int c_ic_jfd\xi,\\
&p=\frac{1}{3}(P_{xx}+P_{yy}+P_{zz}), && p_{ij}=P_{ij}-p, && T=\frac{1}{3kn}\int f|\mathbf{c}|^2d\xi,\\
&q_i=\frac{1}{2}\int c_i|\mathbf{c}|^2fd\xi, && S=-H=-\int \ln f fd\xi, && \mathbf{S}=-\int\xi\ln f fd\xi,
\end{aligned}$$

where the thermal velocity is $\mathbf{c}=\xi-\mathbf{u}$ and indices $i,j=x,y,z$.

We present also other equations. The relaxation model kinetic equation [7] of BGK-type is used. For example for mixtures the model by Andries et al. is as follows

$$\frac{\partial f_i}{\partial t}+\xi\cdot\nabla_r f_i=\nu_i(F_m^i-f_i).$$

Here F_m^i is appropriate Maxwellian for i-th species. These relaxation models come back to the model by Bhatnagar-Gross-Krook [8] which possesses essential physical properties, in particular the H-theorem that is important for the strong nonequilibrium kinetic processes beyond near equilibrium and thermodynamical approximations.

For molecular gases we consider the so-called R-model, i.e., the model kinetic equation by Rykov (see, e.g., [9]), which describes rotational degrees of freedom of gases (for many physically important situations with not very high temperature it is a correct assumption). The so-called 3T model (see [10]) is also applied, which allows us to take into account both rotational and vibrational degrees of freedom and which is easily generalized to the mixtures of molecular gases. In the present paper only the rotational degrees of freedom are considered.

The formulation of the spatially nonuniform (nonhomogeneous) relaxation problem (NRP) is given in [2,3]. For 1D NRP for a steady case for a simple one-component gas the following boundary conditions are accepted:

$$f(0,\xi)=F(\xi), \quad \forall \xi_x>0; \quad f(+\infty,\xi)=0, \quad \forall \xi_x<0,$$

where $F(\xi)$ is the nonequilibrium distribution function. Note that one can try to formulate the problem for the supersonic flows where for the nonequilibrium boundary function there are some particles moving towards the orifice, but the amount of these particles with negative velocities downstream is negligible so the zero condition for the negative velocities gives the same results (for the distribution function and for the main macroparameters) as with the equilibrium distribution function at infinity.

In our numerical simulations we considered velocity space with both positive and negative velocity components. If we put the appropriate value of the Maxwellian for the boundary condition (at infinity) for the negative velocity instead of the zero the influence of this factor on the results was negligible (that has been proved in [11]).

For molecular gases the formulation is analogous. Generalization of the formulation of NRP for mixtures and molecular gases and for 2D is given in [4]. For 2D flow the boundary nonequilibrium distribution function is accepted in a slit. The formulation of NRP for 3D case has a similar form but nonequilibrium distribution is set in a plane orifice.

3 Procedure of closure for strong nonequilibrium states and new transport equations

For obtaining the moment equations we use the expansion of kinetic equations in powers of a small parameter, depending on the longitudinal molecular velocity and consider the first terms. One can demonstrate this technique, for instance, for 1D steady flow. In this case the equation can be written:

$$\frac{\partial f}{\partial x}=\frac{1}{\xi_x}I=\frac{1}{u_0}\big(1-\alpha+\cdots+(-1)^n\alpha^n+\cdots\big)I,$$

where $\alpha\equiv\alpha(\xi_x)=(\xi_x-u_0)/u_0$ and u_0 is mean velocity of a gas mixture for the nonequilibrium distribution in the boundary at $x=0$. Neglecting the influence of the tails of the distribution function, we assume that $f=0$ for $|\xi_x-u_0|>\Delta U$ ($\Delta U>3\sqrt{T}/m$, where T is temperature and m is a mass of the molecule). Then for sufficiently large Mach numbers in the input flow, one can suppose that $\xi_x>0$ and $|\alpha|<1$ for any x in the domain under consideration. We will be restricted by the first order approximation. We assume that inclusion of new terms of this series (that is the Leibniz series) will improve the accuracy of the considered expansion.

For the case of 1D nonuniform relaxation problem (NRP) for a monatomic one-component gas according to [2, 3] this expansion leads to the closure for the first order approximation with the following transport equations (we emphasize that the moment equation are closed for strong nonequilibrium states with the moments treated in the kinetic sense):

$$\frac{\partial u}{\partial x}=\frac{1}{\mu_U}p_{xx}, \qquad \frac{\partial T}{\partial x}=\frac{1}{\lambda_U}q_x, \tag{3.1}$$

where p_{xx} is the nonequilibrium stress tensor component, q_x is the heat flux, the coefficients

$$\mu_U=u_0^2m(m/8K)^{1/2}/(6A), \qquad \lambda_U=3ku_0^2(m/8K)^{1/2}/(8A)$$

(for Maxwell molecules if the Boltzmann equation is used). Here the constant $A=0.343$ and the constant K appears in the expression for the appropriate potential. If the BGK equation is used we have

$$\mu_U=u_0^2mn_0/\nu, \qquad \lambda_U=3ku_0^2n_0/(2\nu)$$

in relations (3.1), where n_0 and u_0 are respectively the density and the velocity of the gas at the boundary and ν is a frequency. It is obvious that Eq. (3.1) differ principally from the ordinary equations of transfer nonequilibrium stress and heat flux in the framework of the Navier-Stokes theory. Note that coefficients μ_U and λ_U depend on the square of mean velocity in the boundary. The closed form of the moment equations for the near equilibrium flows is traditionally deduced with the aid of the Chapman-Enskog formalism, i.e., the expansion in a small Knudsen number. For our case of the strong nonequilibrium state for the boundary conditions (and appropriate of the large local Knudsen number) this approach is not valid.

4 Numerical technique and computational simulations

The Unified Flow Solver (UFS) [5] is used for numerical simulations in all problems under consideration. UFS includes the direct Boltzmann solver both for 1 component, for multicomponent or for mixtures of gases and continuum solver. A uniform mesh of discrete velocities is used for a bounded velocity domain. The collision integral is computed in the full form using the conservative scheme with Korobov's nodes (different collision models can be selected) or in the model form of BGK type: BGK, S-Model, R-model or $3T$-model. Kinetic continuum schemes are used for continuum solver. Cartesian dynamically adapting to the solution meshes are applied in physical space. Automatic selection of the solver type (kinetic or continuum) is done for each cell of physical space using a switching criterion, and the solutions are coupled on the boundaries of kinetic and continuum domains. So it can be said that adaptive mesh and algorithm refinement (AMAR) is applied in the UFS. The parallel automatic domain decomposition and dynamic load balancing are implemented in UFS. In the current study only kinetic modules of UFS are used, and the numerical method of these modules is briefly described in the following paragraphs.

The finite volume technique is applied for the approximation of the Boltzmann equation in physical space. The following numerical scheme can be written after integration of the Boltzmann equation for i-th point in velocity space over j-th cell in physical space, and using the 1-st order finite difference scheme in time:

$$\frac{f_{ij}^{k}-f_{ij}^{k-1}}{\tau}V+\sum_{face}(\xi_i\cdot\mathbf{n})_{face}f_{i,face}^{k-1}S_{face}=I_i(f_{*j}^{k})V, \tag{4.1}$$

where k is the time index, $*$ denotes all points in velocity space for the given cell, $f_{i,face}^{k-1}$ is the value of the function on the cell face, $\mathbf{n}$ is the unit outward normal vector to the face, V is the cell volume, and S_{face} is the face surface area. For calculation of the face values of the distribution function standard interpolation schemes are applied. The calculation of collision integrals is done with the use of semi-regular methods (quasi Monte Carlo with Korobov's sequences).

It is worth mentioning that in order to numerical analogs of the conservation laws to be fulfilled the numerical scheme should be conservative. For scheme (4.1) this means that the moments of collision integral with the weights of collision invariants must be equal to 0:

$$\sum_i I_i(f_{*j}^{k})\phi_\alpha=0, \quad \alpha=0,\, x,\, y,\, z,\, 2, \tag{4.2}$$

where

$$\phi_0=1, \quad \phi_x=\xi_x, \quad \phi_y=\xi_y, \quad \phi_z=\xi_z, \quad \phi_2=\xi^2.$$

For the full collision integral this is performed by introducing the conservative correction of the collisions frequency (the full collision integral is considered to be the sum of direct and inverse parts $I_i(f_{*j}^{k})=-f_i\nu_i(f_{*j}^{k})+G_i(f_{*j}^{k})$)

$$\nu_i^*=\nu_i(1+a_0+a_x\xi_x+a_y\xi_y+a_z\xi_z+a_2\xi^2). \tag{4.3}$$

Substitution of the corrected value of frequency (4.3) into (4.2) results in a system of 5 linear equations for 5 unknowns a_α, $\alpha=0,\, x,\, y,\, z,\, 2$, which is easily solved. If a BGK-type collision integral is considered, the parameters of the equilibrium function are chosen in such a way that the Eq. (4.2) to be true.

Some results for molecular gases (nitrogen and oxygen) are obtained with the R-model equation for two-atomic molecular gas with rotational degrees of freedom for 1D NRP. The nonequilibrium boundary conditions are given by a sum of two Maxwellians. One can recognize in Fig. 1 the anomalous character of heat transfer for the total temperature and heat flux (the signs of the temperature gradient and the heat flux are the same). The difference in profiles for these molecular gases is small.

The problem for 2D case for a plane flow has been considered in [4], now we study 2D case for an axisymmetrical flow. The axisymmetrical solutions are of importance due

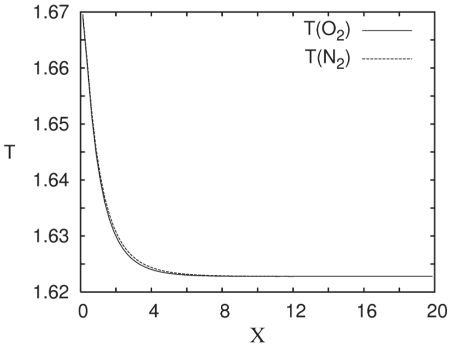

Figure 1: Profiles of total temperature.

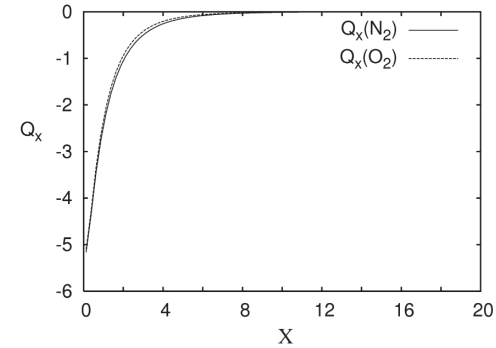

Figure 2: Profiles of total heat flux for oxygen and nitrogen.

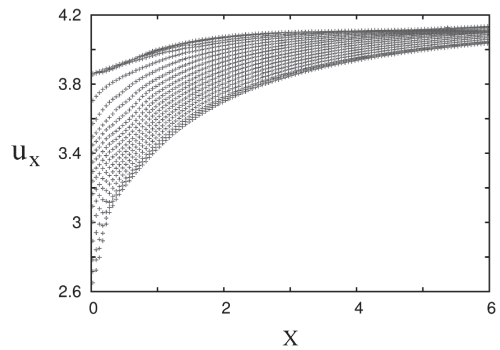

Figure 3: Profiles of the longitudinal velocity at different values of r.

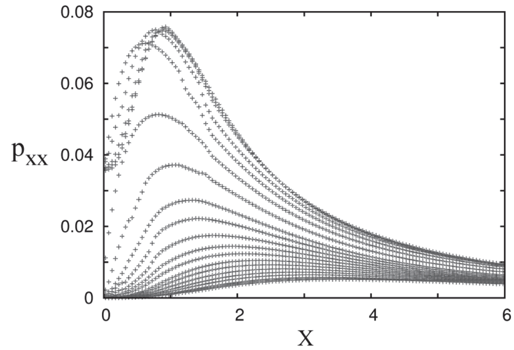

Figure 4: Profile of the component of the nonequilibrium stress tensor at different values of r.

to the obvious physical sense related to the flows of the gas in molecular beams. The R-model is applied (Mach number $M=3$, Knudsen number $Kn=1$). Profiles in Figs. 3, 4 demonstrate the anomalous character of the irreversible momentum transfer for all distances from the axis of the symmetry (the longitudinal velocities increase downstream and the nonequilibrium stresses are positive). For 2D problem there is no, of course, such simple moment relationships as in the case of 1D NRP. But for areas near the symmetry line where the transversal derivatives are small one expects the appearance of the effects similar to the 1D NRP flows. In Fig. 3 greater velocities correspond to the values of transversal coordinate r which are closer to the symmetry line. These calculations confirm that all profiles for any coordinate r demonstrate the anomalous character of the momentum transport. One can see that the change of the velocity in the relaxation zones is relatively large.

A special interest is the computations with the boundary nonequilibrium functions obtained by the simulation related to the real experimental processes, namely to the interactions of the optical lattice with the supersonic molecular beam. The optical lattice is a shallow (mK) periodic optical potentials. The transport and dynamics of ultra-cold atoms have been widely studied [12,13]. Recently deceleration and acceleration of molecular and atomic species travelling in a supersonic beam has been demonstrated using optical lattices [14]. From our point of view it is very interesting that this technique can provide us the strong nonequilibrium functions which is a necessary condition for a realization of NRP flow.

First we considered NRP with the parameters corresponding to the experimental data for nitric oxide (NO) and use the R-model equation for obtaining the mentioned anomalous transport effects. We use two boundary conditions which correspond to nonequilibrium distributions with the positive and negative heat fluxes corresponding to those obtained in the experiment (see Fig. 4 from [14] on the top results with negative flux, on the bottom with the positive heat flux). The temperature of this molecular gas in the experiment was very small (1.8K) so the assumption that the vibrational degrees of freedom can be negligible is valid. Numerical simulations showed that the anomalous transport takes place however the change of the temperature in relaxation zone is not large (of the order of 1%) therefore the experimental observation of these effects is not a simple task. The problem of obtaining experimental conditions for strong nonequilibrium and larger changes of temperature should be posed.

The physical influence of the optical lattice on the molecules in the beam can be described by the appropriate electrical field, see [14]. A periodic optical dipole potential is created by the interaction between a polarisable particle and the field of an optical interference pattern as a result of counter propagating laser fields. The Boltzmann equation is solved in the collisionless limit because the characteristic time of interaction between of the electric field and the molecules is smaller than the time between collisions. We consider a supersonic beam of argon Ar (one can use not only molecular but also atomic gas due to polarization of the atoms). We use a simple atomic beam for simplicity. For considered beam the temperature is 30K. The one-dimensional unsteady free-molecular Boltzmann equation with the force term is written:

$$\frac{\partial f}{\partial t}+\xi_x\frac{\partial f}{\partial x}+\frac{F_x}{m}\frac{\partial f}{\partial \xi_x}=0. \tag{4.4}$$

Here m is a mass of the particle. The electric force is as follows (see [15]):

$$F_x=-\frac{1}{2}\alpha q E_1(t)E_2(t)\sin(qx-\beta t^2),$$

where E_1 and E_2 are the electric field amplitudes (two counterpropagating fields are used), α is a static polarizability for Ar (the polarizability to mass ratio of Ar is presented in [16]), q is the wavenumber, β is the frequency chirp due to the time dependent frequency difference between each of the fields.

Initially particles in the beam are at thermal equilibrium. The nonequilibrium distribution function obtained as a result of the influence of optical lattice is shown in Fig. 5. After obtaining the distribution function from Eq. (4.4) we solve NRP with the Boltzmann Eq. (2.1) for the steady case. For a monatomic gas we use the collision integral

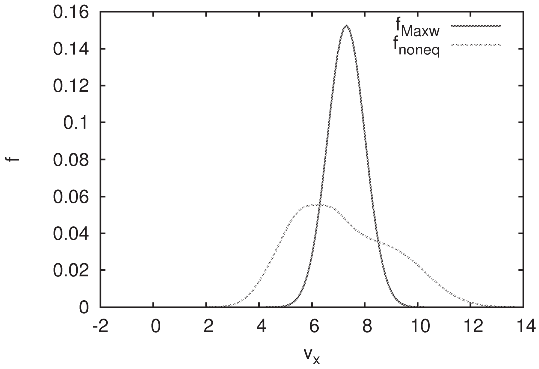

Figure 5: The nonequilibrium distribution function ("prepared" from the initial equilibrium Maxwell distribution function after solving Eq. (4.4)) which is a boundary for NRP.

with the hard sphere model. The nonequilibrium distribution from Fig. 5 was accepted as a boundary condition in 1D NRP. The results of the computations for the Boltzmann equation for Ar are presented in Figs. 6 and 7. One can see the anomalous character of the transport.

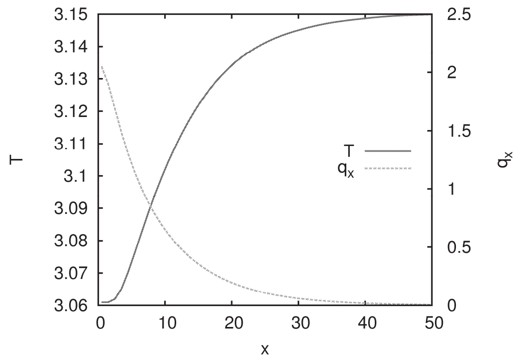

Figure 6: Temperature and heat flux profiles for NRP with the mentioned distribution function as a function of the boundary condition.

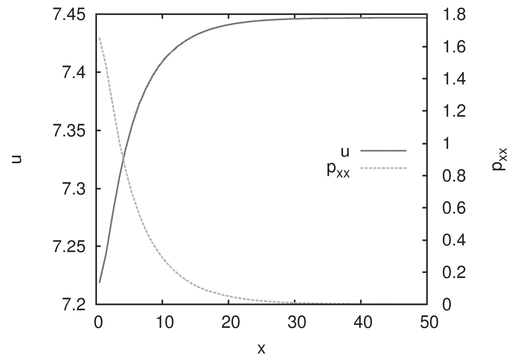

Figure 7: Velocity and nonequilibrium stress tensor component profiles for NRP with the mentioned distribution function as a function of the boundary condition.

5 Computations with a large change of temperature in the relaxation zones

The obvious drawback of the considered NRP is the small change of the temperature in the relaxation zones (change of velocity is larger in some cases). If the change is smaller than 10% it is hard to measure the effects in experiments and the hypothetical model of heat devices (e.g., the microrefrigerator) is not seen very interesting. The problem of max-

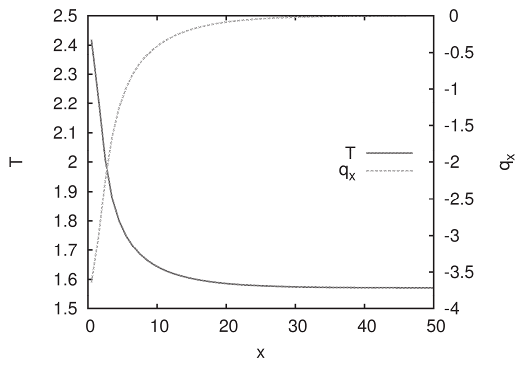

Figure 8: Profiles of temperature T and heat flux q_x.

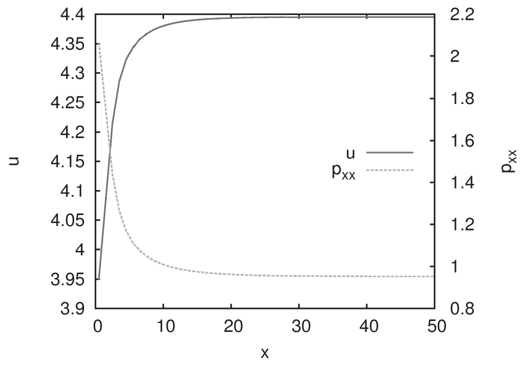

Figure 9: Profiles of longitudinal velocity u and nonequilibrium stress tensor component p_{xx}.

imizing these changes should be posed. The analysis of the relationships representing conservative laws for macroparameters shows that the changes of mentioned quantities depend on the magnitude of the dissipation $(p_{xx},\, q_x/u_0)$ for the boundary nonequilibrium distribution.

Suppose the nonequilibrium distribution function is a linear combination of two delta-functions with different velocities u_1 and u_2, namely $f(0,\xi)=n_1\delta(\xi_x-u_1)+n_2\delta(\xi_x-u_2)$, we assume that the density and mean velocity are constant, in this case $|q_x|$ is proportional to the cube of $|u_2-u_1|$. In the most test examples in [4] the nonequilibrium functions is a sum of two Maxwellians with the difference of the mean velocities of the order of unity. Increasing the value of $|u_2-u_1|$ it is possible to obtain considerable increase both in the boundary heat flux and in changes of macroparameters in the relaxation zone. The following distribution function is used in calculations:

$$F=0.5F_M(1,0,0,0.5)+0.7F_M(5,0,0,0.5), \tag{5.1}$$

where $F_M(u_x,u_y,u_z,T)$ is Maxwellian with the unit density, velocity components u_x, u_y, u_z and temperature T. Results of the numerical analysis are presented in Figs. 8 and 9.

It is seen that the changes of the temperature and velocity are 40% and 15% respectively. It is important to note that in the nonequilibrium boundary there is nonzero zone of the distribution with negative velocities. But for equilibrium at infinity such zone is negligible. Thus we cannot use the mentioned expansion in powers of a small parameter in the entire velocity region. However the numerical analysis confirms the anomalous character of the transport for each spatial point. The flow is supersonic: the Mach number increases from $M\sim 2$ for the nonequilibrium boundary until to $M\sim 3.5$ at infinity.

Obtaining the nonequilibrium distribution with similar characteristics is a future task both for simulation and experimental technique. The method of optical lattices is an interesting and perspective tool for study of these processes and one can suppose, in particular, that it would be possible to create strong nonequilibrium distributions in supersonic beams of particles using two or more optical lattices.

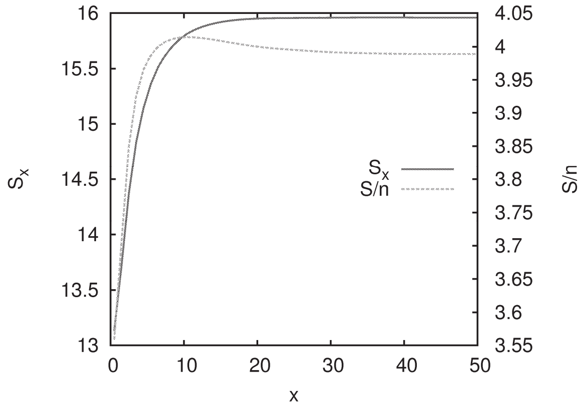

Figure 10: The profiles of the entropy flux S_x and the specific entropy S/n.

6 Discussion and conclusions

To discuss the properties of the kinetic strong nonequilibrium system far from the traditional thermodynamical consideration it is important to present results of behaviour of the H-function (or in other words $S=-H$, i.e., the nonequilibrium entropy in the problems under study). The H-theorem of course is valid for any nonequilibrium state, so we should calculate the appropriate moments. For 1D NRP the analogue of the H-theorem for the uniform relaxation problem is the statement that the entropy flux S_x must increase. However the behaviour of the entropy S and the specific entropy S/n, where n is density is not restricted by the H-theorem. Nevertheless one can suppose that these values also increase. However the analysis based on the expansion in powers of the mentioned small parameter of the entropy evolution in space performed in [3] shows that for the positive heat flux the entropy S and the reduced entropy S/n monotonously increase downstream. For the case of the negative heat flux there is a small maximum for these quantities. The computations with the boundary distributions (5.1) confirm this statement. In Fig. 10 profiles of the entropy flux and the specific entropy are depicted. The flux profile is monotonous and the curve of the specific entropy has a very small local maximum that denotes that for the points downstream with respect to the point of the maximum the specific entropy decreases.

The other issue of discussing is the transition from the nonequilibrium state in NRP to equilibrium at infinity. Strictly speaking we have two characteristic parameters, namely a small parameter mentioned above which depends on the value of the molecular velocity and the Knudsen number which describes the extent of rarefaction of the gas. For a strong nonequilibrium state Knudsen number is of the order of unity (or more) and the mentioned expansion is valid. But for regions downstream where the gradients of all quantities tend to zero the local Knudsen number also tend to zero. Thus there are two concurrent expansions: mentioned earlier and the ordinary Chapman-Enskog series. It is a future task to find the relations between these formalisms. The problem of clarification this mathematical and physical situation needs to be studied.

We can conclude that some computations for different kinetic equations for different gases including molecular gases confirm the possibility of the anomalous transport in relaxation zones. Some 1D and 2D nonuniform relaxation problems are considered (3D free jet problems are now under consideration but one can suppose that they will demonstrate the analogous properties). Nevertheless the anomalous transport in the nonequilibrium zones of the order of the mean free path is observed for some flow regions for all considered problems. It is important that the real physical situation intrinsic for the real experiment is modelled in computations. One can expect that the theoretical and numerical analysis of the conditions of nonuniform relaxation problem can help in observing these effects experimentally.

Acknowledgments

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