Numerical Study of a Gas Flow Inside a Rotating Cylinder Using the Consistent Boltzmann Algorithm

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Abstract: A gas flow inside a high speed rotating cylinder has been studied numerically using the Consistent Boltzmann Algorithm (CBA) as well as the direct simulation Monte-Carlo (DSMC) method. In the CBA and DSMC simulations of axially symmetric flow, hard sphere (HS) and variable hard sphere (VHS) collision models are applied, respectively. The gas flow inside the cylinder can be divided into two parts. The first small part is close to the center of the cylinder which is moderately rarefied and the second major part of the cylinder is dense, especially close to the rotational wall of the cylinder. Since the DSMC method is restricted to dilute gases, the comparison of the results of the DSMC method with the analytical solutions shows discrepancies. The CBA can be used at all densities, therefore it is necessary to apply CBA for simulation of the gas flow. The results of the flow simulation using the CBA such as number density, temperature and swirl velocity are compared both with the results of the DSMC method and the analytical solutions. The results of the flow simulation using the CBA show better agreement than the results of the DSMC method in comparison with the analytical solutions.

Key words: Direct simulation Monte-Carlo method • Consistent Boltzmann Algorithm • Rotating cylinder • Boltzmann equation

INTRODUCTION

In gas dynamics, the Knudsen number (Kn) is defined as the ratio of the molecular mean free path (λ) to the characteristic length of the flow (l) which is described, [1]:

\[ Kn = \frac{\lambda}{l} \] (1)

The Knudsen number is a measure of the rarefaction of the flow. When the Kn number is greater than 0.1, the continuum assumption begins to break down and the Navier-Stokes equations are no longer valid. The mathematical model at the molecular level is the Boltzmann equation and in this case the simulation is usually done using the DSMC method. The DSMC method has been utilized for the simulation of aerospace flows (external flows around bodies) [2], gas flow in the turbomolecular pump [3], shock waves [4] and micro-electro-mechanical systems (MEMS) such as micro- and nanochannels [5-7].

Many researchers have investigated the gas flow between two rotating cylinders (Couette-Taylor flow) [8], while few researchers have simulated the gas flow inside the rotating cylinder. The DSMC simulation of a rotating cylinder in a vacuum casing has been carried out by Roblin and Doneddu [9]. They determined the mechanical power of the rotating cylinder and the heat flux dissipated on the two cylinders. The formation of different kinds of the flow patterns in the range of various values of the cylinder aspect ratio (length/diameter) was investigated by Pourmahmoud [10]. He investigated the effect of this parameter on the flow field characteristics such as the density field and velocity profiles. Garjajei and Nourazar [11] applied the time relaxed Monte-Carlo (TRMC) scheme and the DSMC method in order to simulate the gas flow inside the rotating cylinder. The DSMC method was designed for the modeling of dilute and low density gases. Since the collision rate and transport properties are function of the molecular cross section, the Boltzmann equation and the DSMC method are inconsistent.

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Therefore, many numerical methods have been proposed to solve this problem. Alexander et al. [12,13] introduced a Consistent Boltzmann Algorithm (CBA), which allows the simulation of a hard sphere (HS) gas at all densities. They modified the DSMC method by adding a random displacement in the advection process which leads to consistent flow field characteristics in the low density regimes. The nonideal gas flow and heat transfer in microchannels have been studied using the CBA and the modified DSMC method by Wnag and Li [14]. Since the characteristic length of microchannel is so small, the gas is dense and the nonideal gas effects should be considered.

To our knowledge, none of the researchers in this field so far tried to use the CBA for the simulation of the gas flow inside the rotating cylinder. In the present study, the gas flow inside the rotating cylinder is studied using both the DSMC method and the CBA. The working fluid is Argon and the flow field characteristics such as temperature, number density and velocity are investigated. Special attention is focused on the comparison between the DSMC and CBA results with the analytical solutions. The simulation is carried out for 500000 iterations which is equal to 12.5 seconds of real times.

Mathematical Formulation

Problem Statement: In order to simulate the gas flow inside the rotating cylinder, two numerical methods are used. The axially symmetric DSMC and CBA codes with VHS and HS collision models are applied, respectively. The radius and length of the cylinder are 0.04 m and 0.2 m, respectively. The cylinder rotates with angular velocity of 15000 Rad/sec. The working gas inside the cylinder is Argon with VHS reference molecular diameter of (at 273 K) $4.17 \times 10^{-10}$ m, HS molecular diameter of $3.659 \times 10^{-10}$ m and molecular mass of $66.3 \times 10^{-27}$ Kg. The initial temperature and initial pressure of the gas are 300 K and 2.76 Pa, respectively. The time step of simulation is chosen to be $0.5 \times 10^{-6}$ seconds that is small in comparison with the mean collision time. The sensitivity of computational domain with respect to cells and sub-cells number is checked. Finally the domain is divided into $300 \times 60$ cells and each cell is sub-divided into $10 \times 10$ sub-cells. Also proper boundary conditions for computational domain, as shown in Fig. 1, are taken into account. The rule of diffuse reflection is applied for the top and bottom ends of the cylinder and the rotational wall. The temperature of the top and bottom ends of the cylinder and the rotational wall are considered to be constant and equal to 300 K. The cell size is about 1/3-1/4 times mean free path in order to ignore the change in the flow properties across each cell. After every 5 and 50 simulated time steps, the sampling of flow properties and the averaging of sampled values are performed, respectively. The number of modeled molecules is 50000.

The time of each iteration is equal to $2.5 \times 10^{-5}$ seconds of real time. The calculations are performed up to 500000 iterations which takes about 400 hours (12.5 seconds of real times) by an PC with 2.93 GHz CPU I3 530 and 2 GB RAM.

![Fig. 1: Computational domain and boundary conditions.](image-url)
Governing Equations: The governing equation describing the gas flow inside the rotating cylinder is the Boltzmann equation which is written for a simple and single component dilute gas as, [15]:

\[ \frac{\partial f}{\partial t} + c \frac{\partial f}{\partial r} + v \frac{\partial f}{\partial c} - \int_{0}^{2\pi} \int_{r}^{r'} (f' - f) v_c \sigma d\Omega dk \]  \hspace{1cm} (2)

Where, \( F \) is the external force per unit mass, \( f(r,c,t) \) is the velocity distribution function of the molecules of class \( c \) (with the velocity of \( c \)), \( f'(r,c',t) \) is the velocity distribution function of the molecules of class \( c \), \( f'(r,c',t) \) is the post-collision velocity distribution function of the molecules of class \( c \), \( f'(r,c,t) \) is the post-collision velocity distribution function of the molecules of class \( c' \), \( \Omega \) is the solid angle, \( \sigma \) is the collision cross section, \( r \) is the position vector, \( c \) is the velocity vector, and \( c \) is the relative velocity between two molecules of class \( c \) and \( c' \).

Analytical Solutions: A rotating cylinder with the angular velocity \( \omega \) about its axis, length \( L \) and radius \( R \) as a mathematical model is considered. A gas is supposed to be contained inside the cylinder consists of \( N \) molecules with the molecular mass of \( m \) and the temperature of \( T \). Two assumptions should be considered to find the number density \( n \) of the gas as a function of radial distance \( r \) \cite{16}: 1-The effect of gravity is neglected. 2-The cylinder rotates for a long enough time in order to reach equilibrium in the flow field. The energy of a gas particle inside the rotational cylinder is written as:

\[ E(r) = \frac{1}{2} m \omega^2 = \frac{1}{2} m r^2 \omega^2 \]  \hspace{1cm} (3)

The effect of rotation is the same of additional external field acting on the system can be expressed as:

\[ U(r) = -\frac{1}{2} mr^2 \omega^2 \]  \hspace{1cm} (4)

The Boltzmann distribution is used in order to get number density. By substituting for \( U(r) \) from Eq. 4, the number density is expressed as:

\[ n(r) = A \exp \left[ \frac{U(r)}{kT} \right] = A \exp \left[ \frac{mr^2 \omega^2}{2kT} \right] \]  \hspace{1cm} (5)

Where, \( k \) is the Boltzmann constant. The normalization factor \( A \) can be determined by \( N = \int n(r) dV \), giving:

\[ A = \frac{N m \omega^2}{2 \pi k T L} \exp \left( \frac{m \omega^2 R^2}{2 kT} \right)^{-1} \]  \hspace{1cm} (6)

Numerical Methods

The DSMC Method: The Direct Simulation Monte-Carlo (DSMC) method was introduced by Bird [1] is a numerical method for the modeling of rarefied gas flows. In this method the molecular motion and intermolecular collision are decoupled over the time step that is smaller than the mean collision time. A large number of simulated molecules with a position, a velocity and internal energy are used to simulate the real gas. This number is smaller than the number of real molecules. So each simulated molecule represents a large amount of real molecules. The computational domain is divided into cells and sub-cells. Two conditions should be considered in DSMC method: first, the time step over which the molecular motion and collisions are decoupled should be small enough in comparison with the mean collision time. Second, the cell size should be small in comparison with both the gradient length scale of the macroscopic quantities of the flow field and the local mean free path. In the DSMC method all computation are unsteady and after a long enough time the steady flow is achieved. The No Time Counter (NTC) method introduced by Bird [1] is used to determine the intermolecular collision in a cell.

CBA: The Consistent Boltzmann Algorithm (CBA) was introduced by Alexander et al. \cite{12,13} is an extension of the DSMC method for dense gases while the DSMC method was designed for the modeling of dilute gases. In the DSMC method, molecular velocities are changed by intermolecular collision during the collision process, while the molecular positions are not changed. They are only changed in the movement process. In order to change the DSMC method with VHS model to the CBA with HS model, two assumptions are necessary: First, after the intermolecular collision each molecule displaces a distance equal to the molecular diameter. The displacement vector \( \delta_{s} \) is equal to:

\[ \delta_{s} = \epsilon \hat{D} \]  \hspace{1cm} (7)

Where, \( \epsilon \) is the diameter of hard sphere molecule and \( \hat{D} \) is the unit vector parallel to the connecting line centers at impact calculated from the pre-and post-collision velocities:

\[ \hat{D} = \frac{(c'_1 - c'_2) - (c_1 - c_2)}{\|c'_1 - c'_2\| - \|c_1 - c_2\|} = \frac{c'_1 - c'_2}{c'_1 - c'_2} \]  \hspace{1cm} (8)
Where, \( c_r \) and \( c_v \) are the pre and post-collision relative velocity of the colliding molecules. After the collision, the molecules are advected as:

\[
\begin{align*}
\eta_1(t + \Delta t) &= \eta_1(t) + c_v(t) \Delta t + d_{sel} \\
\eta_2(t + \Delta t) &= \eta_2(t) + c_v(t) \Delta t - d_{sel}
\end{align*}
\]  
(9)

In fact, the colliding molecules are displaced a distance \( e \), one in the direction of \( D \) and the other in the direction of \(-D\). This advection displacement models the attractive force. Second assumption is the dense hard sphere collision frequency which is used to correct the low density collision rate. It is defined as:

\[
\Gamma_{hs} = Y(n) \Gamma_B
\]  
(10)

Where, \( Y(n) \) is the Enersg factor, \( \Gamma_B \) is the Boltzmann (dilute gas) collision rate and \( \Gamma_{hs} \) is the hard sphere collision rate.

**RESULTS AND DISCUSSION**

**Verifying the Validity and Accuracy of the CBA:**
To verify the accuracy and validity of the CBA code, our CBA calculations for the number density are compared with the results of DSMC method and the analytical solution. Fig. 2(a) shows the variation of the number density versus the radial distance for the CBA (500000 iterations), the DSMC method (500000 iterations) and the analytical solution. The analytical solution is obtained by using the Eq. 5. It should be mentioned that the analytical solution is based on the equilibrium assumption, while our simulation is not in the state of complete equilibrium. Therefore, it is assumed that our simulation results reached the equilibrium condition as well and the analytical solution is used as a reference to judge the accuracy of the CBA. Due to the rotation of the cylinder, when the radial distance increases to the radius of 0.03m, the number density increases gradually. But after the radius of 0.03m, the number density increases swiftly until it reaches its maximum value at the radius of 0.04m. This means that the number of molecules and intermolecular collision rate near the rotational wall are much higher than those in the center of cylinder. As it is clear from the Fig. 2(a), the comparison of the results of CBA with the analytical solution indicates a better agreement than the DSMC method. At the lower radii, the results of DSMC method are approximately in good agreement with the CBA due to lack of sufficient molecules near the center of cylinder but with the increase in number of molecules at high radii (increase in simulation accuracy), there is a discrepancy between their results. The comparison between the DSMC results and the analytical solution near the rotational wall shows higher discrepancy than the CBA. In comparison to the center of cylinder, the gas flow near the rotational wall is dense, thus the CBA has higher accuracy than the results of DSMC method. Fig. 2(b) represents the time evolution of...
the variation of gas number density along the radial coordinate using the CBA for various iterations (10000-500000 iterations, 0.25-12.5 seconds of real time). It is obvious from Fig. 2(b), when the number of iterations (time of calculation) increases, the values of number density near the center of cylinder decrease and the computed numerical values of this parameter are in acceptable agreement with the analytical solution. Finally, it can be predicted that at higher iterations (more than 1000000 iterations) the steady state is obtained and the CBA simulation will become identical to analytical solution.

**Temperature:** Other important parameter investigated is the temperature written as:

$$T = \frac{(3\nu + \zeta T_{in})}{(3 + \zeta)}$$  \hspace{1cm} (11)

Where, $T_{v}$ is the translational kinetic temperature, $T_{in}$ is the internal temperature and $\zeta$ is the number of internal degrees of freedom. The internal energy consists of vibrational and rotational energies. Since Argon is a monatomic gas, it has only the translational energy and the translational temperature can be assumed as temperature (overall temperature). Fig. 3(a) shows the time evolution of the variation of gas temperature along the radial coordinate using the CBA for different iterations (10000-500000 iterations, 0.25-12.5 seconds of real time). According to Fig. 3(a) and temperature boundary condition of 300 K, the value of temperature is about 300 K at first. With the increase in radius, the temperature increase until it reaches its maximum at the radius of 0.028 m and then decreases nearly to the value of 300 K at the rotational wall. As mentioned in section 3.1, the number of molecules and number density increase near the rotational wall and consequently the intermolecular collision and the molecular collision with moving surface increase. During the rotation, the momentum transfer occurred from the rotational wall to the cylinder. After the collision of molecules with the rotational wall, the molecules reflect with the higher velocity and thus higher translational energy in comparison with those before the collision with surfaces. Consequently, the reflected molecules diffuse extra energy into flow field of the cylinder. It leads to increase in the gas temperature near the rotational wall. On the other hand, there is a net heat transfer to the surface due to the high rotational speed of the cylinder. It is equal to the work which is done against the shear stress by the rotation of the cylinder. After a long enough time the gas reaches steady state and the fluctuations decrease. Since the momentum transfer is the only energy which is transferred from the rotational wall to the gas, it is predicted that the temperature of gas tends to the boundary temperature (300 K) in the entire flow field and its peak disappears for the high iterations numbers. Fig. 3(b) illustrates the comparison of the results of DSMC method with the results of CBA (500000 iterations). The comparison indicates that temperature results of CBA are in better agreement with the steady state condition (300 K) than the results of DSMC method.
Fig. 4(a): Time evolution of the variations of swirl velocity using the CBA along the radial coordinate from 10000 up to 500000 iterations.

Fig. 4(b): Comparison between the swirl velocity results of simulation using the DSMC method and CBA.

The evaluated temperature peak of CBA is 319 K, while it is 321 K for the DSMC results. The computed values of temperature for the DSMC method at the center of cylinder (r = 0 m) and rotational wall (r = 0.04 m) are 293 and 305 K, respectively, while, for the CBA results are 296 K and 302 K, respectively. Therefore, the CBA results reach steady state sooner than the DSMC results.

Swirl Velocity: Fig. 4(a) depicts the time evolution of the variation of swirl velocity along the radial coordinate using the CBA for various iterations (10000-500000 iterations, 0.25-12.5 seconds of real time). As seen from the Fig 4(a), by increasing the iteration (time), the results tend to increase linearly with the radius and reach steady state that is the swirl velocity of rigid body rotation (\( w = r\omega \)). \( w \) is the swirl velocity, \( r \) is the radial distance and \( \omega \) is the angular velocity. For the low iterations, from the center of cylinder to the radius of 0.02 m, the swirl velocity doesn’t vary linearly with the radial distance due to the lack of sufficient molecules near the center of cylinder. As shown in Fig. 4(b), a comparison between the swirl velocity of CBA and DSMC method (500000 iterations) is performed. From Fig. 4(b), the computed values of CBA reach steady state sooner than the results of DSMC method for the same iteration.
Fig. 6(a): Constant density contours using the CBA (500000 Iterations).

Fig. 6(b): Constant density contours at the left-hand side of the cylinder using the CBA (500000 Iterations).

Fig. 6(c): Constant density contours at the left-hand side of the cylinder using the DSMC method (500000 Iterations).

Streamlines, Constant Density Contours and Constant Temperature Contours: Fig. 5(a) shows the temperature contours using the CBA (500000 iterations). It is obvious from this figure that the contours are symmetric. Figs. 5(b),(c) show a comparison between the results of temperature using the CBA and DSMC method (500000 iterations), respectively. Fig. 6(a) illustrates the density contours using the CBA representing concentric horizontal cylinders with different radii. A Comparison between the density contours using the CBA and DSMC method (500000 iterations) is displayed in Figs. 6(b),(c), respectively. These comparisons show that the density and temperature contours of CBA have less fluctuation than the DSMC contours. The CBA contours are smoother than the DSMC contours and it indicates the high accuracy of density and temperature results using the CBA. Figs. 7(a),(b) show the velocity vectors in a left-hand side of the cylinder using the CBA and DSMC method (500000 iterations), respectively. Because of the vacuum boundary condition for the top and bottom ends of cylinder, two symmetric vortices of approximately equal size (double-vortex flow) are formed. As the figures indicate, the vortex flow which is formed by the velocity vectors using the CBA has less fluctuation in comparison with the vortex flow in the DSMC method. It can be found from Figs. 7(a),(b) that the vortex flow in the CBA is formed sooner than the ones in the DSMC method. Figs. 8(a),(b) show streamlines in the right-hand side of cylinder using the CBA and DSMC method (500000 iterations), respectively.
CONCLUSIONS

In this paper, the gas flow inside the rotating cylinder is studied numerically. The DSMC method and CBA with the HS and VHS collision models, respectively, are applied to simulate the gas flow inside the cylinder. Since the small part of the flow field inside the rotating cylinder is moderately rarefied, it can be predicted that the CBA is more accurate and efficient than the DSMC method for the gas flow simulation. This is due to the facts that, the CBA is a modification of the DSMC method for dense gases with two additions. First, an extra displacement after the intermolecular collision is applied and second, the low density collision rate is replaced by the dense hard sphere collision rate. The flow field characteristics such as number density, temperature and swirl velocity are obtained using the DSMC method and CBA. For all simulation results, the CBA reaches steady state solution sooner than the DSMC method. In comparison with the analytical and steady state solutions, the CBA results show better agreement than the DSMC results.

REFERENCES

