Numerical simulations of complex nonequilibrium flows in finite regions on the basis of the Boltzmann kinetic equation

V.V. Aristov, S.A. Zabelok, A.A. Frolova
Dorodnicyn Computing Center, Federal Research Center of Computer Science and Control of Russian Academy of Sciences. Ul. Vavilova 40, 119333, Moscow, Russia.
aristovvl@yandex.ru

Abstract. A new formulation of the inner boundary problem for description complex nonequilibrium flows between membranes is presented. Solutions by means of the Boltzmann equation and the model kinetic equation for mixtures with chemical reactions demonstrate interesting physical properties in this open nonequilibrium system. Possibility of the anomalous thermal transport where the heat flux and the temperature gradient are of the same sign, is studied. Influence of boundary conditions on the parameters of the structure is considered as well.

Introduction

We study strong nonequilibrium gas flows in which effects of the anomalous heat transfer do not correspond to a continuum law. Note that some researches have investigated nonequilibrium flow regimes and considered questions concerning the correct transition from the microscopic description to the macroscopic description, see for example [1-3]. We use the nonlinear Boltzmann equation and the model kinetic equations. Direct methods for numerical solving these equations are applied [4] for studying new nonequilibrium flows in the boundary steady problems. For different problems with nonequilibrium boundary conditions (see [5, 6]) nonclassical transport in flows appears (this effect for the first time has been described in [7]). In particular, heat can be transferred from the region with the lesser temperature to the region with the greater temperature. Now we consider a problem with “membrane-like” boundary conditions. In the simplest case particles leaving the region under consideration do not collide with particles entering this region. For such a situation even equilibrium distributions for the boundary conditions can lead to nonclassical anomalous transport mentioned above due to complex interaction of the oppositely directed flows. In a more complex situation a part of gas can be reflected from the membrane molecules with the diffuse condition. This problem for a mixture of chemically reacting gases is also solved using the kinetic model equations [8,9] which we have previously applied in study of nonequilibrium structures in the nonuniform relaxation problem [10].

1. Formulation of the problems and governing equations

1.1. Flows of a simple gas in a closed region with membrane type boundary conditions

The stationary flow of a rarefied gas is investigated in 1D geometry that represents an interval with length \( L \). At the ends of the interval, membrane-type conditions are set. In this case it is assumed that
the counter flows of particles do not interact at the boundaries. In other words, the unchanged velocity distribution functions are specified on the left and right boundaries for particles with velocities directed inside the region (the distribution functions can be as equilibrium as nonequilibrium). When solving the problem, the stationary Boltzmann kinetic equation for the velocity distribution function (VDF) \( f(x, \xi) \) is used in the following form:

\[
\xi_x \frac{\partial f}{\partial x} = I(f, f),
\]

where \( x \) is the coordinate of the physical space, \( \xi = (\xi_x, \xi_y, \xi_z) \) is the velocity vector, and \( I(f, f) \) is the integral of elastic collisions. The boundary conditions of membrane-type are as follows

\[
f(0, \xi) = F_0(\xi), \forall \xi_x > 0, \quad f(L, \xi) = F_1(\xi), \forall \xi_x < 0.
\]

Here \( F_0 \) and \( F_1 \) are the distribution functions (generally nonequilibrium). Note that the problem on evaporation and condensation is a particular case of this problem. The gas is assumed to be monatomic with the interaction law being the model of hard spheres. Macroscopic variables, such as particle number density \( n \), velocity vector \( \mathbf{u} \), temperature \( T \), heat flux vector \( \mathbf{q} \) and pressure tensor \( P \) are determined by integrating the VDF with the corresponding weights over the three-dimensional velocity space.

1.2. Flow of a chemically reacting gas in a closed region with membrane type boundary conditions

A more difficult case can be investigated for a chemically interacting gas. We study the flow of a chemically reacting gas of four components \( A \) with masses of molecules \( m^i \) (\( i = 1, \ldots, 4 \)) and the energy of a chemical bond \( E^i \). The regime of slow chemical reactions is considered, that is, it is assumed that the relaxation time due to elastic collisions is much less than the relaxation time during chemical interaction. The gas components are involved into a reversible bimolecular reaction, and the change in the internal chemical energy \( \Delta E \) of the mixture is assumed to be positive.

\[
A^1 + A^2 \leftrightarrow A^3 + A^4, \quad \Delta E = \sum_{i=1}^{4} \lambda^i E^i = E^4 + E^3 - E^2 - E^1 > 0,
\]

where \( \lambda^i \) is the stoichiometric coefficients, respectively \((1, -1, -1, -1)\).

The formulation of a problem with membrane-type boundary conditions for a one-dimensional flow of a gas mixture of four components is similar to that for a single-component gas. Also, as above, it is assumed that the outgoing gas does not interact with the incoming gas.

The solution of the problem is determined by the system of Boltzmann equations, but the calculations of the system of Boltzmann equations are extremely complicated therefore, the use of model equations in the case of a chemically reacting gas is reasonable. The approximating system of BGK type equations is proposed in [8, 9], in which the integral terms are replaced by one relaxation operator for each component of the mixture

\[
\frac{\partial f^i}{\partial t} + \left( \xi^i, \frac{\partial f^i}{\partial \xi^i} \right) = Q^i(f) \equiv v_i (f_{m^i} - f^i), \quad i = 1, \ldots, 4, \quad (1)
\]

where, \( f_{m^i}(\xi) = n_i \left( \frac{m^i}{2\pi k T_i} \right)^{3/2} \exp \left( -\frac{m^i (\xi - u_i)^2}{2k T_i} \right) \), \( i = 1, \ldots, 4 \).

The free five parameters of the equilibrium function for each reacting component, namely the particle number density \( n_i \), the three components of velocity \( u_i \) and temperature \( T_i \) are determined from the equality of momentum, energy and density exchanges for each component in (1) and the
system of complete Boltzmann equations. The boundary conditions are analogous to the mentioned above but now should be accepted for each component.

2. The problem with membrane-like boundary conditions for a simple monatomic gas

The results of computations for the Boltzmann equation for the different variants boundary conditions are presented in figures 1-2. We will mark by a color (blue in the case of monatomic gas and yellow in the case of mixture) the zones with the anomalous thermal transport in the region under consideration.

The results shown in figure 1 are obtained for Knudsen number Kn=1. The boundary condition for the left plot are Maxwellians \( F_L(\xi) = f_M(1.0,3.0,1.0) \) and \( F_R(\xi) = f_M(1.5,\ldots,2.5) \). It is interesting that for equilibrium boundary conditions and moderate Knudsen number there is a significant anomalous zone due to the nonequilibrium flow in region under consideration. In the right plot the results are obtained with \( F_L(\xi) = f_M(1.0,3.0,1.0) \) and \( F_R(\xi) = f_M(1.,0.5,3.0) + f_M(1,1.5,3.0) \), the anomalous heat transport is in the entire region (here is not marked by the color). In figure 2 (the left plot) the dependence of the value of the anomalous zone on Knudsen numbers is presented for the boundary conditions \( F_L(\xi) = f_M(1.0,2.0,1.0) \) and \( F_R(\xi) = f_M(1.0,0.5,1.0) \). The assumption of a full permeability of the membrane can be reduced, namely the coefficient of the permeability \( P \) can be introduced similar to \([9]\). In this case a parameter \( a=1-P \) is related to the part of molecules which are reflected from the membrane with its temperature and with the accommodation. In figure 2 (the right) the dependence of the size of anomalous zone on the coefficient of the reflection is shown for the boundary conditions \( F_L(\xi) = f_M(1.0,3.0,1.0) \) and \( F_R(\xi) = f_M(1.0,\ldots,1.5,1.0) \).

**Figure 1.** The demonstration of the anomalous heat transport for a problem with two variants of the “membrane-like” boundary conditions.
3. The problem with membrane-like boundary conditions for a mixture with chemical reactions

Two main purposes of study of the problem with the “membrane-like” boundary conditions:

1) to find an anomalous transport in the region;
2) to form complex nonequilibrium flows especially for mixtures with chemical reactions, in this case the boundary conditions can influence the structure in this “chemical reactor”.

In figures 3-5 we show the results of calculations with different boundary conditions and different regimes of rarefaction for a mixture of gases undergo slow chemical reactions (with a value \( \Delta E = 1 \)).

Figure 3. The profiles of heat flux \( q_x \) and temperature \( T \) in for gas mixtures with chemical reactions, Kn=0.1 (left), Kn=1.0 (middle), Kn=10 (right).

In figure 3 the following model variant of molecular component masses was used: \( m_1 = 2.2, m_2 = 0.9, m_3 = 1.5, m_4 = 1.6 \). For the left and right boundaries we use equilibrium distribution functions for all components. For the left boundary the velocities of components were as follows: \( u_L = \{1.5;1.0;2.5;0.5\} \) and for the right boundary \( u_R = \{-0.5;-2.5;-1.5;-1.0\} \)

Figure 4. The profiles of heat flux \( q_x \) and temperature \( T \) in for gas mixtures with chemical reactions for different Knudsen number with the left boundary parameters \( n_L = \{1.0;1.0;0.01;0.01\} \) and right values \( n_R = \{0.5;1.0;0.01;0.01\} \). \( u_L = \{1.0;1.0;1.0;1.0\} \) and right \( u_R = \{-0.5;-0.5;-0.5;-0.5\} \) and \( T=1 \) for Kn = 0.1 (the left plot), and Kn = 1 (the right plot).
In figure 4 results for the boundary conditions with parameters \( n_L = \{1.0;1.0;0.01;0.01\} \), \( u_L = \{1.0;1.0;1.0;1.0\} \), \( n_R = \{0.5;1.0;0.01;0.01\} \), \( u_R = \{-0.5; -0.5; -0.5; -0.5\} \) and temperature on both sides \( T=1 \) are presented, one can see that in this case the change of temperature is smaller, nevertheless the anomalous zone is significant.

Figure 5. The profiles of densities and concentrations. Left plot: densities of mixture components for the variant with the following left boundary conditions \( n_L = \{1.0;1.0;0.01;0.01\} \), \( u_L = \{0.05;0.1;0.05;0.05\} \) and right values \( n_R = \{0.01;0.01;1.0;1.0\} \), \( u_R = \{-0.1; -0.05; -0.05; -0.05\} \), temperature \( T=1.0 \). Densities (middle) and concentrations (right) of mixture components for boundary conditions as in Fig. 4 for \( \text{Kn} = 0.1 \).

In figure 5 profiles of densities and concentrations for four components of the mixture for two variants of the boundary conditions, it is seen their influence on the behavior of the quantities.

4. Concluding remarks

A new type of nonequilibrium transport effect is confirmed by the direct solutions for the Boltzmann and the other kinetic equation for the problem with the “membrane-like” boundary conditions. The anomalous thermal transfer does not contradict to the second law of thermodynamics in the form of the H-theorem. This fact has been proved numerically.

There is an interesting question devoted to the experimental tests of this effect. Nonequilibrium flows can be prepared in the region between two thin permeable membranes with the equilibrium boundary distributions. Particles entering the region form the nonequilibrium state. The issue concerns the reliability of these “membrane-like” boundary conditions. Possible experimental tests are discussed. For these purposes mixed cellulose ester (MCE) membranes could be used as a material for the boundaries. As reported in [12], a pore-size of these membranes is 25 nm, so the appropriate Knudsen number is more than unity at the atmospheric pressure. As an method of diagnostics of the nonequilibrium distribution function in the region under consideration could be proposed the Electron Beam Fluorescence (EBF). This problem for the chemical mixture allows us to create different (qualitatively and quantitatively) nonequilibrium structures.

Acknowledgments

This work by the first (V.A.) and second (S.Z.) authors was supported by Russian Foundation for Basic Research, grant 18-01-00899. The calculations were carried out by means of Joint Supercomputer Center of RAS MVS10p multiprocessor computer.

References

[1] Gorban A.N, Karlin I.V. Physica A. 206 (1994) 401-20.
[2] Gorban A.N., Karlin I.V. Physica A. 360 (2006) 325-64.
[3] SoneY, et al. Phys.Fluids. 8 (1996) 628-38.
[4] Kolobov V.I., Arslanbekov R.R., Aristov V.V., Frolova A.A., Zabelok S.A. J. Comp. Phys. 223 (2007) 589-608.
[5] Aristov V.V., Zabelok S.A., Fedosov M.A., Frolova A.A. Comp. Math. Math. Phys. 56 (2016) 854-63.
[6] Aristov V.V., Zabelok S.A., Frolova A.A. Doklady Physics. 62 (2017) 149-53.
[7] Aristov V.V. Phys. Letters A. 250 (1998) 354-9.
[8] Rossani A., Spiga G. Physica A. 272 (1999) 563-73.
[9] Groppi M., Spiga G. Physics of Fluids. 16 (2004) 4273-84.
[10] Aristov V.V., Frolova A.A., Zabelok S.A. EPL (Europhys. Letters). 106 (2014) 20002.
[11] Erofeev A.I., Fridlender O.G., Fluid Dynamics. 45 (2010) 965-74.
[12] Gupta N.K., Gianchandani Y.B. Microporous and Mesoporous Materials. 142 (2011) 535-41.