Angular Momentum Conservative Algorithm of Collisional Process in DSMC Method

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1 Introduction

The traditional algorithm of collisional process in DSMC method, used for calculation of velocities of molecules after collision, is based on the conservation laws for linear momentum and total energy \[1\]. This algorithm does not provide conservation of angular momentum with respect to some axis, but for non-rotating flow this circumstance is insignificant, since the mean value of angular momentum of such kind of flow is equal to zero.

The situation changes for axisymmetric flow with rotation. In this case the traditional procedure leads to some internal source or sink of angular momentum that may distort the flowfield.

In the paper the discussed effect is recognized and investigated. The angular momentum conservative (AMC) algorithm of collisional process is proposed. The draft version of the paper is published in \[2\].

2 Problem Formulation

The investigations were made for one-dimensional axisymmetric flow of monoatomic gas in the tube with specular wall. The evolution of initially swirling flow during the time was studied. The gas in the tube with uniform initial density \(n_0\) and temperature \(T_0\) and equilibrium distribution function was assumed to start rotating as a solid body, the initial tangential velocity on the wall being equal to \(v_\varphi\). For given molecular model the problem contains two governing parameters: the Knudsen number \(Kn\), defined by the ratio of the mean free path \(l_0\) in the gas at \(t = 0\) to the radius of the tube \(r_t\)

\[Kn = \frac{l_0}{r_t}\]

and the speed ratio

\[S_\varphi = \frac{v_\varphi}{\sqrt{2RT_0}}\]
The simulations were made on uniform grid with $10^4$ simulated molecules. Standard NTC DSMC procedure \[1\] was applied. The initial values of total mass $M_0$, angular momentum $I_0$ and energy $E_0$ of the gas may be defined by the relations

$$M_0 = m N_0 = m n_0 \pi r_1^2$$  \hspace{1cm} (1)

$$I_0 = m \sum_{i=1}^{N_0} v_i r_i$$ \hspace{1cm} (2)

$$E_0 = m \sum_{i=1}^{N_0} \frac{V_i^2}{2}$$ \hspace{1cm} (3)

where $N_0$ is the total number of simulated molecules, $m$ - the mass of molecule, $V$ - the velocity vector, $v$ - the tangential component of this vector. By the same relations may be determined the total energy $E$ and total angular momentum $I$ of the gas during the time.

For any values of $Kn$ and $S\phi$ there should be no temporal dependence of $E$ and $I$. The computations show that this condition is satisfied only for $E$.

Fig.1 illustrates the dependencies of $I/I_0$ on the time for some of considered variants for $S\phi = 1$. The time is normalized by the value of $t_0 = 2 \pi r t / \varphi$, so $t/t_0$ represents the number of revolutions of solid body with $v(r_t) = v_\varphi$.

As can be seen from Fig.1 for all of the variants the decreasing of $I/I_0$ with increasing of $t/t_0$ is observed. For given $Kn$ the effect is more pronounced for solid sphere molecules (SS) in comparison with VSS molecular model for Maxwell molecules (MM). The effect depends on the Knudsen number: the less $Kn$ the more the effect. But the highest sensitivity of the effect is observed to the grid size: changing the number $N$ of cells from 50 to 25 causes the same effect as the decrease of the Knudsen number approximately by 4 times.

Due to the dependence of $I(t)$ it is difficult to obtain the steady solution of the problem. The dissipation of rotational contribution of energy into the heat takes place during the time. The only steady solution that may be obtained with traditional collisional procedure is terminal one, when at $t \to \infty$ the gas will stop rotating, having uniform density $n_0$ and getting warm to the temperature

$$T = \frac{2 E_0}{3 R M_0}$$

3 AMC Algorithm

The reason of temporal dependence of total angular momentum is quite clear: the colliding molecules have different radial coordinates $r_1, r_2$, that
leads to the difference in angular momentum

$$m_1 v_1 r_1 + m_2 v_2 r_2$$

of these molecules before and after collision (v denotes the tangential component of velocity of the molecule). To provide the conservation of angular momentum the algorithm of collisional process should be changed. One possible variant of AMC algorithm is as follows.

Let us denote by $u$ the vector containing axial and radial components of the velocity of molecule. The post-collision velocities calculated by traditional procedure will be denoted by symbol $\ast$, while the symbol $'$ will be used for these velocities in the proposed algorithm.

The algorithm is based on conservation law of angular momentum $m v r$ for tangential component of velocity instead of linear momentum $m v$. That is why the post-collision tangential velocities are calculated by usual relations $\Pi$, with the value of $m_i$ being replaced by the product $m_i r_i$. The obtained velocities $v'_1$, $v'_2$ provide precise conservation of angular momentum, but violate the energy conservation. To provide energy conservation the correction of velocities $u'_1$ and $u'_2$ is needed. To do this correction the analysis of energy defects

$$dE_i = m_i (v'_i^2 - v_i\ast^2)$$
should be made. Three possible relations between energy defects \( dE_i \) and velocities \( u_i^* \) are as follows.

1. If
   \[ m_1 u_1^{*2} > dE_1 \]
   and
   \[ m_2 u_2^{*2} > dE_2 \]
   both components of vectors \( u_i^* \) should be corrected by the factors \( c_i \)
   \[ c_i = \sqrt{1 - \frac{dE_i}{m_i u_i^{*2}}} \]

2. If
   \[ m_1 u_1^{*2} + m_2 u_2^{*2} > dE_1 + dE_2 \]
   the correction factor \( c \) for components of both velocities \( u_i^* \) should be the same and equal to
   \[ c = \sqrt{1 - \frac{(dE_1 + dE_2)}{(m_1 u_1^{*2} + m_2 u_2^{*2})}} \]

3. If none of the above conditions is satisfied, the collision is considered to be "bad" and is not performed, i.e. the molecules conserve their pre-collision velocities.

The computations show that the relative number of collisions of types 1 and 2 is about 99% and 1%, respectively. The relative number of "bad" collisions never exceeds \( 10^{-4} \), so the effect caused by the neglecting of these collisions is small.

### 4 Steady Solution

The described algorithm provides precise conservation of angular momentum and energy. All the curves, presented in Fig.1, transform into straight line \( I/I_0 = 1 \), if this algorithm is applied.

AMC algorithm enables to obtain the steady solution of the considered problem. This solution proves to be the same, as the prediction of Navier-Stokes theory and has the following features.

1. The flow is isothermal
   \[ T = \text{const} \] (4)

2. The gas rotates as a solid body
   \[ v = v_w \frac{r}{r_t} \] (5)
3. The radial distribution of density is described by the relation
\[ n(r) = n(0) \exp \left( \frac{v^2}{2RT} \right) \] (6)

4. The solution is completely determined by the values of \( M_0, I_0, E_0 \) and does not depend on the way of initial swirling.

5. The solution does not depend either on the molecular model or on the Knudsen number.

These features of the considered flow are important for clarifying the nature of the Ranque effect \[9, 10\].

Three unknown values \( v_w, T, n(0) \) determining the radial distribution of parameters of steady solution may be defined based on the values of \( M_0, I_0 \) and \( E_0 \) from the relations
\[ \pi r_t^2 m n(0) \frac{\exp S_w^2 - 1}{S_w^2} = M_0 \] (7)
\[ M_0 v_w r_t \frac{\exp S_w^2 (S_w^2 - 1) + 1}{S_w^2 (\exp S_w^2 - 1)} = I_0 \] (8)
\[ \frac{3}{2} RT M_0 + \frac{v_w I_0}{2 r_t} = E_0 \] (9)

where speed ratio \( S_w \) of the flow at \( r = r_t \) is defined by
\[ S_w = \frac{v_w}{\sqrt{2RT}} \] (10)

The left hand sides of the relations 7 - 9 representing the total mass, angular momentum and energy of the flow may be obtained based on the relations 4 - 6 by simple integration.

The comparison between numerical and analytical radial distribution of parameters of steady flow for \( VSS \) molecules, \( Kn = 0.1, S_{\phi} = 1, N = 50 \) is made on Figs. 2 - 4 for density, tangential velocity and temperature, respectively. The numerical results are shown by solid circles while solid lines represent the results of analytical solution 7 - 9. As can be seen from these Figures, numerical and analytical results are in excellent agreement. For \( Kn = 10 \) the steady solution was found to be the same as for \( Kn = 0.1 \).

It should be noted that the steady flow in the considered problem is characterized by locally Maxwellian distribution function for any molecular models and \( Kn < \infty \).

AMC algorithm of collisional process may be applied for simulation of non-rotating flows too. The experience of such application to the flow in gasdynamic window [5] shows that the results obtained with proposed and traditional algorithms are the same within the expected statistical scatter.
To stay the effect of non-conservative nature of traditional collisional procedure in the real conditions, some test computations of considered flow were made by AMC algorithm for adiabatic tube wall with diffuse-specular scattering of molecules for different values of accommodation coefficient $\sigma$. Fig. 5 illustrates the dependencies of $I/I_0$ on the time for VSS molecules, $Kn = 0.1$, $S_\phi = 1$, $N = 50$ and 4 values of $\sigma$ in the range $\sigma = 2 \cdot 10^{-3} - 10^{-4}$. The comparison of these dependencies with those presented in Fig. 4 reveals that the traditional collisional procedure causes the same change in angular momentum as the diffuse-specular wall with the accommodation coefficient $\sigma$. 

Figure 2: Radial distribution of density

Figure 3: Radial distribution of tangential velocity
σ in the range $\sigma = 10^{-3} - 10^{-4}$. Therefore, for flows with real surface $(\sigma \sim 1)$ in the flowfield the studied effect is small, its relative value is about $10^{-3} - 10^{-4}$.

Figure 4: Radial distribution of temperature

Figure 5: Temporal dependence of total angular momentum
5 Conclusion

The proposed algorithm of collisional process provides precise conservation of angular momentum and energy and may be used for direct simulation of flows with rotation.

It should be noted, however, that the improvement of the results, obtained by this algorithm may be important only for the problems without external source or sink of angular momentum. If solid surface with diffuse reflection is present in the flowfield, the changes in angular momentum, caused by this surface will be much greater than those, caused by non-conservative nature of traditional algorithm of collisional process. For such kind of flows there is no need to employ AMC algorithm, especially taking into account that it takes 10% – 15% more CPU time.

Nevertheless, for some problems the application of AMC algorithm is advisable. An example of such kind of problem is the Ranque effect [3], which nature is determined by conservation of angular momentum of the gas flow in the vortex tube [4].

References

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