Computational technologies for determining the collision term in Boltzmann equation

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Abstract. For solution of applied tasks of mathematical modeling it is required to know the properties of the medium, which are difficult or impossible to determine experimentally or by semi-empirical formulas. In such cases it is important to be able to correctly evaluate capabilities of theoretical methods. Since the values of the transport characteristics of the medium are influenced by microprocesses, it is reasonable to use the approach of the molecular-kinetic theory of gases, the Boltzmann equation in particular. The right side "collision" part of this equation contains multiple improper integrals with singularities whose values are used in determining the transition coefficients. In this paper, we present computational technologies for determining the values of such integrals, which allows to reasonably determine the calculated values of the transfer coefficients in media based on the first principle of the molecular-kinetic theory of gases in mathematical modeling of problems of fluid and gas mechanics on the basis of macroequations of heat and mass transfer.

1. Introduction

At present in a number of scientific organizations works are being carried out for the purpose of studying of physical and physic-technical characteristics of liquids and gases in a wide range of temperatures and pressures on the basis of heat and mass transfer macroequations [1-3]. In many cases for solution of current mathematical modelling tasks it is necessary to know the characteristics of the medium, which are difficult or simply impossible to determine directly even at the modern level of experimental equipment. Thus, thermal diffusion, self-diffusion and some other medium transfer coefficients cannot be determined by means of the experimental approach at this point. However, on the basis of their value it is possible to interpret some natural phenomena: reduction of hydrodynamic resistance of vessels due to use of microbubble gas mixture; reduction of the thermodynamic resistance in technical systems used for gas transport [4-6]. In such cases it is very important to be able to correctly evaluate the possibilities of theoretical methods and when deriving heat and mass transfer equations to take into account the influence of microprocesses on the transfer characteristics of the medium occurring at the molecular level. In this connection, in the numerical modeling of various physical and technical processes on the basis of continuous medium mechanics macroequations, it is necessary to use the molecular-kinetic theory of gases, the Boltzmann equation in particular. The right-side "collisional" part of this equation contains multiple improper integrals, the values of which are used in the computation algorithm for determining the transport coefficients. It should be noted that one of these integrals contains an oscillating integrand parametric function. In this paper, various
computational technologies were used to determine their values: orthogonal polynomials method, spline interpolation. The method of presenting of the initial unbounded domain of integration into a square domain was applied, the node partition algorithm, which takes into account the boundary layers and the oscillation of the integrand function, was proposed. This approach allows to make substantiated determination of calculated values of transfer coefficients in gaseous media, relying on the first principle of the molecular-kinetic theory of gases.

2. Formulation of the problem
It should be noted that hydromechanics macroequations are derived from the Boltzmann equation [7-9]. In which case the collision part of this equation consisting of six-fold improper integrals describes dissipative processes of interacting molecules in the medium. In calculation of kinetic coefficients of transfer using the Chapman-Enskog method [7, 8], Sonin orthogonal polynomials [10] and integral parenthesis the collision term of the Boltzmann equation is reduced to the integrals as seen in [4-9]:

$$\Omega_{ij}^{(\gamma)} = \left(\frac{kT}{2\pi m_{ij}}\right)^{\frac{3}{2}} \int_{0}^{\infty} \exp(-\gamma^2) \gamma^{2\gamma^{\frac{3}{2}}} Q_{ij}^{(\gamma)} d\gamma$$

where \( \gamma = (m_{ij}/2kT)^{\frac{1}{2}} \cdot g^* \) is a non-dimensional variable related to the reduced kinetic energy \( g^* \); \( m_{ij} = m_{ij}^i + m_{ij}^j \) is the averaged mass of molecules of the \( i \) and \( j \) type. As follows from expression (1), in order to determine the value of \( \Omega_{ij}^{(\gamma)} \) it is necessary to know the values of the three improper integrals. One of them is a part of the function \( \chi_{ij}(g^*, b^*) \) [9]:

$$\chi_{ij}(g^*, b^*) = \pi - 2b^* \int_{(r_0^s)_{\min}}^{\infty} \frac{dr^*}{(r_0^s)^2 \left( 1 - \varphi_{eff}^*/(g^*)^2 \right)^{\gamma/2}}$$

where \( \varphi_{eff}^* = \varphi^*(r^*) + (g^* b^*/r^*)^2 \), and \( \varphi^*(r^*) \) takes the form [9].

The value of the lower limit \( (r_0^s)_{\min} \) in the integral expression (3) is determined from the nonlinear algebraic equation [1, 8, 9]. In order to determine its value, the authors proposed asymptotic and numerical algorithms [9]. It is shown that \( (r_0^s)_{\min} \approx AI \) [11].

3. Calculation methods of determining the value of the \( \Omega \)-integral
Another problem of determining the values \( \chi_{ij}(g^*, b^*) \) is the behavior of the integrand in the integral of expression (3). It must be noted that if the reduced kinetic energy of interacting molecules is equal to their reduced potential energy, i.e. \( g^2 = \varphi_{eff}^* \), then the integrand in (3) turns to zero. If \( g^2 > \varphi_{eff}^* \), then trajectories of interacting molecules have an on-returnable pattern and coordinates of points on it are determined by the set of real numbers \( R \). In case if \( g^2 < \varphi_{eff}^* \), then trajectories of interacting molecules have a returnable pattern and coordinates of these trajectories are determined by a set of complex numbers \( C \) [9]. Points \( b_{\text{ext}} \), \( g_{\text{ext}} \), laying on a “critical” surface (of the curve) dividing these sets, are the bifurcation points of solution [12]. The bifurcation points coordinates were determined by solving a system of nonlinear equations.
The integrand function improper integral (7) in the vicinity of the points located on the “critical” surface has large gradients. Therefore for correct determination of values of the function \( \chi(g^*, b^*) \) it is proposed to use calculation methods based on spline quadrature and Gauss-Christoffel quadrature using orthogonal polynomials [13]. In this respect the partition nodes of the integration segment of [0,1] in the spline quadrature during calculation of the values of the function \( \chi(g^*, b^*) \) were determined from the condition of fixed value of error of interpolation of the integrand by cubic splines. For the Gauss-Christoffel quadrature, in which orthogonal polynomials are used, the integration nodes on an interval [0,1] were distributed on the basis of minimizing the error of approximation of the integrand by orthogonal polynomials. The results of numerical calculations of the function \( \chi(g^*, b^*) \) (7) with the above quadrature sat the same number of partition nodes had a satisfactory concurrence of values differing from each other in the fourth decimal.

Let us proceed to the analysis of calculation techniques which are proposed for determination of values of the improper integral (1). The integrand function of this integral includes the expression for the improper integral \( Q_{00}^0(2) \) with a rapidly oscillating integrand. To determine values of the integral (1) the initial domain \( \Omega = \{0 \leq b^* < \infty, 0 \leq r < \infty \} \) with the use of transformations
\[ b^* = -\frac{x}{1-x}, \quad \gamma = \frac{y}{1-y} \left( \frac{2kT}{m_y} \right)^{\frac{1}{2}}, \quad \left( g^* = \left( \frac{2kT}{m_y} \right)^{\frac{1}{2}} \cdot \gamma \right) \]  

(8)

the quadrant \( G = \{0 \leq x \leq 1, 0 \leq y < 1\} \) is shown. In the new variables \((x, y)\) the expressions for the improper integrals (1)-(2) take the following form:

\[ \Omega_y^{(c)} = \int_0^1 \exp(-z) \cdot z^{\frac{1}{2}} Q_{yj} \cdot \frac{1}{(1-y)^2} dy \]  

(9)

\[ Q_{yj} = 2\pi \int_0^1 1 - \cos \chi_j \left( \frac{2kT}{m_y} \cdot \frac{y}{(1-y)^2} \cdot \frac{x}{1-x} \right) \cdot \frac{x}{(1-x)^3} dx \]  

(10)

where \( z = g^* \cdot m_y / 2kT \).

In (10) the integrand function is rapidly oscillating, and the frequency of oscillations depends on the value \( \left( \frac{2kT}{m_y} \right) \cdot \frac{y}{1-y} \), i.e. the magnitude of \( g^* \). Therefore, for correct calculation of values (10) let us use the Gauss-Christoffel quadrature, in which the nodes of partition of the segment \( x \in [0,1] \) are selected based on condition of minimization of the quadrature error.

When determining the values of the integral (10) initially the value of \( g^* \) magnitude, reduced relative velocity of the interacting molecules were recorded, respectively the value \( y \). The \( G \) domain was partitioned into rectangular stripes:

\[ G = \{0 \leq x \leq 1, y_1 = i_1 \cdot h_2, i_1 = 0,1, \ldots, N_2\} \]

where \( h_2 = 1/N_2, \) \( N_2 \) is the number of partitions of the \( G \) domain into rectangular stripes.

Assuming that \( i_1 = 0 \) and using the Gauss-Christoffel quadrature the values of the integral (10) along the line \( y_0 = 0 \) were determined. Then consecutively assuming that \( i_1 = 1,2,3, \ldots, N_2 \), the values of the integral \( \forall y_1 \) were calculated. Further the analytical view of the integrand function for the integral (9) was forming:

\[ \Phi(y) = \exp(-z) \cdot z^{\frac{1}{2}} \cdot \check{Q}_{yj} \cdot \frac{1}{(1-y)^2} \]  

(11)

where \( \check{Q}_{yj} = \Phi(y) \) \( (y \in [0,1]) \) is the function obtained by means of interpolation of the integral (10) values on the lines \( y_1 = i_1 \cdot h_2 (i_1 = 0,1,2, \ldots, N_2) \).

After determining of the analytical expression for the \( \Phi(y) \) function (11), the value of integral (9) is calculated using algorithm described above. The algorithm of determination of values of the double two-parameter improper integral with oscillating integrand function consists of:

A) algorithm of displaying of the initial unlimited domain \( H \) in the limited domain \( G \), having a square shape;
B) calculation of values of the integral (10) at fixed values of the parameter \( g^* \) (respectively \( y_0 = i_1 \cdot h_2, h_2 = 1/N_2, i_1 \in 0,N_2 ) \) using the Gauss-Christoffel quadrature (spline quadrature);
C) forming of the function (11) using the interpolation algorithm [14-16];
D) calculation of the initial integral (9) using the quadrature used in B).

It should be noted that accuracy of the calculation of the values of the double improper integral using the proposed calculation techniques not only depends on the accuracy of the quadrature but also on the
accuracy of performing the operation in C), which can be always made less than the error of the quadrature equations.

4. Results of numerical experiments
The table 1 shows the comparison of the experimental and calculated values of $\Omega_{i}^{(l,r)}$, using a PC software [9]. Normalizing was used in the process

$$\Omega_{i}^{(l,r)} = \frac{\Omega_{i}^{(l,r)}_{ex}}{\Omega_{i}^{(l,r)}_{rs}}$$

where $\left[ \Omega_{i}^{(l,r)}_{ex} \right]_{rs}$ is the value of the integral of collision for the model of solid media. The values of $\Omega_{i}^{(l,r)}(T^{*})$ obtained by using the proposed calculation techniques were compared to its calculated values given in the paper [17].

Table 1. Comparison of the calculation of $\Omega_{i}^{(l,r)}(T^{*})$ value, performed in this paper, with the results of the paper by L. Monchick and E.A. Mason. Transport properties of polar gases: J. Chem. Phys., 35 (5), Nov. 1961, 1676–1697 [17] and evaluation of relative error of $\delta\Omega_{i}^{(l,r)}(T^{*}),\%$

| $T^{*}$ | 0.1 | 0.4 | 0.6 | 1.0 | 1.6 | 1.8 | 2.0 |
|---------|-----|-----|-----|-----|-----|-----|-----|
| This paper | 4.0119 | 2.3174 | 1.8800 | 1.4420 | 1.1688 | 1.1181 | 1.0763 |
| Paper by L. Monchick and E.A. Mason [17] | 4.0079 | 2.3144 | 1.8767 | 1.4398 | 1.1679 | 1.1166 | 1.0753 |
| $\delta\Omega_{i}^{(l,r)}(T^{*}),\%$ | 0.09 | 0.12 | 0.17 | 0.15 | 0.07 | 0.13 | 0.09 |

The given evaluation of relative error of $\delta\Omega_{i}^{(l,r)}(T^{*})$ in the interval of the given temperatures $T^{*} \in [0.1;2]$ is $\delta\Omega_{i}^{(l,r)}(T^{*}) \in [0.07;0.17]\%$, which is indicative of high accuracy of calculations. The qualitative analysis and comparison with data by other authors allows us to claim the correctness of the results obtained using the proposed calculation techniques of determination of values of the collision part of the Boltzmann equation.

5. Conclusion
Simulation of gas dynamic processes occurring in nature, equipment, based on macroequations of heat and mass transfer requires the use of substantiated values of transfer coefficients. At present in order to determine them there are approaches of experimental or semi-empirical equations and methods of numerical simulation. In this paper the approach of molecular-kinetic theory was used, in which it is proposed to determine calculated values of the medium transfer coefficients in the heat and mass transfer equations based on the collision part of the Boltzmann equation. However a number of difficulties emerge related to the structure of this part: it is a multiple improper integral with oscillating parametrical integrand function. In this paper in order to determine the values of such integrals different calculation techniques are used: orthogonal polynomials method, spline interpolation. The method of presentation of the initial unlimited integration domain into square domain was used, nodes partition algorithmis proposed, which takes into account the boundary layers and oscillation of the integrand function. This allows to make substantiated and high quality determination of the calculated values of coefficients of transfer in media on the basis of the first
principle of the molecular kinetic theory of gases in the process of mathematical modelling of liquid and gas mechanics simulation tasks.

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