On the determination of the transfer coefficients in the heat and mass transfer equations, based on the Boltzmann equation

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Abstract. At present, as a rule, the determination of the transfer characteristics of viscosity, diffusion, heat conduction and other characteristics in macro-equations of aerohydromechanics is carried out experimentally or on the basis of the kinetic theory of gases - the Boltzmann equation. The right “collisional” part of the Boltzmann equation contains multiple improper integrals with an oscillating integrand function, the values of which are used in determining transfer coefficients. This article proposes numerical algorithms suitable for calculating integrals of this type. They are based on the use of the Gauss - Christoffel quadrature formula that applies orthogonal polynomials. The oscillation nature of the integrand requires control of the quadrature error. In this case, the split nodes of the integration interval are distributed on the basis of minimizing the error of approximation of the integrand by orthogonal polynomials. Such an approach, in contrast to others, allows determining the values of integrals with oscillating integrand functions more qualitatively and efficiently and does not contain an "iterative" procedure for increasing the split nodes of the integration segment to achieve a given accuracy.

This article is devoted to the problem of constructing quadrature formulas for calculating improper integrals, which are used in determining the transfer coefficients, based on the Boltzmann equation.

1. Determining transfer coefficients in heat and mass transfer equations based on the molecular-kinetic theory

The problem of determining the coefficients of transfer of viscosity, diffusion, thermal conductivity, etc. in the macro-equations of aerohydromechanics is relevant and attracts the attention of a large number of scientists [1-6]. As a rule, at present, the determination is carried out experimentally or on the basis of the kinetic theory of gases - the Boltzmann equation [7]:

\[
\frac{\partial}{\partial t} + \mathbf{c}_i \cdot \nabla + \mathbf{F}_i \cdot \nabla \mathbf{c}_i \right) f_i(\mathbf{r}, \mathbf{c}_i, t) = \sum_{j} \int \int \int \int \int \left( f'_j - f_j \right) gbdde^d \mathbf{c}_j ,
\]

here \( f_i \), \( f_j \) – distribution functions of molecules of sort \( i \) and \( j \), \( \mathbf{F}_i \) is the external force on the molecule, \( \mathbf{c}_j \) – the speed of molecules of sort \( i \), \( e \) and \( b \) – geometric parameters of colliding molecules.

The right-hand side of the Boltzmann equation, consisting of multiple improper integrals, describes dissipative processes in gases and is used in the algorithm for determining the values of the transfer characteristics of the medium. Based on the Chapman - Enskog method, Sonin polynomials, integral
brackets, these multiple integrals are transformed into expressions consisting of linear combinations of three-fold improper integrals, which are called collision integrals \( \Omega^{(l,r)} \):

\[
\Omega^{(l,r)} = \left( \frac{kT}{\pi m} \right)^{\frac{1}{2}} \int_{0}^{\infty} \exp\left(-\gamma^2\right) \gamma^{l+r+3} \Omega^{(l,r)} d\gamma.
\]  

(1)

Here \( \Omega^{(l)} \) are the average cross sections for the scattering of molecules (transfer cross-sections):

\[
\Omega^{(l)} = \Omega^{(l)} \left( g^* \right) = 2\pi \int_{0}^{\infty} \left(1 - \cos^l \left( \chi \left( b^*, g^* \right) \right) \right) b^* db^* ,
\]

(2)

\( \chi \left( b^*, g^* \right) \) – the function of the angle of molecules scattering:

\[
\chi \left( b^*, g^* \right) = \pi - 2b^* \int_{(\eta)}^{\infty} \frac{dr^* / r^{*2}}{\sqrt{1 - \varphi_{eff} / g^{*2}}}.
\]

(3)

The algorithm for calculating their values consists of several procedures [7, 8]. First, the values of the function of the scattering angle of interacting molecules (3), which describes the deviation of the direction of their movement from the original, are determined. The expression for the function of the scattering angle contains an improper integral, the lower limit value of which is found from the solution of a nonlinear algebraic equation. Since the values of the scattering angle function are used in a combination of threefold improper integrals, the authors in [9, 10] carried out a qualitative analysis of its uniform convergence. It is shown that the values of the scattering angle function are determined on the set of real numbers \( R \) in the case of non-return trajectories of interacting molecules, and in the case of return paths - on the set of complex numbers \( C \). An equation of the surface is obtained, at the points of which a trajectory bifurcation occurs.

To determine the mean cross-section for interacting molecules (2), which is expressed by means of the second improper integral in the collisional part of the Boltzmann equation, effective quadrature formulas are proposed. Since this improper integral contains an oscillating integrand function depending on the parameter, it is recommended to use the Gauss - Christoffel quadrature modification to determine its values.

To calculate the values of the third improper integral, which is part of the collisional part of the Boltzmann equation, the molecular collision integral \( \Omega^{(l,r)} \) (1), the authors of this article proposed computational technologies based on Gauss - Christoffel cubages and the theory of splines [8]. These technologies allow obtaining an analytical form of the integrand in an improper integral and use quadrature formulas for its calculation.

2. Another section of your paper

The value of the integral \( \Omega^{(l)} \left( b^*, g^* \right) \) is one of the determining factors in the algorithm for computing the transfer characteristics of media. Consequently, the accuracy of the values of the transfer coefficients depends largely on the correctness of its calculation. In the kinetic theory of gases, the integral is used to describe the mean scattering cross-section of interacting molecules and has the form [7]:

\[
\Omega^{(l)} = \Omega^{(l)} \left( g^* \right) = 2\pi \int_{0}^{\infty} \left(1 - \cos \left( \chi \left( b^*, g^* \right) \right) \right) b^* db^* ,
\]

(4)

where \( g^{*2} \) is the reduced kinetic energy of relative motion, \( b^* \) is the reduced aim parameter (dimensionless). This improper integral contains an oscillating integrand function in which the value of the parameter characterizes the frequency of its oscillations.

To calculate the values of the mean cross-section for the scattering of interacting molecules (1), the Gauss - Christoffel quadrature based on orthogonal polynomials [11] is considered. One of the problems of constructing this quadrature is the definition of the splitting nodes of the integration segment and the
weight values of the quadrature in them, which are found from the condition of minimizing the quadrature error. It is important to note that the oscillatory nature of the integrand in (4) is taken into account by the Gauss - Christoffel quadrature since its algorithm is based on minimizing the quadrature error.

To determine the nodes and weights in the Gauss - Christoffel quadrature, it is proposed to use a system of algebraic equations

\[ \sum_{k=1}^{n} c_i x_k^\alpha = \int_{a}^{b} \rho(x)x^\alpha dx \quad (\alpha = 0, \ldots, m) \quad (5) \]

In system (5) \( n \) is the number of split nodes and \( m \) is the value of the highest order of the polynomial in question. To determine the weights \( c_i \) (\( i = 1, 2, \ldots, n \)) and split nodes \( x_i \) (\( i = 1, 2, \ldots, n \)), the system of algebraic equations (5) is split into two systems: linear and nonlinear. It is proposed to use a linear system of algebraic equations to determine the weights of the quadrature, and a non-linear system to determine the nodes of the integration segment. To determine the values of unknown weights \( c_i^{(0)} \) (\( i = 1, 2, \ldots, n \)) with known (specified) values \( x_i^{(0)} \) (\( i = 1, 2, \ldots, n \)), it is proposed to use SLAE (a system of linear algebraic equations), the solution of which is determined by the method associated with the construction of an interpolation polynomial, the roots of which are the unknown values. The existence and uniqueness of the solution of this system of equations are ensured by the fact that its matrix is the Vandermonde matrix.

To determine the values of nodes \( x_i \) (\( i = 1, 2, \ldots, n \)), it is proposed to use a nonlinear system of algebraic equations. We will analyze this system:

\[
\begin{align*}
    f_1(x_1, x_2, \ldots, x_n) &= c_1 x_1^\alpha + c_2 x_2^\alpha + \ldots + c_n x_n^\alpha - \int_{a}^{b} \rho(x)x^\alpha dx = 0, \\
    f_2(x_1, x_2, \ldots, x_n) &= c_1 x_1^{\alpha+1} + c_2 x_2^{\alpha+1} + \ldots + c_n x_n^{\alpha+1} - \int_{a}^{b} \rho(x)x^{\alpha+1} dx = 0, \\
    &\vdots \\
    f_n(x_1, x_2, \ldots, x_n) &= c_1 x_1^{2\alpha-1} + c_2 x_2^{2\alpha-1} + \ldots + c_n x_n^{2\alpha-1} - \int_{a}^{b} \rho(x)x^{2\alpha-1} dx = 0,
\end{align*}
\]

or in abbreviated form:

\[
\mathbf{F}(\mathbf{x}) = 0 \quad (7),
\]

where

\[
\mathbf{F} = (f_1, f_2, \ldots, f_n)^T, \quad \mathbf{x} = (x_1, x_2, \ldots, x_n)^T.
\]

To determine the values of nodes and weights in the Gauss - Christoffel quadrature, a method based on splitting the system of equations (6) into two is proposed: a linear system of algebraic equations for determining the values of weights \( c_i \) (\( i = 1, 2, \ldots, n \))
\[
\begin{align*}
\int_a^b c_1 + c_2 + \ldots + c_n &= \int_a^b \rho(x)dx, \\
\int_a^b c_1x_1 + c_2x_2 + \ldots + c_nx_n &= \int_a^b \rho(x)x dx, \\
\int_a^b c_1x_1^2 + c_2x_2^2 + \ldots + c_nx_n^2 &= \int_a^b \rho(x)x^2 dx, \\
&\vdots \\
\int_a^b c_1x_1^{n-1} + c_2x_2^{n-1} + \ldots + c_nx_n^{n-1} &= \int_a^b \rho(x)x^{n-1} dx,
\end{align*}
\]

and a nonlinear system for determining the location of split nodes on the integration segment

\[
\begin{align*}
\int_a^b c_1x_1^n + c_2x_2^n + \ldots + c_nx_n^n &= \int_a^b \rho(x)x^n dx, \\
\int_a^b c_1x_1^{n+1} + c_2x_2^{n+1} + \ldots + c_nx_n^{n+1} &= \int_a^b \rho(x)x^{n+1} dx, \\
&\vdots \\
\int_a^b c_1x_1^m + c_2x_2^m + \ldots + c_nx_n^m &= \int_a^b \rho(x)x^m dx.
\end{align*}
\]

The authors of the article proved a theorem on the convergence of solutions of split systems of algebraic equations to the solution of the original system (6).

Theorem. Suppose that in the ball \( S_r(x_0) \) operator \( F(x) \) (4) is differentiable and its derivative satisfies the Lipschitz condition with a constant \( l \) in it. Suppose that in \( S_r(x) \) the operator \( F(x) \) is continuously invertible and there is such a constant \( m > 0 \) that:

\[
\left\|F'(x)\right\| \leq m.
\]

Let it further be \( \left\|F'(x_0)\right\| \leq \eta \). Then, if \( q = \frac{1}{2} m^2 \eta < 1 \) \( r' = m\eta \sum_{j=0}^{\infty} q^{j+1} < r \) and, then the equation \( F(x) = 0 \) has a solution \( \bar{x} \in S_r(x_0) \), to which Newton’s iterative process converges. And \( x^{(k)} \) converges to \( \bar{x} \) with the speed \( \left\|x^{(k)} - \bar{x}\right\| \leq m\eta q^{2k-1} \).

The weight values \( c_i (i = 1, 2, \ldots, n) \) from the linear algebraic system of equations (8) were determined by the Gauss method. The node values \( x_i (i = 1, 2, \ldots, n) \) from the nonlinear system (9) were determined by the Newton iterative method, using the values found \( c_i (i = 1, 2, \ldots, n) \). After the condition for local iterations to determine the values \( x_i (i = 1, 2, \ldots, n) \) was fulfilled, global iterations were performed until the fulfillment of the condition

\[
\max_{1 \leq i \leq n} \left\{ \left| x_i^{(k+1)} - x_i^{(k)} \right|, \left| c_i^{(k+1)} - c_i^{(k)} \right| \right\} \leq \varepsilon \quad (k = 0, 1, \ldots)
\]
3. The results of numerical calculations of the mean cross-section of interacting molecules
The numerical algorithm proposed by the authors was tested using an example of a model integral with an oscillating integrand function, similar in appearance to \( Q^{(i)}(g^*) \):

\[
\int_0^1 f(x) \cos(\omega t) \, dt.
\]  

(10)

Calculation of the integral (10) for various values of \( \omega \) was performed using an algorithm that includes determining the values of nodes and weights of the Gauss - Christoffel quadrature and calculating the value of the integral having an oscillating integrand function. In this case, in the integral (4), the transformation \( b^* = x/(1-x) \) maps the semi-infinite integration domain \( b^* \in [0; \infty) \) into a segment \( x \in [0;1] \).

The values of transfer sections \( Q^{(i)}(g^*) \), calculated on the basis of the potential \((2(n+3),6)\), proposed by the authors in [12], were obtained for various values of the parameter \( n \). The calculations were performed on the basis of the proposed numerical algorithms in the Wolfram Mathematica package. Figure 1 shows the curves for several transfer sections.

![Figure 1. Transfer sections \( Q^{(i)}(g^*) \), calculated on the basis of the potential \((2(n+3),6)\), for different values of the parameter \( n \).](image)

The presented graphs have a satisfactory agreement with the curves for the transfer sections given in [7].

Conclusion
In determining the transfer characteristics of media, improper integrals with an oscillating integrand function are used. To determine their values correctly, it is necessary to use mathematically justified quadratures. To calculate integrals of this type, the authors used the Gauss - Christoffel quadrature. To determine the number of split nodes (their coordinates) and weights of this quadrature formula, the authors divided the original nonlinear system of equations into two systems: linear and nonlinear. A linear system of algebraic equations is used to determine the weights of the quadrature, and the nonlinear system is applied to determine the split nodes of the integration segment. A theorem on the global convergence of solutions of these systems to the solution of the original non-decomposed system of equations has been proved. Calculations were performed for a model integral with an oscillating integrand function, similar to the integrand function of the integral \( Q^{(i)}(g^*) \), as well as calculations of the transfer section itself. It has been reasonable concluded that the use of numerical algorithms based
on the Gauss - Christoffel quadrature formula allows calculating the values of both definite and improper integrals correctly from the molecular-kinetic theory with a complex form of continuous integrand functions, including the oscillating ones.

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