Laminar Hypersonic Separated Flows Modeled With the DSMC Method

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Abstract. The computations of a near-continuum flow with separation were performed using the DSMC method for a hollow cylinder flare configuration with the Reynolds number of 15,000 and 26,000. An efficient spatial correlator is developed for the DSMC method to estimate an impact of the statistical dependence between molecules on simulation results. Good agreement between the numerical results and available experimental data is obtained for the least dense case, where the DSMC requirements for cell size and the number of molecules are satisfied. For more dense cases, even 80 million molecules and 20 million cells do not satisfy the DSMC requirements, resulting in the underprediction of the separation zone size.

INTRODUCTION

One of the most challenging problems of hypersonic computational aerodynamics is the accurate prediction of laminar flow separation in the near-continuum regime. Numerical solution of this problem for hypersonic laminar flows is traditionally performed using the Navier-Stokes (NS) equations, and the initial effects of rarefaction for low Reynolds numbers are taken into account with the velocity slip and temperature jump boundary conditions. However, for modeling the flow near the leading edge of a slender body, the use of the NS equations even with these boundary conditions is questionable. This is because the rarefaction effects are significant due to the merging of the shock wave and the viscous layer; and the flow physics is complicated when there is the flow separation. To reliably predict hypersonic laminar flows, one should respect the area of applicability of the continuum approach, which depends not only on the free-stream parameters, but also on the body geometry.

To improve understanding of laminar separated flows, experimental and computational studies have been actively promoted by the NATO Research Technology Organization for two axisymmetric configurations, a hollow cylinder flare and a double cone. Those axisymmetric configurations allow one to avoid three-dimensional effects inherent in the flow near a compression ramp. Significant contributions have been made in the modeling of these configurations using both the kinetic (the direct simulation Monte Carlo method, DSMC) and the continuum (NS) approaches [1, 2, 3, 4, 5].

The main goal of this work is to study the applicability of the DSMC method to compute the near-continuum laminar flows with separation over a hollow cylinder with a flare. A special attention has been paid to the analysis of the impact of the statistical dependence between simulated particles and the cell size, and also to the detailed comparison of the obtained DSMC results with the experimental data.

FLOW CONDITIONS AND NUMERICAL METHOD

The free stream conditions used in this work are those observed in the experiment [6] for Runs 9 and 11, and are listed in Table 1. A small difference from Ref. [6] are the conditions for Run 11, for which the corrected data were obtained from Ref. [7]. The geometric parameters for the hollow cylinder flare model are shown in Fig. 1.

A DSMC-based computational tool SMILE [8] is used to calculate the axisymmetric flow about the hollow cylinder flare and double cone configurations. The following DSMC models are used in the computations. The variable hard sphere (VHS) model [9] is used for molecular collisions, with a molecular nitrogen diameter of 4.17Å and the exponent in the viscosity-temperature dependence taken from Ref. [10], of 0.74. The continuous Larsen-Borgnakke model [11] with temperature-dependent rotational relaxation number is used for the energy exchange between translational and...
rotational molecular modes. The Maxwell model with the full energy and momentum accommodation is utilized to simulate the gas-surface interactions. The DSMC computations were performed using 64 processors IBM SP/RS6000 POWER3 computer, and the average parallelization efficiency was 90%.

STATISTICAL ACCURACY OF THE DSMC METHOD

The DSMC method is an accurate statistical approach for solving the spatially nonuniform master Leontovich equation for the N-particle distribution function \( f_N \) [12]. The master kinetic equation for a one-species gas consisting of unstructured molecules may be written as

\[
\frac{\partial f_N(t, \vec{C})}{\partial t} + v_i \frac{\partial f_N(t, \vec{C})}{\partial x_i} = \frac{n}{N} \sum_{i<j} \int_0^\infty b_{ij} \times (\bar{\vec{v}}_i - \bar{\vec{v}}_j) \left\{ f_N(t, \vec{C}') - f_N(t, \vec{C}) \right\} de_{ij} db_{ij},
\]

where \( \vec{C} = (\bar{v}_1, \ldots, \bar{v}_N) \) is 3N-dimensional vector of particle velocities; \( \vec{C}_{ij} = (\bar{v}_1, \ldots, \bar{v}_i', \ldots, \bar{v}_j', \ldots, \bar{v}_N) \); \( b_{ij} \) and \( e_{ij} \) are the impact parameters of \( i \) and \( j \) collision partners; \( (\bar{v}_i, \bar{v}_j) \) and \( (\bar{v}_i', \bar{v}_j') \) are pre- and post-collisional velocities of \( i, j \) molecules, \( n \) is the number density.

The main equation of kinetic theory of gases is the Boltzmann equation which is a nonlinear integral-differential equation closed with respect to a one-particle distribution function \( f(t, \bar{x}, \bar{v}) \). In the simplest case of a monoatomic gas it determines the numerical density of particles in a six-dimensional phase space \( (\bar{x}, \bar{v}) \) of particle coordinates and velocities. It can be written as

\[
\frac{\partial f}{\partial t} + v_i \frac{\partial f}{\partial x_i} = \int (f(t, \bar{x}, \bar{v}) \cdot f(t, \bar{x}, \bar{v}_1') - f(t, \bar{x}, \bar{v}') \cdot f(t, \bar{x}, \bar{v}_1))|\bar{v} - \bar{v}_1| b\, db\, d\bar{v}_1.
\]

Here, after-collision quantities are primed.

Since the Boltzmann equation may be derived [13] from the master kinetic equation for an N-particle system under the conditions of molecular chaos, the DSMC method may be regarded as a statistical method for solving the Boltzmann equation. The molecular chaos hypothesis is strictly valid only for an infinite number of particles and a finite number of particles introduces correlations. Therefore, a significant level of correlations (statistical dependence) may cause the DSMC solution to be different from the solution of the Boltzmann equation.
The molecular chaos hypothesis may be written in terms of one- and two-particle distribution functions, \( f_1 \) and \( f_2 \), as
\[
f_2(v_A, v_B) = f_1(v_A)f_1(v_B),
\]
where \( v_A \) and \( v_B \) are the velocities of the two collision partners, \( A \) and \( B \).

For some function of velocity, \( x \equiv x(v) \), we can write
\[
\int_{-\infty}^{+\infty} f_2(v_A, v_B)x(v_A)x(v_B)dv_Adv_B =
\]
\[
= \int_{-\infty}^{+\infty} f_1(v_A)f_1(v_B)x(v_A)x(v_B)dv_Adv_B =
\]
\[
= \int_{-\infty}^{+\infty} f_1(v_A)x(v_A)dv_A\int_{-\infty}^{+\infty} f_1(v_B)x(v_B)dv_B
\]
This expression may be rewritten as
\[
\langle x(v_A)x(v_B) \rangle = \langle x(v_A) \rangle \langle x(v_B) \rangle
\]
where \( \langle \cdot \rangle \) denotes averaging. This expression can further rewritten as
\[
\frac{\langle x(v_A)x(v_B) \rangle}{\langle x(v_A) \rangle \langle x(v_B) \rangle} - 1 = 0
\]
(1)

As was mentioned above, the molecular chaos hypothesis is not strictly valid for a finite number of particles, which means the left side of Eq. (1) is not equal to zero.

Let us introduce the following correlator \( G_2 \),
\[
G_2 = \frac{\langle x(v_A)x(v_B) \rangle}{\langle x(v_A) \rangle \langle x(v_B) \rangle} - 1
\]
(2)
The value of this correlator may serve as an indicator of the presence of molecular correlations, the smaller the correlations, the closer \( G_2 \) is to 0.

The value of \( G_2 \) may be directly calculated in the DSMC method for each cell in the computational domain. However, such a direct use of \( G_2 \) in a DSMC code would imply a computational time proportional to \( N^2 \), where \( N \) is the number of particles in a cell. Let us transform Eq. (2) to have a computation time proportional to \( N \).

\[
\langle x(v_i)x(v_j) \rangle = \frac{1}{L} \sum_{l=1}^{L} \frac{2}{N_l(N_l-1)} \sum_{i=1}^{N_l} \sum_{j=i+1}^{N_l} x(v_i)x(v_j)
\]
\[
\langle x(v_i) \rangle = \frac{1}{L} \sum_{l=1}^{L} \frac{1}{N_l} \sum_{i=1}^{N_l} x(v_i)
\]

Here, \( l \) is the summation over time steps, \( L \) is the number of time steps, \( N_l \) is the number of molecules in a cell, and \( i \) and \( j \) are the indices of molecules in a cell. Let us denote \( x(v_i) \equiv x_i, x(v_j) \equiv x_j \),
\[
G_2 = \frac{\langle x_ix_j \rangle}{\langle x_i \rangle \langle x_j \rangle} - 1 = \frac{\langle x_ix_j \rangle - \langle x_i \rangle \langle x_j \rangle}{\langle x_i \rangle \langle x_j \rangle} =
\]
\[
= \frac{\frac{1}{L} \sum_{l=1}^{L} \frac{2}{N_l(N_l-1)} \sum_{i=1}^{N_l} \sum_{j=i+1}^{N_l} x_ix_j - \left( \frac{1}{L} \sum_{l=1}^{L} \frac{1}{N_l} \sum_{i=1}^{N_l} x_i \right)^2}{\left( \frac{1}{L} \sum_{l=1}^{L} \frac{1}{N_l} \sum_{i=1}^{N_l} x_i \right)^2}
\]
\[
= \frac{\frac{1}{L} \sum_{l=1}^{L} \frac{1}{N_l(N_l-1)} \left( \sum_{i=1}^{N_l} x_i \right)^2 - \sum_{i=1}^{N_l} \left( \frac{1}{N_l} \sum_{i=1}^{N_l} x_i \right)^2}{\left( \frac{1}{L} \sum_{l=1}^{L} \frac{1}{N_l} \sum_{i=1}^{N_l} x_i \right)^2}
\]

The computation time necessary to calculate \( G_2 \) using the above expression is linearly proportional to the number of particles, and therefore only slightly increases total CPU time. \( G_2 \) was calculated at steady state over background cells, and the square of the velocity in the \( X \) direction was used.
FIGURE 2. Pressure coefficient (left), skin friction coefficient (center) and Stanton number (right) for different grids. Run 11.

**COMPUTATIONAL RESULTS**

**Hollow cylinder flare, Run 11 conditions**

The modeling of flows with separation in a near-continuum regime is challenging for the DSMC method. In this section the DSMC results obtained for the lowest Reynolds number conditions (Run 11) considered in [6] are presented.

The calculations were performed for three different collision grids. Linear cell size was adapted to the local mean free path during the computation using the constraint that the number of simulated particles in a cell should not to be less than 4. Therefore, the number of cells and their sizes depend on total number of molecules.

The coarse grid has about 1.2 million cells, and the linear cell size is larger than the local mean free path. The intermediate grid has about 5 million cells, and the linear cell size is close to the local mean free path. The fine grid has the cell size in both Cartesian directions smaller than the local mean free path, and the total number of cells is more than 10 million (see details in [14]).

The distributed pressure coefficient along the surface is shown in Fig. 2 (left) for the three different grids. Generally, the grid refinement leads to an increase of the pressure maximum on the are, and an earlier pressure rise on the cylinder part associated with the separation region. There is no noticeable impact of the grid on the cylinder upstream of the separation region and on the are downstream of the shock interaction region. The results for the fine and intermediate grids almost coincide. A cell size the same or slightly smaller than the local mean free path is therefore sufficient for this case to obtain the grid converged results.

Comparison of the skin friction distribution presented in Fig. 2 (center) for different grids show that there is a significant impact of the cell size on the skin friction coefficient inside the separation region and near the shock interaction region. The coarser grid overpredicts the $C_f$ values and visibly underpredicts the size of the separation region. There is no impact of the grid on the second half of the are ($X/L > 1.6$). The impact of the grid on the Stanton number distribution is shown in Fig. 2 (right), and is generally similar to the grid influence on $C_f$.

Comparison of the DSMC results with the available experimental data [6] for pressure and Stanton number surface distributions are also given in Fig. 2. There is a good agreement observed between the DSMC (fine and intermediate grids) and experimental results for the $C_p$ distribution. The size of the separation region estimated based on the pressure distribution is accurately captured by the DSMC method. The agreement of the Stanton number distribution is somewhat worse, especially on the last portion of the are.

In this case, the DSMC applicability conditions (cell size, time step, and the total number of molecules) were satisfied, enabling us to obtain the results that are in good agreement with the numerical and experimental data, and thus prove the applicability of the DSMC method to model this flow.
Hollow cylinder flare, Run 9 conditions

The flow for Run 9 is more dense and the Reynolds number is higher by a factor of 1.67 than for Run 11. The local mean free path is therefore on average less by a factor of 1.67. The total number of cells and molecules should therefore be at least 1.67^2=2.78 times larger. The computations for Run 9 have been performed for different total numbers of molecules ranging from 2.5 million to 80 million. The average number of molecules in a collision cell was equal to 4 in all computations. Both parameters are important for obtaining accurate results. The cell size is critical for resolution of large gradients inside the shock waves and in the very thin boundary layer, and the number of particles should be large enough to avoid any significant impact of statistical dependence between them.

The impact of the number of molecules and cells on the distributed pressure, friction, and heat transfer coefficients is given in Fig. 3. Several conclusions may be drawn based on these results. The separation zone increases with the number of particles both upstream and downstream. The positions of the maxima of pressure, friction, and heat transfer coefficients on the flare shifts downstream slightly. In fact, the locations of the maxima essentially do not change for more than 10 million molecules. The magnitude of the pressure maximum increases, and the values of friction and heat transfer maxima decreases for larger number of molecules. The pressure values downstream from the separation zone are not affected by the change in the number of molecules, while the skin friction and heat transfer coefficients decrease on the second half of the flare for large numbers of molecules.

It should be noted that even with the use of 80 million particles the results are not converged in terms of the number of molecules, and the distributed parameters are expected to change if a larger number of molecules is used. In order to understand the impact of statistical dependence between simulated molecules, the spatial distribution of G_2 correlator was calculated. The G_2 field is shown in Fig. 4 for the maximum number of molecules used. It may be seen that the statistical dependence increases around the separation zone and on the flare downstream from the shock interaction region. Inaccuracies may therefore be expected in these regions due to particle correlations.

The results may also change for a larger number of cells. The DSMC requirement for the collision cell size (linear cell size smaller than one third of the local mean free path) is not strictly satisfied even when 20 million cells are used. The field of the ratio of the mean free path to the cell size in the X direction is given in Fig. 5. The cell size is less than two times smaller than the local mean free path for the entire region between the flare generated shock wave and the cylinder surface. In the separation region and near the flow reattachment point, the linear cell size is also about two times smaller, which may not be sufficient for the accurate resolution of flow gradients in the vicinity of the separation point.

The structure of the separation zone is shown in Fig. 6 where the Mach number field and the streamline contours inside the separation region are presented. Similar to the calculations presented in [3], a counter-rotating vortex was not observed in the vicinity of the corner point.

Comparison of the computed and measured pressure and heat transfer coefficients is presented in Fig. 7. In addition to the present DSMC results for 80 million molecules, the DSMC [1] and NS [3] solutions are given. The present size of the separation region is smaller than that observed in the experiment, but larger than computed by [1]. The pressure maximum on the flare is slightly smaller than those observed in the experiment and continuum modeling. The pressure values downstream from the separation region agree well with the continuum values, being somewhat higher than those in the experiment. The maximum heat flux on the flare is larger than the experimental value.

Generally, since the size of the separation zone increases and the heat flux on the flare decreases with the increase
in the number of molecules and cells, the agreement between DSMC solutions and experiment would be better if a larger number of molecules and finer grid were used.
CONCLUSIONS

The computations of a near-continuum axisymmetric flow about a hollow cylinder flare and a double cone configuration have been performed using the direct simulation Monte Carlo method. Three different test cases were considered, Runs 9, 11, and 28, with the Reynolds number based on the cylinder/first cone length changing in the range from 12,000 to 26,000. For all the cases, the application of the DSMC method to model a flow with a large separation region and shock interaction is extremely computationally intensive. The modeling was conducted on parallel computers, and about 80 million molecules and 20 million cells were used in the largest simulations.

A correlator $G_2$ was introduced that may serve as a quantitative indicator of statistical correlations between simulated particles, and therefore the reliability of results obtained. The use of the correlator in the DSMC code does not require any significant additional computational cost, since its calculation time is proportional to the number of particles in a cell. The correlator is calculated over cells, and shows the regions where statistical correlations may impact the solution. Additional work is needed to establish the connection between $G_2$ values and the error induced by particle dependence.

The results of computations show that the DSMC method is capable of predicting all the details of laminar flow separation in the near-continuum regime only when all the requirements of the time step, cell size, and number of molecules are satisfied. Very good agreement between the DSMC results and available experimental data for the pressure and heat transfer distributions on the hollow cylinder flare was observed for the least dense case, Run 11. The grid and number of molecules requirements are less strict in this case, and were satisfied in the modeling.

More efforts are required to accurately capture large separation regions for more dense flows with the DSMC method (Runs 9 and 28). Even in the largest computations with 80 million molecules, the above mentioned DSMC requirements are not satisfied. The size of the separation zone is larger than in all previous DSMC computations performed by other researchers, but smaller than that obtained in experiments. The DSMC predictions tend to the experimental data with the increase in the number of molecules. Comparison with the continuum solutions shows, that even with a smaller separation region, the DSMC solutions correctly reproduce such complicated details as the shock interaction structure and a counter-rotating vortex near the corner point. The general availability of more powerful computers will certainly further expand the applicability of the DSMC method to model near-continuum flows with separation.

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