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Conservative Species Weighting Scheme for the Direct Simulation Monte Carlo Method

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The direct simulation Monte Carlo method (DSMC) finds application to nonequilibrium gas flows including hypersonic aerodynamics, spacecraft propulsion, materials synthesis, and flows in micromachines. In many of these problems, the species of most interest are present in very small quantities. This presents a resolution problem for the DSMC technique in which a finite number of particles is employed. This study proposes a new numerical scheme for the simulation of trace species. Unlike an existing scheme, the new method explicitly conserves both linear momentum and energy during collisions. The scheme is applied to a number of problems to demonstrate its accuracy and utility. Reduced execution times and improved resolution of trace species properties may be obtained simultaneously with the new method.

Introduction

THE direct simulation Monte Carlo method (DSMC) is a physically accurate method for the computation of nonequilibrium gas flows. The technique is most useful in circumstances where there are insufficient numbers of collisions in the flow to maintain the equilibrium forms of the distribution functions describing the various energy modes of the gas. Generally, such conditions prevail when the average distance between successive collisions of each particle, the mean free path, is comparable to the characteristic length scale of the flow. This type of nonequilibrium condition occurs in a variety of problems of current interest. These include hypersonic flows around vehicles flying at high altitude in planetary atmospheres, flows from small rockets used on satellites for control, flows involved in the synthesis of thin films, and flows in micron-scale mechanical structures.

The DSMC method employs particles simulated in the computer to represent the motions and collisions of real molecules and atoms. A typical simulation employs a few million particles to represent the much larger number of real molecules. The particle weight W is the number of real molecules that each simulated particle represents. The basic assumption of the technique is that particle motion may be performed separately from particle collisions over a time step that is small compared to the average time between successive collisions of the same particle. In the DSMC method, particle motions and collisions are performed in the physical domain. Particles are moved through the length specified by the product of the time step and the velocity vector of each particle. The particles are then collected into cells, and only those particles that occupy a particular cell are considered possible collision candidates. Collision selection is performed using statistical probability models that are derived from basic kinetic theory. Macroscopic flow properties are obtained by time averaging particle properties in the computational cells over several thousand iterations of the basic algorithm.

In many of the applications of interest, the chemical species of most importance occur in very small quantities. To illustrate this point, one particular example is considered. The Bow Shock Ultra Violet (BSUV) flight experiments[1,2] were designed to better understand basic radiation phenomena in the flowfields surrounding hypersonic re-entry vehicles. In the two flights, radiative emission was measured in the uv region for nitric oxide (NO) over a range of altitudes in the upper atmosphere. For the highest altitudes considered, which were above 85 km, the mean free path became sufficiently large to suggest application of the DSMC method. However, the amount of NO existing in these flows was very small. Typically, the mole fraction of NO present was less than 10^{-5}. This presents a major difficulty to the DSMC algorithm. To simulate one particle of NO in a computational cell at this mole fraction would require simulation of 100,000 other particles. This approach would therefore require at least 100 million particles for a simulation of modest size. Even with a numerically efficient DSMC code implemented on vector computers,[3] this simulation would require hundreds of hours of execution time.

To circumvent this difficulty, a scheme is required for the DSMC technique in which the physical weight of a particle W is dependent upon its chemical species. Thus, a particle representing a trace species, such as NO in the BSUV flights, would be given a lower weight than particles representing more abundant species such as N_2 and O_2. The purpose of the present study is to introduce a new weighting scheme that explicitly conserves both linear momentum and energy in each collision. First, an existing, nonconservative weighting scheme is described. Next, the development of a conservative scheme is provided. Finally, the performance of the new scheme is assessed through application to a number of typical problems.

Nonconservative Weighting Scheme

A species-dependent weighting scheme was first proposed by Bird.[4] The use of different particle weights in the DSMC technique for different species mainly affects the computation of collisions. Other portions of the basic DSMC algorithm affected by weights include sampling flow properties, and the generation of new particles. These are all discussed in the following sections.

Effect of Particle Weights on Collisions

In the weighting scheme proposed by Bird,[4] each particle i is assigned an individual weight W_i, and this is usually performed so that all particles of the same chemical species have the same weight. This change to the basic DSMC algorithm affects the computation of collisions in two ways. First, it affects the computation of the number of collisions. The most common scheme for determining which particles in a cell collide is the no time counter method of Bird.[5] In this scheme,

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the number of pairs of particles to be considered for collision is given by

$$N_c = \tfrac{1}{2} n N \Delta t (\sigma g)_{\max} \tag{1}$$

where n is the real number density, N is the number of simulated particles in the cell, Δt is the simulation time step, σ is the collision cross section, and g is the relative velocity of a collision. For each of the N_c pairs, the probability of collision is

$$P_c = \sigma g / (\sigma g)_{\max} \tag{2}$$

The number density in the traditional DSMC algorithm is simply given by

$$n = NW/V \tag{3}$$

where W is the weight of all particles, and V is the volume of the cell. When the weight of each particle is a variable, the number density becomes

$$n = \sum W_i \Big/ V \tag{4}$$

where W_i is the weight of particle i. Care must be taken in the computation of the number of collisions to be considered when using species-dependent weights. It may be shown that for collisions between particles of species a and particles of species b, the number of pairs to be formed is

$$(N_c)_{a,b} = \frac{n_a N_b \Delta t (\sigma g)_{\max}}{P_{a,b} + (W_b/W_a) P_{b,a}} \tag{5}$$

where W_a and W_b are the particle weights of species a and b, respectively. In Eq. (5), the quantity $P_{a,b}$ is the probability that the properties of a species a particle are changed in a collision with a particle of species b. This probability accounts for the fact that when particles of different weights collide, the amount of change in the properties of the particle with the larger weight is reduced. When particle b is a trace species, so that $W_a > W_b$, then

$$P_{a,b} = W_b/W_a \quad \text{and} \quad P_{b,a} = 1 \tag{6a}$$

otherwise

$$P_{a,b} = 1 \quad \text{and} \quad P_{b,a} = W_a/W_b \tag{6b}$$

When the weights of species a and b are equal, Eq. (5) reduces to the result obtained using n_a and N_b in Eq. (1). The use of species-dependent particle weights makes the selection of candidate collision pairs more complicated than the traditional no time counter scheme, as the number of a, b pairs given by Eqs. (5) and (6) must be explicitly generated for each type of species pair.

The second effect of varying particle weights on the DSMC algorithm is in the manner in which the mechanics of collisions is performed. When only one weight is used throughout a simulation, the properties of both particles that participate in a collision are changed using the simple rules of conservation of linear momentum and energy. Consider a collision between two particles with precollision velocity vectors $\boldsymbol{U}_1 = (u_1, v_1, w_1)$ and $\boldsymbol{U}_2 = (u_2, v_2, w_2)$. As given in Ref. 4, the postcollision velocity vectors $\boldsymbol{U}_1'$ and $\boldsymbol{U}_2'$ of particles 1 and 2 are given by

$$\boldsymbol{U}_1' = \boldsymbol{U}_m + [m_2/(m_1 + m_2)]\boldsymbol{g} \tag{7a}$$

$$\boldsymbol{U}_2' = \boldsymbol{U}_m - [m_1/(m_1 + m_2)]\boldsymbol{g} \tag{7b}$$

where m_1 and m_2 are the masses of particles 1 and 2, $\boldsymbol{U}_m$ is the center of mass velocity vector, and $\boldsymbol{g}$ is the relative velocity vector. In the weighting scheme of Bird,[4] when two particles of different weights collide, the probabilities that the properties of particles of species a and b are changed by collision are given by Eqs. (6a) and (6b). Thus, the properties of the particle with the lower weight, i.e., the trace particle, are changed according to Eqs. (7a) or (7b) with a probability of 1. The properties of the particle with the higher weight are changed with probability given by the ratio of the particle weights, e.g., W_1/W_2, if particle 1 is the trace species. Under equilibrium conditions, this scheme will approximately conserve linear momentum and energy over a sufficiently large number of collisions. However, the scheme does not conserve these properties explicitly at each collision on the occasions when the properties of both particles are not changed according to Eqs. (7). Indeed, Bird[6] recommends against the use of this scheme. Hence, there is a requirement for development of a particle weighting scheme for the DSMC technique that does conserve linear momentum and energy.

Other Effects of Particle Weights

The use of varying particle weights also affects the generation of new particles and sampling of flowfield properties. The use of a lower weight for a trace species evidently will reflect the need to generate a larger number of particles to represent this species. In sampling flowfield properties, two counters must be updated when variable weights are employed. As with the traditional DSMC algorithm, one of the counters keeps track of the number of simulated particles that have occupied each cell, ix. At each time step, this is achieved by summing over all particles in each cell using

$$\text{array}(ix, 1) = \text{array}(ix, 1) + 1 \tag{8}$$

The second counter keeps track of the relative contribution of each particle to the total number density of the cell and is obtained by summing the following over all particles in each cell:

$$\text{array}(ix, 2) = \text{array}(ix, 2) + W_i \tag{9}$$

In the case where all particles have the same weight W, Eq. (9) is obtained simply by multiplying Eq. (8) by W.

Conservative Weighting Scheme

The total linear momentum in the x direction represented by two particles of different weights involved in a collision may be written

$$p_x = W_1 m_1 u_1 + W_2 m_2 u_2 = W_1 (m_1 u_1 + \phi m_2 u_2) \tag{10}$$

where $\phi = W_2/W_1$, and it is assumed that particle 2 represents a trace species, and hence, $W_2 < W_1$. The first stage in the new weighting scheme involves splitting the first (nontrace) particle into a particle with weight W_2 and a particle with weight $W_1 - W_2$. Conservation of linear momentum is then written

$$p_x = W_1 [(1 - \phi) m_1 u_1 + \phi (m_1 u_1 + m_2 u_2)] \tag{11}$$

A collision is then performed using the traditional DSMC mechanics given in Eqs. (7) on the two particles that have weight W_2. Thus

$$p_x = W_1 [(1 - \phi) m_1 u_1 + \phi (m_1 u_1' + m_2 u_2')] \tag{12}$$

where $'$ indicates postcollision properties. The final stage is to merge together the two particles that were split such that

$$p_x = W_1 (m_1 u_1'' + \phi m_2 u_2') = W_1 m_1 u'' + W_2 m_2 u_2' \tag{13}$$

where the postcollision velocity of the first (nontrace) particle is

$$u_2'' = (1 - \phi)u_1 + \phi u_1' \tag{14}$$

The previous scheme is applied in all three physical directions and explicitly conserves linear momentum. Unfortunately, it does not explicitly conserve total energy. The total precollision energy represented by the two particles is

$$E = W_1 \tfrac{1}{2} m_1 (u_1^2 + v_1^2 + w_1^2) + W_2 \tfrac{1}{2} m_2 (u_2^2 + v_2^2 + w_2^2) \tag{15}$$

Using the splitting and merging scheme described by Eqs. (11–14), the total postcollision energy is

$$E' = W_1 \tfrac{1}{2} m_1 (u_1''^2 + v_1''^2 + w_1''^2) + W_2 \tfrac{1}{2} m_2 (u_2'^2 + v_2'^2 + w_2'^2) \tag{16}$$

so that the difference in energy between the pre- and postcollision states is

$$\Delta E = W_1 \tfrac{1}{2} m_1 \phi (1 - \phi)[(u_1 - u_1')^2 + (v_1 - v_1')^2 + (w_1 - w_1')^2] \tag{17}$$

Note that for $W_1 = W_2$, $\phi = 1$ and $\Delta E = 0$, so that energy is conserved exactly when the weights of the two particles are equal.

If the split–merge scheme is employed at each collision, then energy is continually lost from the system because $\Delta E > 0$. This problem is addressed by keeping track of these energy losses in each cell. When one collision loses energy through Eq. (16), this energy is then added to the c.m. energy of a subsequent collision. In general, this energy should only be added to collisions between particles having the maximum weight used in the simulation; that is, between two nontrace particles (leading to a nontrace collision). The energy addition is performed by increasing the relative velocity of the next nontrace collision to make up the energy lost in the previous split–merge collision. In this manner, the maximum energy lost is only that caused by a single collision. When it is noted that the magnitude of ΔE is proportional to ϕ, it becomes clear that the amount of energy lost is very small indeed, and particularly so for those species present in very small amounts for which ϕ is itself very small. The amount of energy to be added to the next nontrace collision is a variable maintained in each cell of the simulation. Whenever several collisions occur sequentially in which $W_2 \neq W_1$ (i.e., the split–merge procedure is employed), then the energy to be made up for each of these collisions is summed until a nontrace collision occurs. Thus, energy conservation is maintained over all iterations of the simulation.

This particle weighting scheme is not unique. For example, an alternative approach could be imagined in which the particle splitting is performed so as to ensure conservation of energy, and then a correction made to augment the change in momentum to the following collision. However, this approach is disregarded as it is mathematically much more complicated, requiring the root of a quadratic equation.

Simulation of internal energy exchange and chemical reactions can also be accomplished for trace species using the splitting–merging technique. For example, the total postcollision rotational energy is given by

$$E_r = W_1 E_{r_1}'' + W_2 E_{r_2}' \tag{18}$$

where

$$E_{r_1}'' = (1 - \phi)E_{r_1} + \phi E_{r_1}' \tag{19}$$

in which E_{r_1} is the precollision rotational energy of particle 1, and E_{r_1}' is the postcollision rotational energy of particle 1 obtained from the collision between the split particle and particle 2. A similar approach may be used for vibrational energy, except that care must be taken when employing a quantized energy distribution. Simulation of chemical reactions requires considerable care. An additional opportunity of using particle weights is that slow chemical reactions may have their reaction probabilities increased by a large factor that may then be put into creating trace species with relatively low particle weights.

Results

The particle weighting scheme outlined previously is attractive as it explicitly conserves linear momentum in each collision. It is also asserted that very little energy is lost from the system because of the use of the energy counter. To prove that this is true, a number of demonstration simulations are performed.

Single-Cell Simulations

The first test of the particle weighting scheme considers a collection of over 100,000 particles initially in thermal equilibrium at a specified temperature. The particles are allowed to undergo several million collisions, after which the velocity distribution functions are determined. In Fig. 1 the results are shown for a simulation involving a mixture of 1% argon in 99% helium at a temperature of 1000 K. The particle weights are assigned by species such that $W_{Ar}/W_{He} = 0.01$. It is clear that the expected equilibrium forms for the velocity distribution functions are accurately reproduced by the new weighting scheme. After 10-million collisions, linear momentum in all three directions is explicitly conserved (within machine accuracy). In this case the total energy is also explicitly conserved. This is because the very last collision computed in the simulation is between two particles of equal weight. In this case, the energy lost from the previous collision between a helium and argon particle is exactly replaced. In the case where the final collision is between particles of different weight, the total energy lost is typically 1% of the average collision energy. Thus, the total energy lost by the system averaged over all 10-million collisions is about 10^{-9} times the average collision energy in this case. Hence, to very high order, energy is also explicitly conserved with the new scheme.

The same heat bath is used to illustrate the problems with the nonconservative weighting scheme. The composition and temperature are identical to the previous case and a small velocity component of 100 m/s is applied in the x direction. This system is simulated for 1000 time steps. In Fig. 2a, the total momentum in the x direction of the system computed using

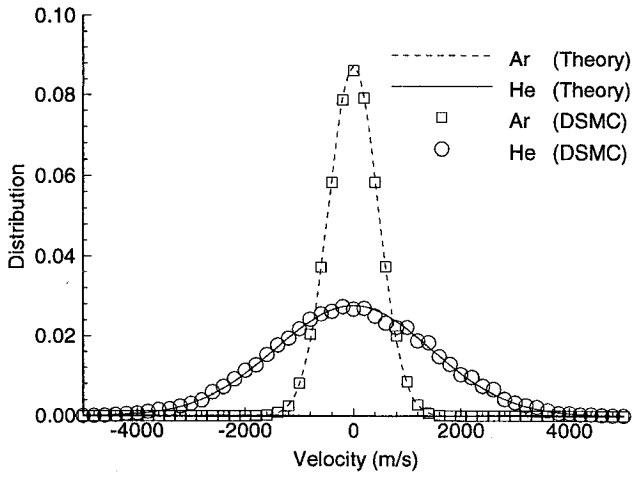

Fig. 1 Velocity distribution functions in a single-cell simulation at T = 1000 K.

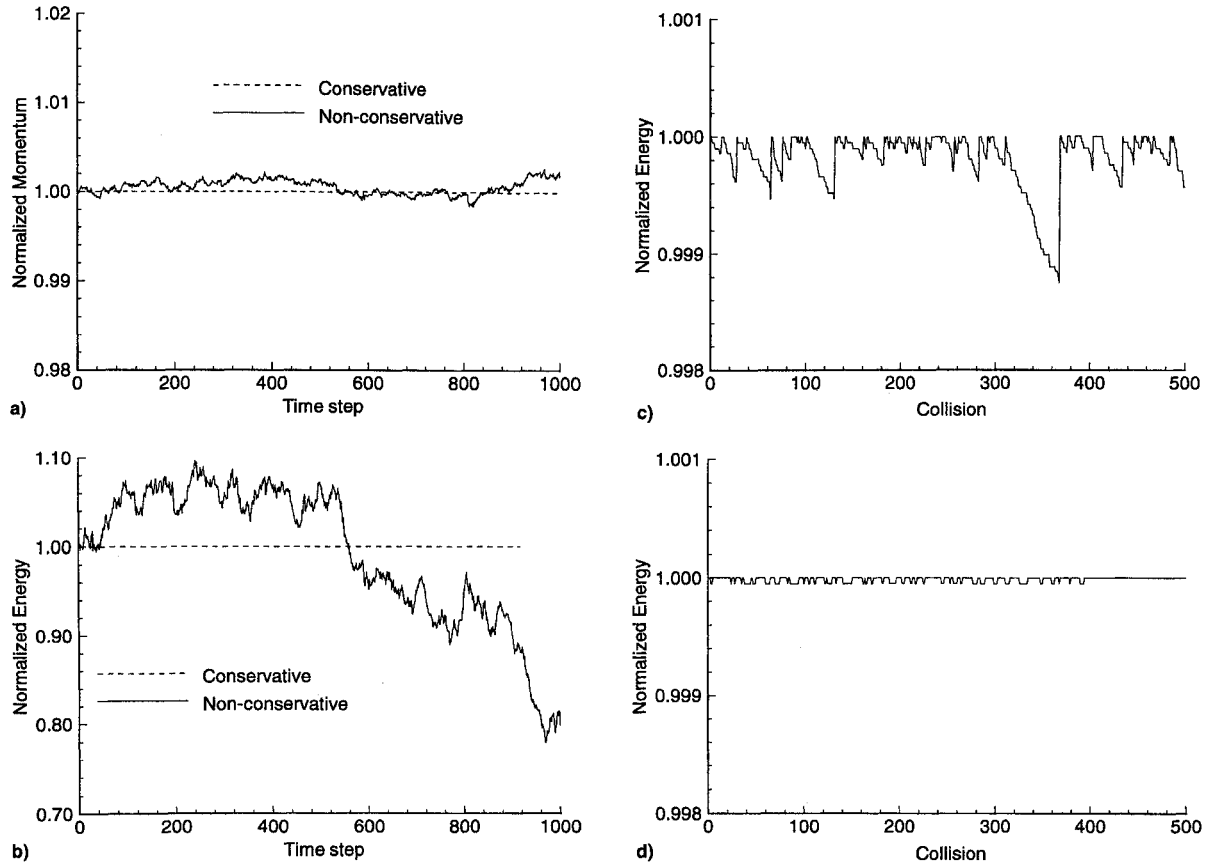

Fig. 2 Total system a) momentum and b) energy (normalized) as a function of time for an equilibrium heat bath using two different weighting schemes, and variation of total system energy (normalized) after each collision for an equilibrium heat bath of c) 20% argon in 80% helium using $W_{Ar}/W_{He} = 0.1$, and d) 1% argon in 99% helium using $W_{Ar}/W_{He} = 0.01$.

the new conservative scheme and the old nonconservative scheme are compared. For each simulation, the momentum is normalized by the value at the start of the computation. The conservative scheme conserves momentum exactly at each collision, and hence, no fluctuations are present. By comparison, the nonconservative scheme exhibits fluctuations of about 0.2%. In Fig. 2b, the variation in the total energy of the system for the two simulations is shown. In this case, the fluctuations in the total energy of the nonconservative scheme are found to be significant and exceed 20%. By comparison, the conservative scheme conserves energy exactly.

In principle, the conservative scheme conserves both momentum and energy for any ratio of weights ϕ. However, there are practical limits. Consider the case where species 2 is the trace component. As the value of ϕ is decreased, the number of collisions simulated between species 2 and species 1 will become much greater than the number of collisions between two species 1 particles. Recall that the system energy is only conserved in the scheme when a 1–1 collision takes place. Thus, when the weight ratio is very large, a 1–1 collision will occur relatively infrequently. For each of the many 1–2 and 2–1 collisions that occur before a 1–1 collision, the total system energy will decrease. When a 1–1 collision does take place, the total energy will be increased back to its original value. It is therefore recommended that the ratio of weights for trace and nontrace species be chosen to be approximately equal to the ratio of mole fractions of trace and nontrace species.

These issues are illustrated in Figs. 2c and 2d where the total system energy is shown at the end of each collision in two different equilibrium simulations, both conducted at the same temperature and velocity used to generate the data in Figs. 2a and 2b. For the results shown in Fig. 2c, a mixture of 20% argon in 80% helium is computed using a weight ratio of $W_{Ar}/W_{He} = 0.1$. In this case, the weighting scheme shows a large maximum error in the total system energy of 0.1%. The physical and numerical parameters for this calculation are chosen to illustrate a condition where the weighting scheme should not be employed. First, the weight ratio is relatively large, leading to large losses in energy at each Ar–He collision, as dictated by Eq. (17). Second, the trace to nontrace weight ratio is smaller than the trace to nontrace mole fraction ratio. This leads to there being about seven times more Ar–He collisions than He–He collisions; hence, in this case, there can be many energy-losing Ar–He collisions before total system energy is restored through an He–He collision.

The results shown in Fig. 2d are for physical and numerical parameters that are more representative of a case where the weighting scheme is needed and should be used. Here, the mixture is 1% Ar in 99% He, and $W_{Ar}/W_{He} = 0.01$. It is clear in this case that the impact of making up the lost energy is much reduced in comparison to the results of Fig. 2c. Indeed, the maximum error in the total system energy is now just 0.005%. This improvement is because of both the lower weight ratio employed and that the weight ratio is approximately equal to the ratio of trace to nontrace mole fractions.

One-Dimensional Shock Wave

In many experimental investigations of rate processes, the species of interest is seeded in small quantity in an inert gas. This applies to shock-tube experiments, and to molecular beams that are considered in the next section. In the present case, a one-dimensional normal shock wave is considered. The flow consists of 1% Ar in 99% He at a Mach number of 5. Normalized profiles of density and temperature are shown in Figs. 3a and 3b, respectively. Notice how the translational temperature of the trace heavy species rises downstream of the helium temperature and shows a significant overshoot. In these

figures, comparison is made between results obtained with and without species-dependent particle weights. In the latter case, the weights used are such that $W_{Ar}/W_{He} = 0.01$. Clearly, excellent agreement is obtained between the two simulations. In the simulation that used the same weight for both helium and argon, the total number of particles employed is 175,000 (of which 1750 are Ar) and the total execution time on a workstation is 29 h. By comparison, the simulation with species-dependent weights employs 17,500 particles (of which 8750 are Ar) and only 3 h execution time.

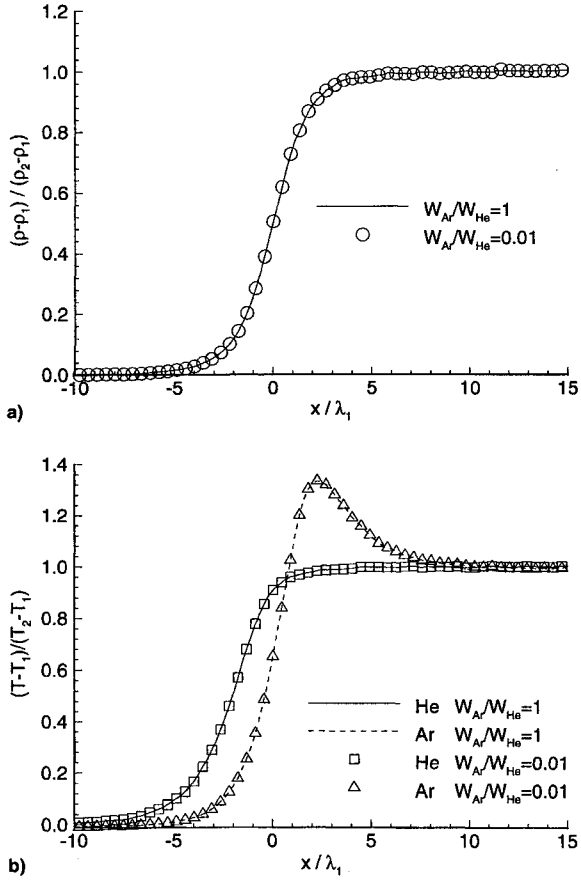

Fig. 3 Normalized a) density and b) translational profiles in a normal shock wave of 1% argon in 99% helium at Mach 5.

Supersonic Molecular Beam

Supersonic beams are used in a variety of processes to accelerate heavy molecules seeded in a light carrier gas. One such process is investigating beams as a candidate mechanism for deposition of silicon films through dissociation of silicon-based molecules by colliding them with a substrate at hyperthermal energies.[7] In these studies, molecular hydrogen is heated and accelerated through an orifice and skimmer configuration. Molecules such as silane (SiH_4) and disilane (Si_2H_6) are seeded at the level of about 1% into the hydrogen and accelerated through intermolecular collisions to substrate impact energies in excess of 1 eV.

The trace species, either silane or disilane, is the species of most interest in these flows. To perform useful DSMC simulations of such processes, it is necessary to resolve the properties of these species in great detail. This system is an excellent example of the need for particle weights. Simulation is performed for a representative axisymmetric system. The geometry is illustrated in Fig. 4 and consists of a point source representing flow through a sonic orifice. The total temperature is 300 K and the flow rate is 200 standard cubic centimeters per minute (sccm). A mixture of 1% silane in hydrogen is considered. A conical skimmer with entrance diameter of 1.3 mm and exit diameter of 2 cm is located at a distance of 5 mm along the axis from the point source. A 10-cm-diam substrate is oriented perpendicular to the axis and is located at a distance of 10 cm from the original source. The substrate temperature is 300 K and the sticking coefficient for silane is assumed to be 1.0, i.e., all silane molecules impacting the substrate are adsorbed onto the surface.

Comparison is made of results obtained with and without species-dependent weights. In the case where weights are employed, the ratio of weights is $W_{SiH_4}/W_{H_2} = 0.04$. Profiles of concentrations and velocities along the flow centerline are shown in Figs. 5a and 5b. The results of Fig. 5a indicate that the two gases expand quite uniformly toward the substrate. Some of the complicated kinetics involved in these flows are illustrated. Initially, the gas expands rapidly out of the orifice and through the skimmer without any appearance of a shock

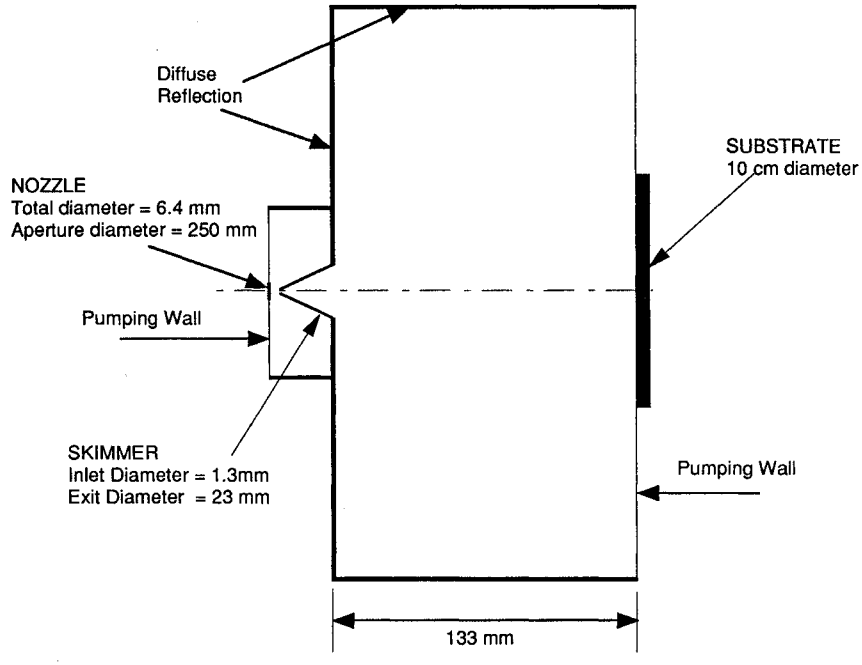

Fig. 4 Schematic diagram of the silicon thin film deposition system.

being formed at the skimmer entrance. As the gas approaches the substrate, the density of the hydrogen particles is raised slightly. The density of the silane particles continues to decrease monotonically as these particles are assumed to be deposited on the surface. The velocity profiles shown in Fig. 5b illustrate why supersonic beams are useful for thin film deposition. Close to the orifice, the hydrogen particles are rapidly accelerated because of their expansion. Through intermolecular collisions, the silane particles are also accelerated in this region. Because of the relatively low densities encountered between the skimmer exit and the substrate surface, there is almost no reduction in the speed of the silane particles and they impact the substrate with high energy.

In Fig. 5, the conservative particle-weighting scheme gives results that are in excellent agreement with the more expensive computations. The simulation without weights employs a total of 375,000 particles and achieves a numerical performance of 17 μs per particle per time step on a workstation. The total simulation requires 44 h execution time. This total number of particles provides an average of 3.6 silane particles per cell. The simulation with species-dependent weights employs 70,500 particles and achieves a performance of 21 μs per particle per time step. In this case, the total solution time is 10 h on the same computer. This simulation provides 13.3 silane particles per cell. Thus, the total execution time is reduced by a factor of 4 at the same time as the resolution of the trace species is improved by a factor of 4.

Bow Shock Wave of Air

Finally, the new particle-weighting scheme is employed to compute one of the flows for which radiative emission measurements are available from the second BSUV flight experiment.[2] The flow conditions are an altitude of 80 km, a velocity of 5.1 km/s, and the body geometry is represented by a sphere of radius 0.1016 m. The freestream mole fraction of nitric oxide at this altitude is about 10^{-6}. Therefore, without variable weights, it is numerically infeasible to include NO in the simulation. In Fig. 6a, the temperatures of the various internal energy modes of the bulk gas are compared along the stagnation streamline. One simulation is performed without variable weights (and therefore has no nitric oxide in it), and one simulation used a low weight to allow resolution of NO. In this case, the weights are such that $W_{NO}/W_{N_2} = 2 \times 10^{-5}$. It is clear that the bulk properties of the gas flow computed in the two simulations are in excellent agreement.

The number densities of nitric oxide and atomic oxygen along the stagnation streamline obtained with the variable-weight DSMC simulation at 80-km altitude are compared with a continuum solution [computational fluid dynamics (CFD)] in Fig. 6b. At this altitude, the Knudsen number is about 0.03 so that the continuum approach should provide good physical accuracy. The CFD simulation solves the Navier–Stokes equations with coupled thermochemical relaxation.[8] Every effort is made to use equivalent thermochemistry models in the DSMC and CFD simulations. While the DSMC results for nitric oxide show some degree of statistical scatter, the comparison of the DSMC and CFD profiles indicates that the weighting scheme is working effectively.

The degree of thermal and chemical nonequilibrium under hypersonic conditions should increase with altitude. An example of the strong degree of nonequilibrium in the BSUV-2 flight is illustrated in Fig. 7 in which the temperatures of the

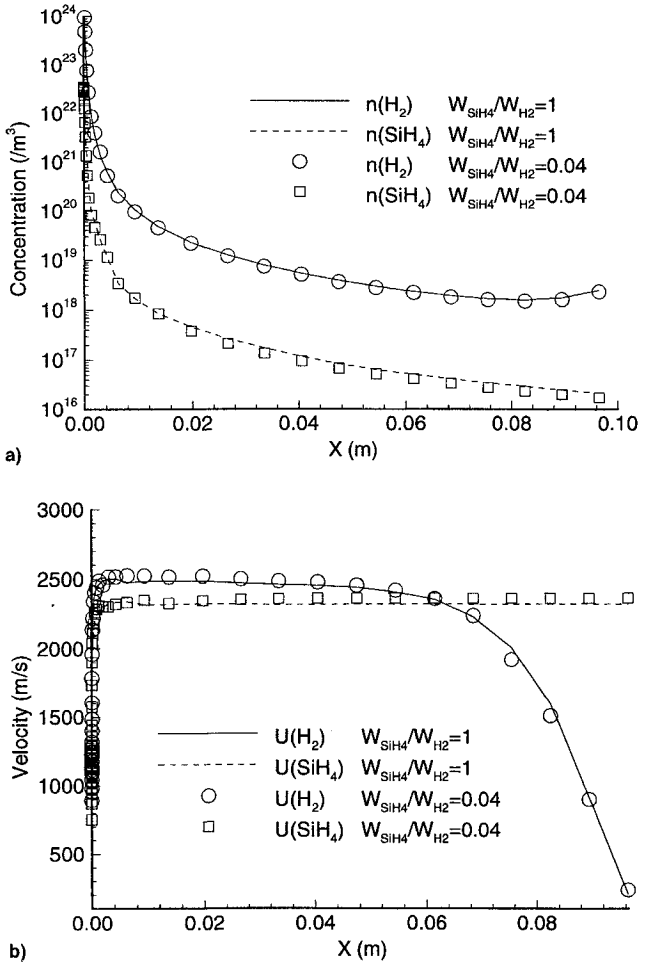

Fig. 5 a) Number density and b) velocity profiles along the flow centerline of a supersonic molecular beam flow consisting of 1% silane in 99% hydrogen.

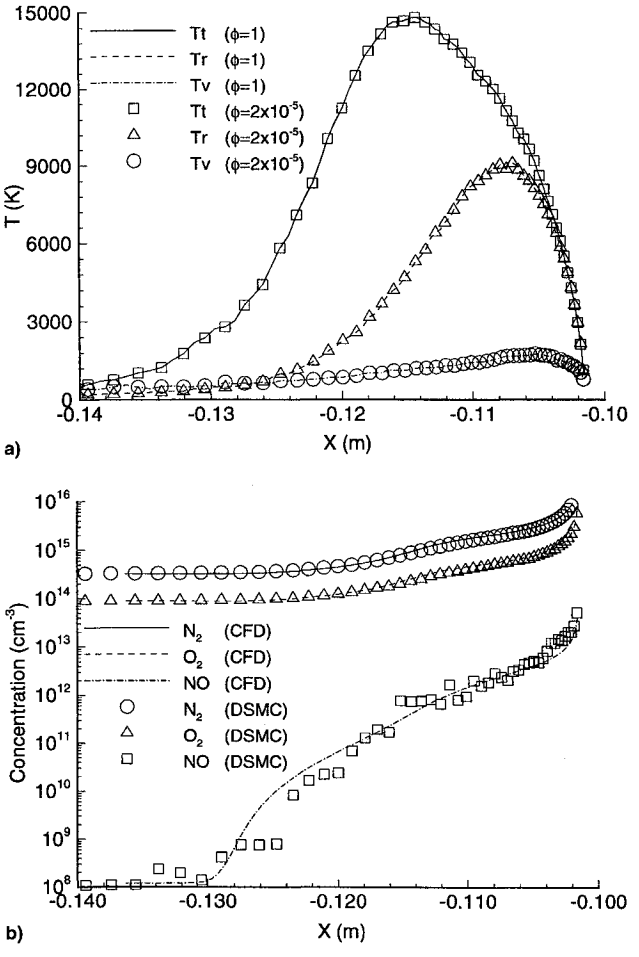

Fig. 6 a) Temperature and b) number density profiles along the stagnation streamline of the BSUV-2 vehicle at an altitude of 80 km and a velocity of 5.1 km/s.

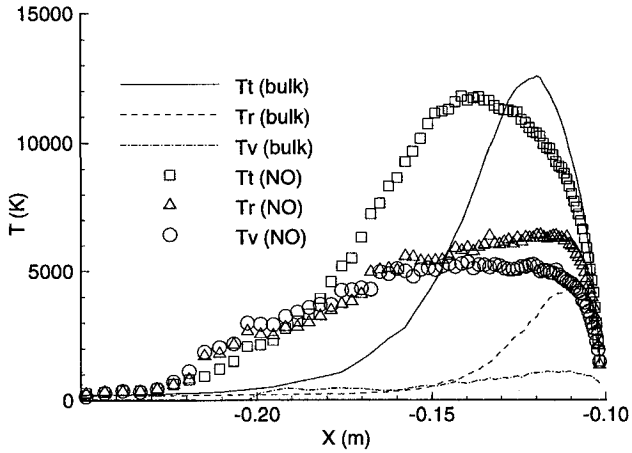

Fig. 7 Temperature profiles along the stagnation streamline of the BSUV-2 vehicle at an altitude of 87.5 km and a velocity of 5.1 km/s.

NO molecules are compared with those of the bulk gas along the stagnation streamline at an altitude of 87.5 km. It is clear that the rotational and vibrational modes of NO are more excited than the bulk gas, whereas the translational modes are comparable. The rotational and vibrational temperatures affect the widths and relative heights of the spectral lines. The ability to include direct simulation of the NO using the weighting scheme has therefore been of particular importance in this application.

Conclusions

A new particle-weighting scheme has been developed for the DSMC. The scheme permits the resolution of species that occurs in low concentrations by assigning lower weights to particles representing these trace species. The new scheme is demonstrated to explicitly conserve linear momentum for every collision. Total energy is conserved by carrying over a small amount of energy from one collision to the next. This provides a convenient mechanism to conserve energy to very high order.

Application of the scheme gave results in excellent agreement with more expensive computations performed without the use of variable particle weights. The total number of particles required and the total execution time were significantly reduced through the use of variable weights. For application to a trace species seeded in a molecular beam, the total cost was reduced by a factor of 4, while resolution of the trace species was improved by a factor of 4. In application to simulation of NO in a hypersonic flow, the use of weights permitted resolution of this very rare species that was not possible to include in the simulation previously.

The use of the scheme is recommended only for the simulation of trace species at mole fractions of 0.1 and less. As indicated by Bird,[6] the statistical fluctuations associated with the use of particle weights appear to be larger than would normally be expected from a DSMC simulation. This is attributed to additional random walk effects. Therefore, the weighting scheme should only be used where absolutely necessary. In general, it is feasible to obtain adequate resolution of species present in mole fractions above 0.1 without requiring the use of weights.

It is also recommended that the ratio of the weights of trace and nontrace species be chosen to be approximately equal to the ratio of the mole fractions of the trace and nontrace species. This approach ensures that the addition of energy lost through each collision between a trace and nontrace particle is recovered rapidly within the simulation.

The implementation of the variable weighting scheme is quite straightforward and required a relatively small overhead in terms of execution time and memory.

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