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Review of Code Validation Studies in High-Speed Low-Density Flows

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Nomenclature

a	= adjustable parameter
C_D	= drag coefficient
C_H	= heat-transfer coefficient
D	= diameter, m
E	= collision energy, J
E_{ion}	= ionization threshold, J
Kn	= Knudsen number, λ/D
n	= number density, $1/\text{m}^3$
nu	= number flux, $1/\text{m}^2/\text{s}$
P	= reaction probability
Q	= heat flux, W/m^2
s	= coordinate along surface, m
T	= temperature, K
U, V	= velocities, m/s
X, Y, Z	= spatial coordinates, m
δ_s	= shock thickness, m
ζ_B	= average number of degrees of freedom
λ	= mean free path, m
ρ	= density, kg/m^3
ϕ	= exchange restriction factor

Subscripts

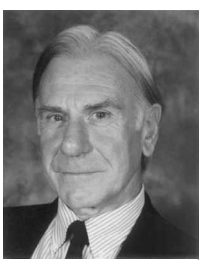
p	= parallel
r	= rotational
x	= transverse
1, 2	= upstream and downstream of a shock wave
∞	= freestream

Introduction

FEW would dispute that when Bird, in 1970,[1] first formulated his direct simulation Monte Carlo (DSMC) method, it would mark a milestone in the evolution of fluid mechanics. It brought within grasp practical solutions to important engineering problems where the flow was rarefied. Although probably not appreciated then, the method had enormous power, and, as time went on, it was possible to demonstrate that solutions to very complex flows involving chemical reactions, ionization, and high degrees of molecular nonequilibrium were achievable.

When Bird first published his method, interest in nonequilibrium gas phenomena was being spurred on by a pressing need to assess the aerodynamics of spacecraft during reentry. Solutions obtained using Navier–Stokes methods had proved inadequate, and practical solutions to the more fundamental governing Boltzmann equation were totally beyond the scope of either analytical or numerical methods. Bird's new scheme bypassed the direct solution of this equation with a probabilistic simulation, which was achieved by calculating the motions of a large ensemble of simulator particles. Initially the number was in the hundreds of thousands, but with today's computers it can be of the order of 10^8. These simulators moved and collided with each other within physical space in a realistic manner and built up a statistical picture of the flow phenomena being studied.

Bird's DSMC method had a very significant numerical advantage over other rival particle simulation schemes. For this reason it was possible to apply it to quite complex flows, and the evidence then available indicated that the method yielded good estimates of all of the desired flow properties. Furthermore the realization



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was quickly made that it had another enormous advantage over alternative approaches in that it could readily be extended to multispecies flows—even the inclusion of chemical reactions between constituents was within its scope. This was extremely significant because the spacecraft reentry high-temperature flows, at the time of particular interest to engineers, inevitably included dissociation and other chemical effects, which could not be ignored.

Despite this success, Bird was not without his critics. His inability to provide a formal proof that his numerical results were equivalent to those that would have been obtained from the Boltzmann equation was seen to be a serious drawback. It was left to experimentalists to confirm the validity of the method and to demonstrate that the solutions were, in fact, quite precise. Eventually in 1990 an analytical proof[2] was published that more or less silenced the criticism. Even so, this proof was limited to a simplified representation of the gas molecules, and it is not possible to establish the accuracy of the method in complex situations where, for instance, reactions occur. The need for experiments to validate the DSMC computational procedures is seen to be indispensable, and as each new step in the extension of the method is introduced, further validation is required to demonstrate that the modeling is correct. Fortunately, over the years, a series of such experiments have been undertaken for which closely matched DSMC simulations have been performed specifically for the purpose of code validation. Some of these will be described in this paper. But, as will be seen, as the scope of the DSMC method has been extended into increasingly more complex situations (both in terms of high-enthalpy real-gas effects and flowfield geometrical detail), the experimentalists have found it increasingly difficult, if not impossible, to provide suitable data.

What, then, is the evidence that DSMC provides valid and verifiable solutions to real engineering problems?

DSMC Method

The only precise way to predict flows that are in thermodynamic nonequilibrium and/or rarefied (by which we mean that the Knudsen number is of the order of 0.001 or greater) is to use a method based on the assumptions of Boltzmann equation. Within this equation[3] the state of the gas is expressed in terms of a time-dependent molecular velocity distribution function. This function gives the probability at any time of a particle occupying a position in physical and velocity space. The Boltzmann equation was originally formulated for simple gases, but it can be extended to include internal energy, multiple species, and radiation by adding an additional dimension for each energy mode or species. These extra dimensions add considerable complexity to the equation, and even in an approximated form it is totally intractable for engineering applications. Only when the Knudsen number is very small is it legitimate to bypass the Boltzmann equation formulation and use instead the Navier–Stokes equations. Even then this is conditional on the gas being in a state where there are only minor perturbations from molecular equilibrium.

An attractive and viable alternative to the direct solution of the Boltzmann equation is a group of numerical simulation methods. These methods recognize the particulate nature of the gas and describe it in terms of information (values of velocity, position, energy state, etc.) on an ensemble of sample particles (or simulators) that move through the computational domain. These sample particles closely mimic the progress of the gas molecules in the real flow. Because, even in the most rarefied cases of engineering interest, the flowfield contains an enormous number of molecules, we are obliged to use a relatively small number of simulators to represent the real particles as they move through the physical domain of interest. Simulations of this type have proved to have enormous advantages over any attempted direct solution to the Boltzmann equation in that they can handle complicated problems and are amenable to realistic modeling of the complex molecular energy exchange and chemical processes. Particle simulation methods are notoriously computationally expensive. However with the advent of increasingly more powerful computers this is no longer seen to be a serious drawback if valid solutions can be obtained that otherwise would not have been forthcoming. High-performance computing and massively parallel architecture machines have already made an impact on the types of problems that are currently being tackled using particle simulation methods.

As already noted, one such particle simulation method that has proved especially effective is Bird's DSMC.[4] In DSMC the movement of the particles is decoupled from their collisions by advancing each of these processes alternately and independently over small, equal time increments. The size of the time step has to be chosen to be significantly smaller than the local mean collision time. Candidates for intermolecular collisions are selected from neighboring particles in a probabilistic manner by comparing a random number with the collision probability of each pair. The outcome of each collision has to be determined using appropriate models, and although the properties of the particles after each collision can be derived deterministically, almost universally they are obtained using statistical and, very often, phenomenological methods. These methods typically define appropriate probability density functions from which the postcollision properties can be determined by random selection. These functions are calculated in advance for each phenomenon, and the postcollision properties (velocity components, internal energies, etc.) are obtained from them by random selection. At high enthalpies particle pairs must also be considered for possible chemical reactions or even ionization at each collision.

The behavior of molecules during a simulated collision depends on the choice of the intermolecular force potential. Models used in DSMC range in complexity from simple hard spheres and inverse power representations to Morse and Lennard–Jones potentials.[5] These latter two potentials include a realistic long-range attraction between molecules as well as the short-range repulsion, but it is generally accepted that they impose too high a computational overhead for their use to be justifiable in an engineering context. Alternative ingenious extensions of the hard sphere model have been proposed that have proved to be very good at reproducing the macroscopic behavior of a gas yet remain computationally efficient. The first was the variable hard sphere (VHS) model introduced by Bird.[6] More recently Koura and Matsumoto[7] devised a variant called the variable soft sphere (VSS) model, which is now used extensively. Both models assume a hard sphere interaction between the particles, but their diameter changes with the collision energy according to some power law. The exponent is calculated by matching the viscosity of the simulated gas to that of its real counterpart. The VSS model adds a second degree of freedom by introducing anisotropic postcollision scattering. The second free parameter of the VSS model is set so that it also reproduces the diffusion coefficient of the gas correctly.

For polyatomic particles the transfer of energy to and from the internal modes has to be considered. The most popular model is a stochastic one devised by Borgnakke and Larsen.[4,8] Their model has proved to be very successful in describing the macroscopic distribution of energy in the gas even though the treatment of individual collisions is not rigorous. Uncertainties about the real distributions that prevail led Borgnakke and Larsen to adopt an implicit local equilibrium assumption so that the post collision properties are sampled from a varying but equilibrium distribution for each collision. As we will see, the evidence indicates that this model works well for nonreacting collisions. The reason is probably that, for these interactions, all available energy states tend to be populated without any specific preference. This leads to rapid equilibration within just a few collisions.

For collisions involving chemical reactions a very different picture emerges; for more details the reader is referred to the discussion in Gallis and Harvey.[9] The position of the energy barrier along the interaction path depends on the species involved in the collision. Variations in this position result in the energy that is released by an exothermic chemical reaction being distributed preferentially into either the translational or internal energy modes. The nascent products thus emerge from a collision in a perturbed and nonequilibrium state. The current methods widely used in DSMC codes to model the internal energy thermal relaxation for reactions, based on selecting postcollision properties from an equilibrium distribution, are not strictly correct especially if the flow is rarefied. New models based on maximum entropy concepts have been proposed in an attempt to overcome these difficulties (see, for example, Ref. 9). The errors that result from the use of approximate collision models for reactions,

in particular those that employ equilibrium distributions, have not been quantified. There is thus a pressing need for correctly targeted and sufficiently accurate experiments to be performed to assess the significance of these shortcomings within the context of practical applications such as reentry flight.

What then is the evidence that the DSMC method provides accurate answers to real flow problems? Comparisons with corresponding solutions to the more fundamental Boltzmann equation are not an alternative because these do not exist. Navier–Stokes solutions are recognized as being inaccurate in the range of the Knudsen number of interest. Thus the task has to be approached by comparing solutions with reliable experimental evidence. This presupposes that both the numerical solutions and the experiments are performed accurately. In both instances this is not a forgone conclusion especially for complex and higher-enthalpy situations. The DSMC method requires skill to implement especially in terms of grid definition and time step. Within boundary layers in complicated two-dimensional or, worse, three-dimensional problems, achieving adequate resolution is often difficult. Deciding whether a solution is properly resolved temporally and spatially can be difficult for the person running the code, yet alone anyone independently reviewing the work. Thus whenever possible, independent solutions to the identical problem should be attempted to verify the results. On the experimental side there are severe measuring difficulties in obtaining validation quality data in any low-density flow. As the enthalpy is increased, these difficulties mount up to the point where the sourcing of any suitable information on flows involving, for instance, ionizing reactions is currently almost beyond the scope of any contemporary wind-tunnel facility.

This paper is concerned with evidence that exists for the validation of the DSMC method. From the foregoing remarks one can see that to address this task it is not only necessary to categorize the examples in terms of complexity of flow geometry, but it is also important to examine a hierarchy of levels of complexity of the molecular interactions that are involved. At the simplest level we have flows involving monatomic particles with only translational energy being exchanged. Increasing in complexity there are the polyatomic flows where the collisions are inelastic and internal energy also is exchanged. At the next level there are the chemically reacting flows where there is the requirement to model both the reaction kinetics and a new set of complex internal energy exchange processes that take place associated with the reactions. At the highest level we have the plasma flows. The level of ionization in fluids that have to be represented can vary from slight to high. In all of these flows, except those for which the ambipolar diffusion approximation can be made, Coulomb forces have to be taken into account in addition to all of the other effects that we have already listed. This means that the influence of longer-range multibody collisions has to be included in the computations and, as a minimum, a Poisson solver added to the DSMC code. This clearly adds significantly to the complexity.

Real-Gas Effects in Nonreacting Flows

Virtually all of the validation data for DSMC so far available is for nonreacting flows. The studies that have been made within this category can be divided broadly into two areas:

1) The first area is where tests are devised to establish that the basic DSMC method yields legitimate solutions equivalent to those that would have been obtained using the Boltzmann equation and that it does so for a variety of flowfield geometries.

2) The second area is where tests are performed to evaluate the accuracy of the various approximate molecular models used in the DSMC calculations. These cover the evaluation of the appropriateness of the choice of the intermolecular potential and of the internal energy exchange scheme.

Early attempts at validation of the DSMC method were made in the mid 1970s and generally involved comparisons with results either for basic flow elements such as shock waves or for simple classical body shapes such as flat plates or cones in rarefied hypersonic flows. By this time a number of low-density, high-Mach-number wind tunnels had been constructed, and these provided a useful medium for experiments at the appropriate Knudsen numbers. Direct measurements of surface pressure and heat transfer were available, but large and uncertain correction had to be applied to these measurements because of rarefaction effects. Hence the accuracy of these data was generally not acceptable for code validation purposes. However one new method of measurement, the electron beam fluorescence technique,[10] had recently been developed, which proved invaluable. In this method a beam of collimated electrons is fired through the test gas to produce a pencil of light from which the density and temperature can be inferred using photometric and spectrometric techniques, respectively. The method is nonintrusive, and this was particularly important because physical probes caused interference that was undesirable and difficult to quantify. Thus the conventional sources of flowfield data were not suitable for code validation purposes. However, with care, it was possible to use the electron beam fluorescence method to yield data of sufficient accuracy. Some small and quantifiable corrections had to be applied to the density measurements, for example, to take into account the influence of secondary electrons. Good quality results were possible to obtain by avoiding absolute measurements, but instead normalizing the results with observations made in the undisturbed freestream (where the conditions were known). Early experiments on the use of this technique to determine the structure of shock waves were reported by Alsmeyer[11] and Robbens and Talbot.[12] Hickman[13] and Davis and Harvey[14] also obtained profiles of density for a flat-plate boundary layer in rarefied hypersonic flow.

The electron beam fluorescence method can also be used to make measurement of flow temperature. In nitrogen flows the rotational temperature is usually derived from the R-branch of the O-O vibrational band of the first negative system of the spectrum. Such tests are difficult to perform well and have been almost exclusively restricted to continuously operating wind tunnels. This is because at the low flow densities where the DSMC method is applicable the intensity of the fluorescence is very low. To resolve the spectrum adequately, it is usually necessary to perform a time-integrated observation over several minutes. Davis and Harvey[14] obtained very good spectra, but they had to revert to powerful digital filtering techniques to obtain them. This work illustrated well the care that had to be taken to obtain validation quality data.

Although conceptually all of the components of temperature can be derived from the fluorescence, the rotational value for a diatomic gas is the simplest to obtain, followed in order by the vibrational and the translational components. These latter two involve sizeable corrections and assumptions, and there is considerable doubt as to whether data of sufficient accuracy for code validation purposes can be derived for these quantities using this technique.

Other nonintrusive optical techniques are now available for flow diagnosis. Various manifestations of the laser-induced fluorescence (LIF) method are the most well developed and widely used in aerodynamic experiments. These techniques rely on the presence of certain specific species, for example, nitric oxide (NO). In high-enthalpy flows NO is a transient reaction product, and it also occurs during combustion. The various LIF techniques are generally not suitable for the code validation of nonreacting flows. Furthermore, as there is some doubt about the absolute accuracy of the technique and because it is not well suited to low density flows, no attempt so far appears to have been made to use it to validate DSMC codes.

Shock Waves

One of the simplest and most fundamental gas dynamic phenomena that can be used for code validation is the structure of a normal shock wave. Bird in his book[4] quotes a series of results he obtained, all for his VHS molecular models, which he compares with Navier–Stokes and Burnett equation solutions. As expected, some discrepancies arise. He states that the DSMC results are consistent with the experiments of Muntz and his coworkers who have made a detailed study of shock structures (see, for example, Refs. 15 and 16). In the second of these references, their computed results for shock waves in helium and argon at Mach numbers between 1.5 and 9 are compared with electron beam fluorescence data for density, temperature, and distributions for the components of molecular velocity parallel and transverse to the flow. The DSMC computations were made using the VHS collision model and one based on the

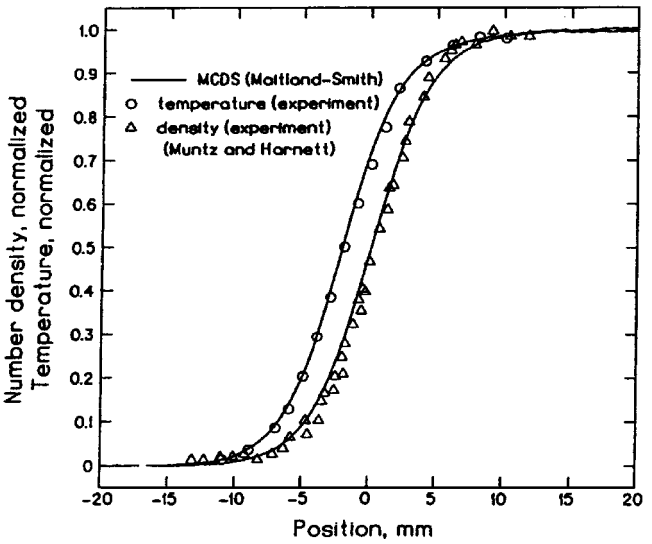

Fig. 1 Density and temperature profiles for a helium shock wave at Mach 1.59. DSMC compared with electron beam measurements (reprinted from Ref. 16).

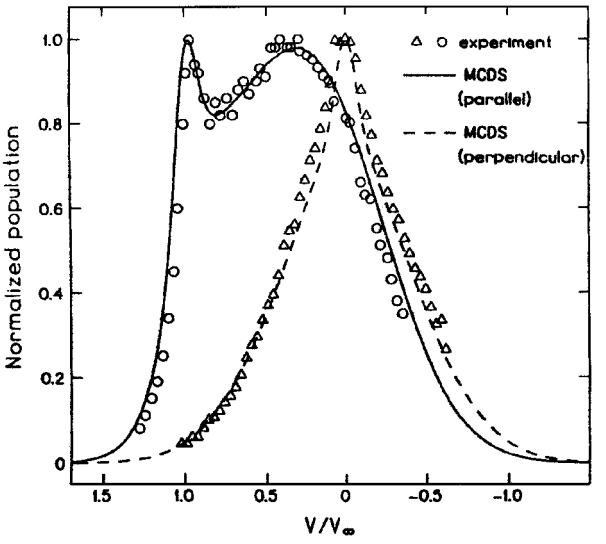

Fig. 3 Velocity distribution function for a shock wave in He at Mach 25. Electron beam measurements compared with DSMC computations (reprinted from Ref. 16).

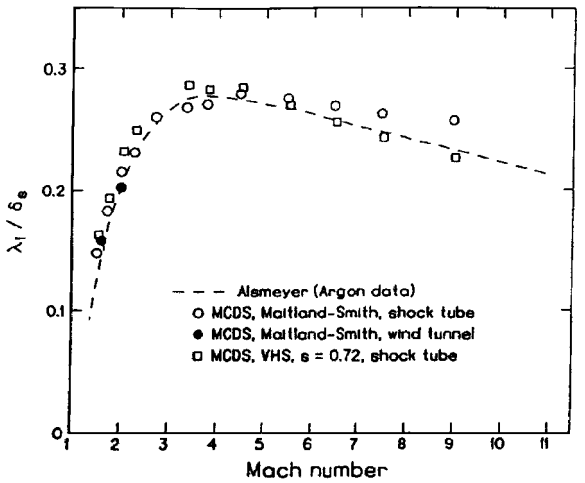

Fig. 2 Normalized inverse maximum shock thickness vs Mach number for argon (reprinted from Ref. 16).

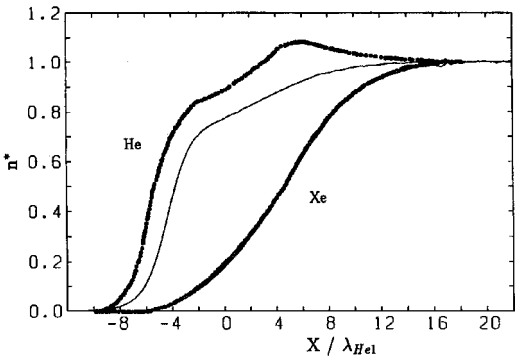

Fig. 4 Shock-wave number density profiles in a mixture of He and Xe. M = 3.89; Mole fraction of Xe = 0.03. DSMC computed results shown as symbols compared with electron beam fluorescence measurements (reprinted from Ref. 19).

Maitland–Smith potential[17] (which, from spectroscopic and transport coefficient evidence, is acknowledged as being very realistic), and the agreement with the experimental results is excellent. Some of their plots are reproduced here in Figs. 1–3. In particular, the velocity distribution functions are very faithfully predicted, which adds confidence in the DSMC code at a fundamental level.

Shock structures for mixtures of helium and xenon have been investigated experimentally by Gmurczyk et al.[18] using the electron beam fluorescence technique. Matsumoto and Koura,[19] using their VSS molecular model, compared these measurements with their DSMC computations of the density profiles (Fig. 4). They found that the profiles for the denser xenon gas were generally closely represented but the shape for the helium, which exhibits a complex profile, was not reproduced well. In his book Bird[4] shows his computed results for some of these examples using his VSS molecular model. Comparison between the two calculated profiles for helium indicates that there are certain differences that can be attributed to the two intermolecular potentials, but these are far less than the discrepancy with the measured values. Bird alludes to a recognized problem with the experiment, which he does not substantiate. This highlights one of the difficulties in validating codes—that of truly assessing how well and independently the experiment and computations have been executed. If a researcher has access to the measurements, there is the inevitable temptation to redo the calculations until good agreement with the measured data is achieved. Furthermore, most authors are reluctant to submit for publication results that show serious discrepancies between their calculations and experiments.

Data are also available for diatomic shock waves, one example being the results of Macrossan.[20] He examines sensitive factors such as the thickness and asymmetry of the density profile and compares these with classical experimental results of Alsmeyer[11] and Robbens and Talbot.[12] He concludes that, within the scatter of the computations, very good validation of DSMC profiles is achieved. The accuracy of the correlation appears to depend on the choice of the collision model. There is a trend in the results for the more sophisticated and supposedly better model based on the Morse potential, which has an attractive far-field force, to perform slightly worse than the purely repulsive inverse power models. But, the scatter in the data is larger than the difference between calculation and experiment, and this conclusion is not a robust one.

Nanbu and Watanabe[21] give an interesting example of the verification (as opposed to validation) of the DSMC method. They contended that the Bird scheme does not rigorously reproduce solutions to the Boltzmann equation, whereas their method, which they claim has a more solid mathematical foundation, does. The authors present comparisons between the results for both codes for the structure of monatomic shock waves. Interestingly the results of the two codes are indistinguishable within the numerical scatter, (Figs. 5 and 6). For this very simple one-dimensional example this paper provides corroboration that the Bird code does in fact do what it sets out to do, namely, effectively provide a valid solution to the Boltzmann equation.

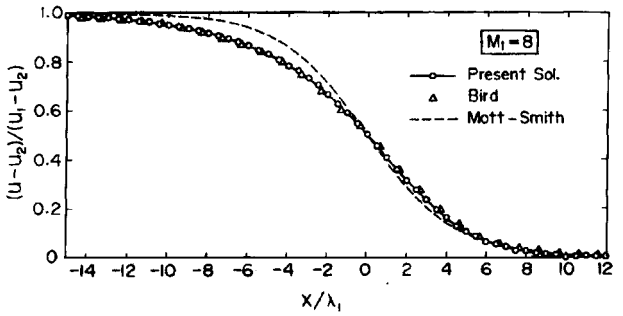

Fig. 5 Comparison of shock-wave velocity profiles computed using Bird's and Nanbu's simulation methods (reprinted from Ref. 21).

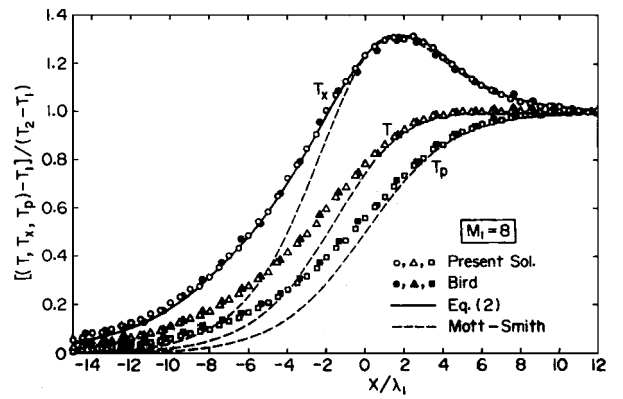

Fig. 6 Comparison of shock-wave temperature profiles computed using Bird's and Nanbu's simulation methods (reprinted from Ref. 21).

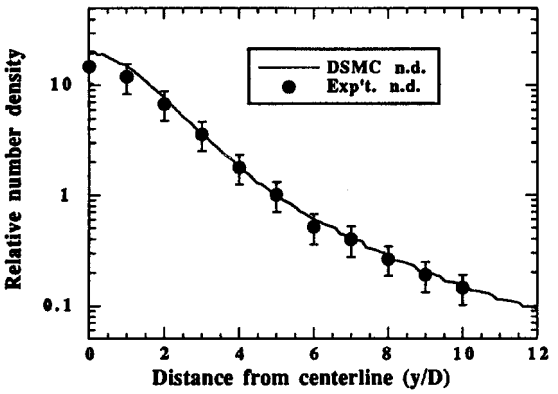

Fig. 7 Radial number density profile at $x/D = 3$ in a nitric oxide freejet. LIF measurements compared with DSMC (reprinted from Ref. 22).

Wysong and Campbell[22] and Weaver et al.[23] compared results using the DSMC method with LIF and electron beam measurements in free jets of NO and Argon and N_2, respectively. They obtained good results for the axial and radial number density distributions (Figs. 7 and 8), although in the first case some adjustments had to be made to normalize the DSMC computations. These results demonstrate the DSMC code's ability to predict well rapidly expanding flows—in contrast to the Navier–Stokes (NS) codes, which do not perform well in these circumstances.

Flat-Plate and Cone Flows

An attempt to correlate DSMC results with experimental measurements for a flat plate at zero angle of attack in rarefied hypersonic flow was first made by Vogenitz et al.[24] in 1969. This attempt did not turn out very satisfactorily because of inadequate experimental data. Two subsequent wind-tunnel studies by Hickman[13] and Davis and Harvey[14] proved to be more suitable for the purpose of DSMC validation. Vogenitz and Takata[25] used the Hickman experiment to

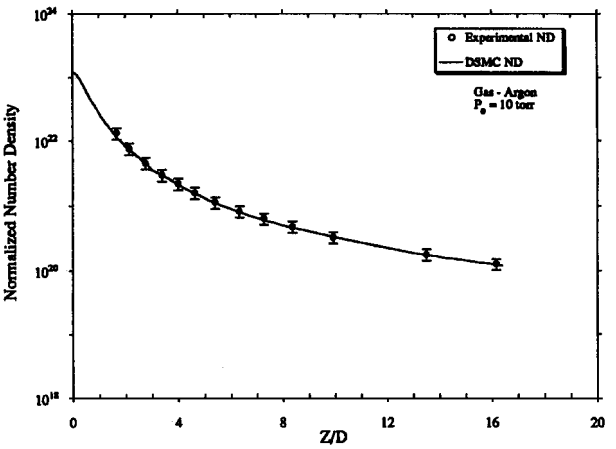

Fig. 8 Centerline number density in an argon freejet. Electron beam measurements compared with DSMC (reprinted from Ref. 23).

evaluate their DSMC computations, but their results show some numerical scatter. Davis and Harvey compared their measurements with results from their own DSMC code in which a variety of intermolecular models were tried. Because the Davis data appear to be the most consistent, we will concentrate on those data here.

To avoid problems with three-dimensional effects on a finite span flat plate, the Davis experiment was performed on the axisymmetric analog to the flat plate—a hollow sharp leading-edge cylinder. Density and rotational temperature profiles were recorded at several stations along the cylinder, which are reproduced in Figs. 9 and 10. Axisymmetric DSMC computations were performed using the following:

1) A Borgnakke–Larsen (B–L) stochastic exchange model with one of two fixed values for the exchange restriction factor ϕ. This determines the fraction of collisions treated inelastically and hence the internal energy exchange rate. The B–L model was combined with an inverse power collision model.

2) A hybrid model combining a classical Morse potential interaction for high-energy collisions with a B–L model for low energy collisions.

Generally, the predictions are close to the experimental values, and on the whole the B–L model performs satisfactorily on its own. The variations in the rotational temperature at different stations along the plate are a direct consequence of the internal energy exchange process, and the results illustrate the effectiveness of the B–L model. Changes in the value of ϕ that was used with increasing distance along the plate would have been desirable. Such an option had been suggested by Pullin in what he had termed his variable-ϕ model.[26]

The conclusion is made from this experiment that the DSMC method appears to be very effective in yielding realistic solutions to real flow problems. The internal energy exchange modeling using the stochastic B–L scheme works well, at least as far as the rotational excitation is concerned. In these flows the vibrational temperature is completely frozen, and so nothing can be concluded about the effectiveness of modeling this mode.

Planetary Probe and Blunt-Ended Cylinder

A project that captured the imagination of many researchers and proved invaluable as a validation exercise is the so-called Planetary Probe problem. This problem originated at NASA as the basis of a proposed reentry capsule and consisted of a 70-deg spherically blunted, cone with a flat base. This geometry became the object of an extensive study in which many laboratories throughout the world contributed experimental or computational resources. An AGARD Working Group (WG18) adopted it as a test problem. It was also the subject of an international blind computational fluid dynamics contest, which was included in the Fourth European High Velocity Database Workshop, organized by the ESA in November 1994 at the European Space Research and Technology Centre (ESTEC) at Noordwijk in the Netherlands.[27] It was designated test case 6, and,

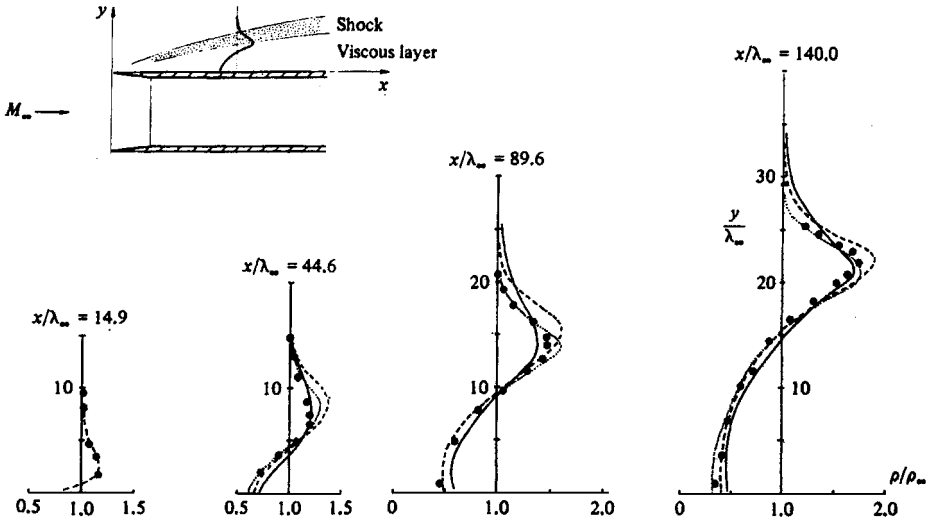

Fig. 9 Density profiles obtained using electron beam fluorescence with a hollow cylinder model. Comparison with DSMC using · · · ·, hybrid Morse; - - - -, variable phi Morse; and ——, variable-ϕ inverse power models (reprinted from Ref. 32).

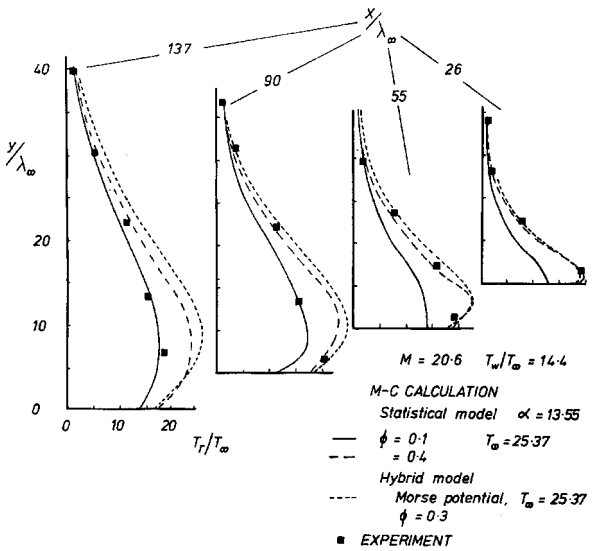

Fig. 10 Rotational temperature profiles obtained using electron beam fluorescence on a hollow cylinder (reprinted from Ref. 33).

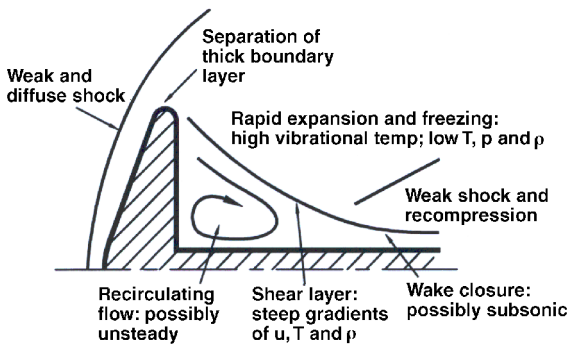

Fig. 11 Schematic of the planetary probe flow.

in the workshop, groups were invited to submit solutions for this flow for specified freestream conditions. Models of the cone were made available to experimental groups, and tests were conducted in several hypersonic wind tunnels in the United States and Europe at conditions that included rarefied ones.

The shape of the probe is indicated in Fig. 11. To support the wind-tunnel model, a long sting was provided, which changed the base flow from that of the free-flying probe. A schematic of the expected flow structure is shown in the figure. Separation takes place on the outer lip of the cone, giving rise to a recirculating base flow. Reattachment of the shear layer occurs downstream on the sting. The very rapid expansion of the flow around the lip of the cone gives rise to rarefaction and nonequilibrium effects in the base flow even at freestream conditions where the forebody flow is within the continuum range. Despite the low densities in the base-flow region, transition to turbulent flow is also possible in the vicinity of the reattachment point at least at conditions at the high-density end of the DSMC range of applicability. Thus a mixture of effects caused by rarefaction and thermodynamic nonequilibrium at one extreme and turbulent transition at the other can occur simultaneously with this configuration. This configuration provides an excellent test case where compression, separation, rapid expansion, and reattachments all play key roles. The forebody flow proved to be a relatively trivial task to compute, and much of the attention became focused on the fascinating wake flow.

Good quality measurements of drag, surface pressure and heat transfer and electron beam flowfield density and number flux surveys were obtained in various wind tunnels and were made available during the course of this study. The experiments were divided into two groups:

1) The first group consists of tests that were performed in the SR3 tunnel at Centre National de la Recherche Scientifique (CNRS) in Meudon, France, and in the V2G and V3G tunnels at DLR in Göttingen, Germany. These were performed in nitrogen at low-enthalpy conditions where the real-gas effects were restricted to rotational energy nonequilibrium.

2) Group two consists of tests at higher enthalpy that were performed in the High Enthalpy Shock Tunnel Göttingen (HEG) at DLR, Göttingen, and in the Large Energy National Shock Tunnel (LENS) at Calspan in the United States. These were performed in air and nitrogen, respectively, at conditions that were at the extreme upper range of density for DSMC and included greater degrees of internal energy nonequilibrium and some chemical activity. Details of the test conditions chosen are given in Ref. 28. The test Mach numbers ranged from about 9 to 20.

Solving this problem proved to be very popular, and over a dozen groups attempted DSMC and NS computations at one or more of the specified freestream conditions. Results were collected and correlated for the AGARD Working Group by J. Moss at NASA Langley Research Center (see, for example, Ref. 28) and by the present authors for the ESTEC Workshop. A considerable volume of data was assembled and disseminated by Moss. At the ESTEC Workshop "contestants" were not given prior access to the experimental results nor other people's solutions, and, for this reason alone, it proved to be an exceptional opportunity to verify and validate the DSMC codes without bias. This test case represents by far the most comprehensive validation exercise so far performed on the DSMC code.

We consider here only the lower-enthalpy nonreacting cases. Figure 12 shows density contours computed at NASA Langley Research Center using Bird's G2 code.[28] These are compared with measurements obtained at CNRS using an electron beam. A remarkably close correlation is seen even for the difficult wake region. At the ESTEC workshop[29] Coron from Aerospatiale (Fig. 13) and the present authors submitted two other solutions, which are almost identical to the NASA solution and equally accurate. What is particularly interesting is that the Aerospatiale and Imperial College solutions were produced without any prior knowledge of the experimental results, which were withheld by the CNRS staff until the start of the workshop. Furthermore, they were generated by codes that had been independently written, which were not derivatives of the Bird code. They provide therefore excellent evidence to both verify and validate the codes.

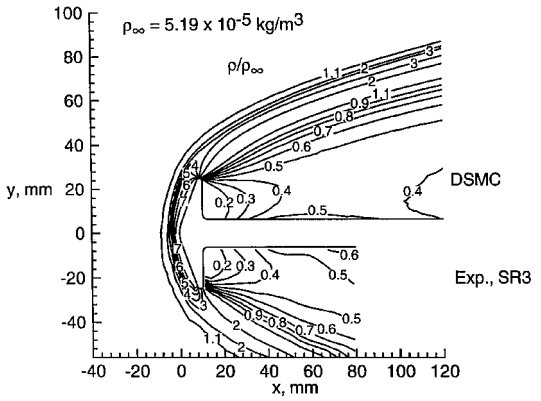

Fig. 12 Density contours calculated by Moss and Price[28] using DSMC compared with those measured with an electron beam: Mach 20, nitrogen at 1.5 km/s, and *Kn* = 0.0045 (reprinted from Ref. 28).

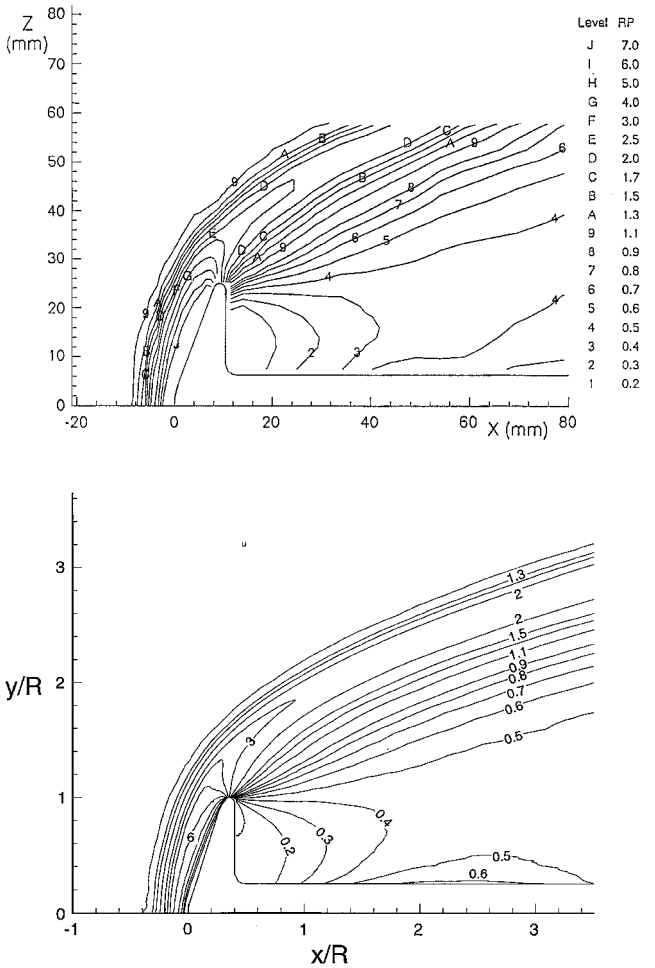

Fig. 13 Comparison between electron beam density measurements obtained in SR3 wind tunnel (top) and those calculated by Coron using DSMC (bottom) (reprinted from Ref. 29).

Examples, taken from Moss and Price,[28] of the distributions of heat transfer along the body from the stagnation point to the downstream end of the sting are given in Figs. 14–16. Comparisons of the total heat flux, drag coefficient, and particle number flux are shown in Figs. 17–19. All of these results show that a close match between calculation and experiment has been achieved, and a high level of confidence can be placed in the prediction of these quantities if the computations are performed carefully. The close agreement with the experimental results is very good evidence for the validity of the DSMC method at least for flows that involve only rotational energy exchange.

Several other solutions to this problem were submitted to the ESTEC workshop,[29] but these failed to achieve the precision of those just considered, which demonstrated convincingly that obtaining accurate solutions with DSMC codes is not always a forgone conclusion! This is a strong reminder that, in common with performing experiments satisfactorily, writing and running a DSMC code is a demanding task that requires considerable skill, care, and experience.

Experiments were also conducted at CNRS and DLR on the planetary probe at incidence to the flow. Coron and Harvey[27] and Moss

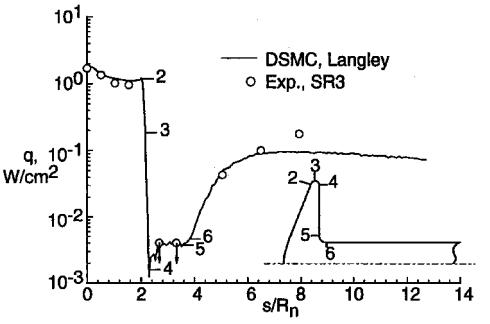

Fig. 14 Planetary probe heat-transfer measurements made in SR3 compared with DSMC computations: *Kn* = 0.0045 and *Re* = 4.18E+3 (reprinted from Ref. 28).

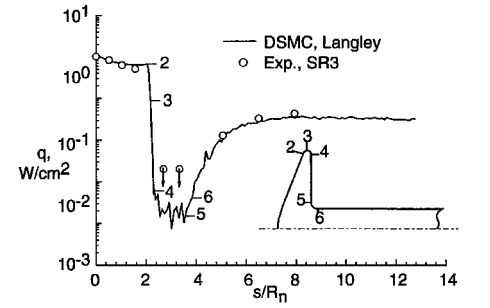

Fig. 15 Planetary probe heat-transfer measurements made in SR3 compared with DSMC and NS computations: *Kn* = 0.0134 and *Re* = 1.42E+3 (reprinted from Ref. 28).

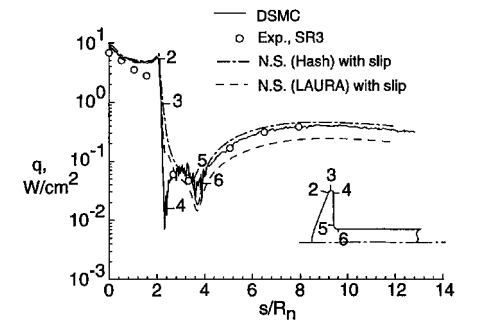

Fig. 16 Planetary probe heat-transfer measurements made in SR3 compared with DSMC and NS computations: *Kn* = 0.0005 and *Re* = 3.626E+4 (reprinted from Ref. 28).

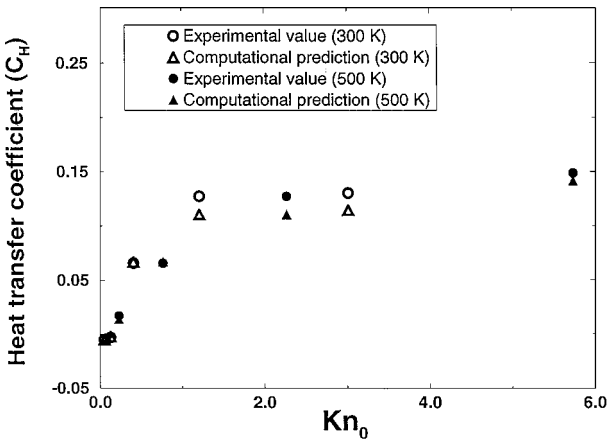

Fig. 17 Authors' own predictions of the heat-transfer coefficient of the planetary probe in the V2G experiment.

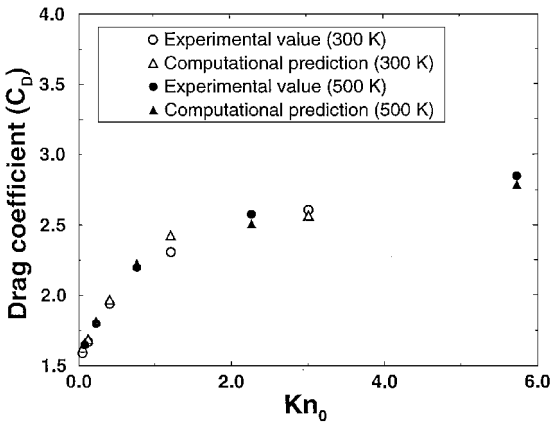

Fig. 18 Authors' own predictions of the drag coefficient of the planetary probe in the V2G experiment.

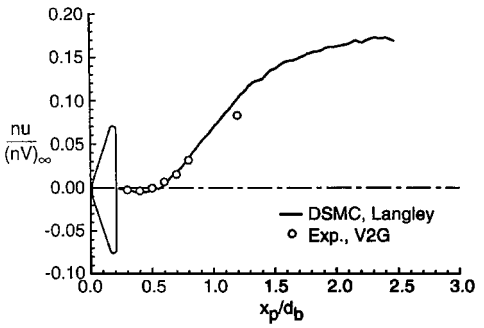

Fig. 19 Number flux profile along the wake centerline of the planetary probe in the V2G wind tunnel. Measurements made with a Patteson probe compared with DSMC (reprinted from Ref. 28).

and Price[28] used three-dimensional DSMC codes to obtain solutions for this, and both obtained excellent correlation with the density contour data and heat transfer on the windward side (Fig. 20). The three-dimensional DSMC codes use a core algorithm that is the same as in the two-dimensional versions. Thus the principal differences are confined to the complexity of the mesh and particle searching routines and to the much heavier memory and computing resources required. However these results are important as they extend the confidence in the method already demonstrated in the plane and axisymmetrical problems to fully three-dimensional and, hence, more demanding flows.

DSMC computations on the flow establishment time for the planetary probe wake are given in Holden et al.[30] These computations were for the lowest-enthalpy LENS tests conditions where some chemical activity took place. These computations show that the

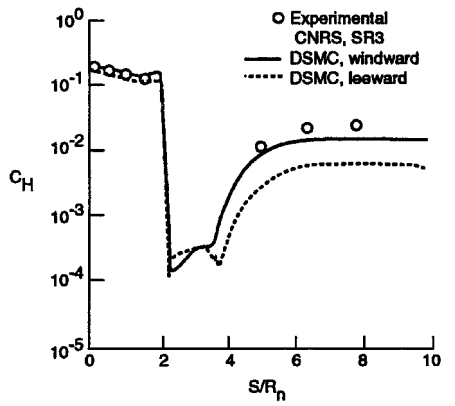

Fig. 20 Comparisons of SR3 experimental and computed heating rates at 10-deg incidence (reprinted from Ref. 28).

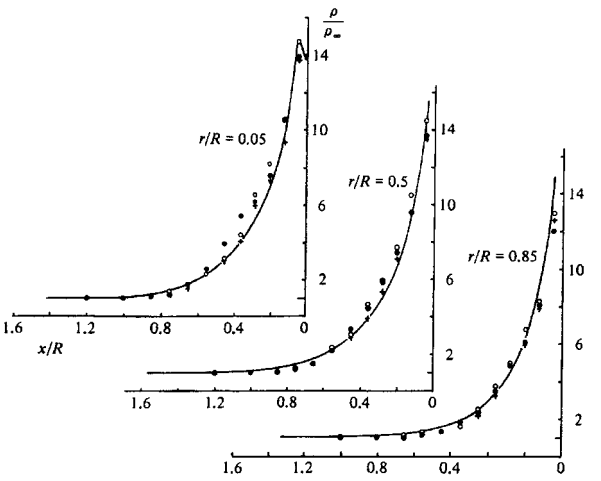

Fig. 21 Streamwise number density profiles at three radial positions ahead of blunt-ended cylinder. Electron beam measurements compared with DSMC computations using ○, hybrid Morse potential model; ●, variable-ϕ, Morse potential model; and +, variable-ϕ, inverse power model (reprinted from Ref. 32).

wake flow takes about 3 ms to establish and that the heat transfer does not reach its final distribution before this time. This conclusion was confirmed by the experiment. Interestingly the calculations also show that the pressure distribution reaches its final level in about half this time. The difference is attributed to the pressure being established though the mechanism of wave propagation at about the sonic speed, whereas the heat transfer is dependent on the convection of flow within the recirculating base flow, which is a slower process. Although not precise, these observations give some validation that time-resolved DSMC computations can be relied upon.

Another blunt-body configuration that has attracted considerable attention is the blunt-ended circular cylinder axially aligned with the flow. This was tested experimentally by Harvey et al.[31] using an electron beam technique to obtain density and rotational temperature measurement ahead of its front face. The tests were conducted in nitrogen at Mach 25 for Knudsen numbers based on cylinder diameter of the order of 0.03. Results for the density and rotational profiles along the stagnation streamline are cited in Figs. 21 and 22, respectively.[32,33] This flow is very similar to the planetary probe's just described in that the only real-gas effect that plays a significant role is the rotational energy exchange. Very good agreement with the density profiles is observed, and the conclusion is made that the computations and experiments agree within the expected errors in the measuring technique. Taking into account the uncertainties in the wind-tunnel test conditions and the problems imposed using a sophisticated technique such as electron beam fluorescence, these errors are estimated as being of the order of ±3% for the density ratio and ±10% for the rotational temperature. Although quite good agreement is seen with one set of rotational temperature

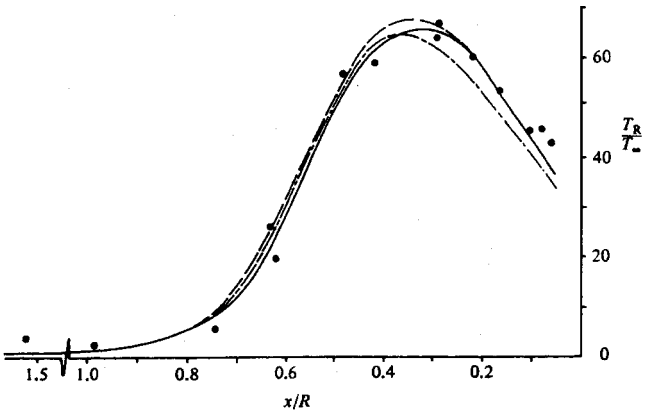

Fig. 22 Rotation temperature distribution along stagnation streamline of blunt-ended cylinder: M = 20.6 and Kn = 0.02. Electron beam measurements compared with various DSMC models (reprinted from Ref. 33).

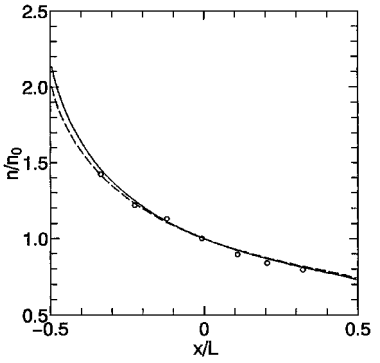

Fig. 23 Nitrogen number density distribution between two heated plates. Electron beam measurements compared with DSMC (reprinted from Ref. 34).

measurements, in a second set, not reproduced here, there is some evidence that the B–L internal energy exchange model underpredicted the rate at which energy is transferred into the rotational mode. This could be simply attributed to an inappropriate value being employed for the exchange restriction factor ϕ used in B–L model. (This quantity is approximately the inverse of the rotational relaxation number.) However, these calculations were performed using a variable ϕ, which was collision energy dependent and hence purported to reproduce correctly the variation of the rotational relaxation with temperature. These computations appear to point to a possible weakness in the B–L formulation.

This experiment specifically addressed the detailed behavior of the flow in a merged shock layer. This flow exhibited a very distinct difference to what would have been expected had the flow been in the continuum range. Under these rarefied conditions a monotonic increase in density is observed along the stagnation streamline. In a continuum flow the first disturbance in the density would be a sharp rise corresponding to the presence of a Rankine–Hugoniot shock wave. This would give an increase of a factor of about six in density ratio. Behind the shock wave there would be a plateau before a further gradual rise takes place because of cooling of the flow near the wall. The good agreement between DSMC computation and experiment again adds evidence to validate the method for low-enthalpy hypersonic flow.

Koura[34] used the example of rarefied nitrogen gas contained between two parallel plates at a large temperature difference to evaluate the use of statistical inelastic collision cross sections used in his DSMC code. Good experimental data are available for this fundamental problem. An excellent agreement for the number density profile was obtained, as can be seen from Fig. 23, which shows results for a Knudsen number of 0.11 with the plates at 79 and 293 K. The closest agreement was achieved when the almost universally used fully accommodating surface boundary condition was abandoned for one with a coefficient of 0.82. This inevitably raises a question about the unchallenged assumption of a fully accommodating, diffuse boundary condition normally employed in all DSMC computations involving so-called engineering surfaces that can only be answered with careful experimentation using, for example, molecular beams.

From these cited cases the conclusion is made that there is overwhelming evidence that the DSMC method yields very good results for flows involving only internal energy exchange. The simplified VSS and B–L molecular interaction models appear to work satisfactorily within an engineering context.

Flows with Chemical and Ionizing Reactions

Many workers have made extensions to the DSMC method to take into account the complex chemistry that takes place in N_2/O_2 mixtures, air, or CO_2/N_2 planetary atmospheres. Experimental validation of these codes has presented a major problem for several reasons. First, the relevant flows are of low density and hence difficult to investigate. Second, significant chemical activity only takes place in flows with stagnation enthalpies in excess of 5 MJ/kg. This restricts the experiments to a small number of expensive-to-run ground facilities or upper atmospheric flight tests. In either case the difficulty in obtaining validation quality data is exacerbated. As the enthalpy is increased, greater uncertainty is experienced in characterizing the freestream flow conditions in ground facilities. The combination of low density and high enthalpy produces test flows that are in a state of nonequilibrium, yet the properties of these flows have to be carefully characterized before any meaningful measurements can be attempted. Instrumentation systems to measure the quantities of interest in the flow, such as species mass faction or number density, are in their infancy. They tend to be very complicated, hard to use in ground facilities, and almost impossible in flight tests. To date they cannot be described as precise. These difficulties are added to the fact that most suitable ground facilities are intermittent and have running time measured in milliseconds or less. Data such as heat transfer or pressure are more readily obtainable, but these tend to be the least sensitive indicators of how well the reacting flow code is performing. All of this goes to explain why information suitable for direct DSMC validation is virtually nonexistent. Evaluation of the codes has only been possible indirectly from, for example, surface flux measurements or from observations of thermal radiation intensity or spectrum.

For these reasons most of the published attempts to validate DSMC for reacting flows have been made using flight-test data. However, uncertainties in the ambient conditions and the severe difficulties posed in performing such experiments have, almost inevitably, meant that the quality of the information falls below that required for validation purposes. Nevertheless, some data are better than none, and we will now examine the main evidence that currently exists.

Computations have been made by Moss et al.[35] on the forebody flow over the Japanese Orbital Reentry Experiment (OREX) vehicle. This had a 3.4-m-diam, 50-deg spherically blunted conical shape. The calculations were made for a velocity of 7.4 km/s at zero incidence for altitudes ranging from 80 to 200 km. The Knudsen numbers thus ranged from 0.0009 to 58. The computations were made with a VHS molecular model, constant ϕ, B–L rotational relaxation, and five species air chemistry. Interaction with the surface was assumed to be diffuse, fully thermally accommodating, and have finite catalyticity. Results for the stagnation point heat transfer are shown in Fig. 24, where comparison between DSMC results, flight inferred data, and Navier–Stokes computations is shown. Good agreement is indicated, but the fact that NS computations are also very close emphasizes the insensitivity of this measurement to rarefaction and chemistry. Axial acceleration measurements were available from the flight tests from which the variations in the drag were inferred. The DSMC computations agreed well with these, but again they are insensitive to, and hence are unlikely to show up, shortcomings in the chemical modeling.

Computations by Rault[36] of the flow about the Space Shuttle Orbiter using a full reacting flow representation for air gave moderately good predictions for the forces acting during reentry, but the heat transfer was not well represented in these calculations. This may well have had more to do with the difficulties in performing the demanding three-dimensional computation on the complex shape than with shortcoming of the DSMC algorithm.

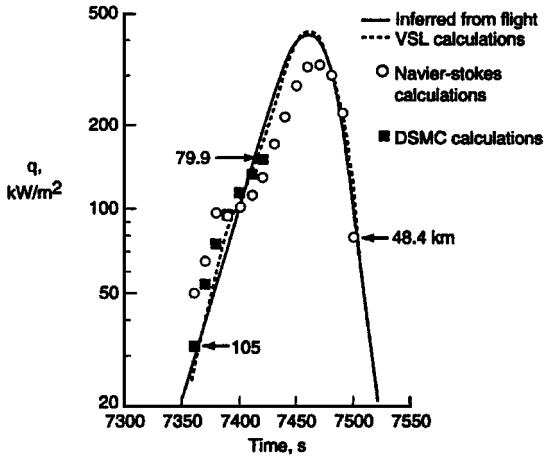

Fig. 24 OREX stagnation-point heating rates (reprinted from Ref. 35).

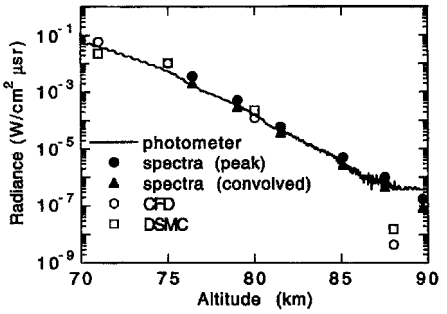

Fig. 25 BSUV experiment. Emission of nitric oxide at 230 nm (reprinted from Ref. 37).

There have been other attempts to compare DSMC computations with flight data. A good example is the study by Boyd et al.[37] of the flow ahead of the bow of two sounding rockets used in the bow-shock ultraviolet (BSUV) flight tests. One of these vehicles achieved a velocity of 5.1 km/s at altitudes in the range of 65–90 km. Spectroscopic measurements of nitric oxide and atomic oxygen emission in the ultraviolet were available for comparison with DSMC and NS computations. The paper quotes spectrally resolved results for the NO emission at 230 nm and O at 130.4 nm. Figure 25 shows one set of results, and close agreement is seen with the measurements for the higher densities. However at 88 km the measurements are underpredicted by a factor of about 30. The authors attributed this to inappropriate modeling of the nonequilibrium radiation and of the exchange reactions:

$$N_2 + O \leftrightarrow NO + N, \qquad O_2 + N \leftrightarrow NO + O$$

The paper indicates that the NS results are very similar to the DSMC even at 80 km, which is somewhat surprising. The rarefaction and, in particular, nonequilibrium effects appear to manifest themselves quite suddenly above this altitude where both codes performed equally badly. This experiment does not give great confidence in the accuracy of the DSMC code in the area in which it should be performing well.

The Skipper project was the third of these missions that were aimed at investigating the aerothermal chemistry of reentering spacecraft. Higher velocities (8 km/s) were achieved, and spectrally resolved measurements of the radiation from the bow-shock region were obtained. DSMC computations of this flow have been reported by Moss and Price,[28] but comparisons with the radiance measurements do not appear to have been published.

A major difficulty in interpreting the results of this sort of exercise is that the experiments generally do not provide the type of information that is particularly useful for evaluating the accuracy of the codes at a fundamental level. Radiation is the end product of a complex series of events involving the flow formation, complex chemical and ionic interactions, and the thermal radiation process itself, and all occur under conditions of chemical and thermodynamic nonequilibrium. If discrepancies occur, it is usually not possible to pinpoint which part of the code is at fault.

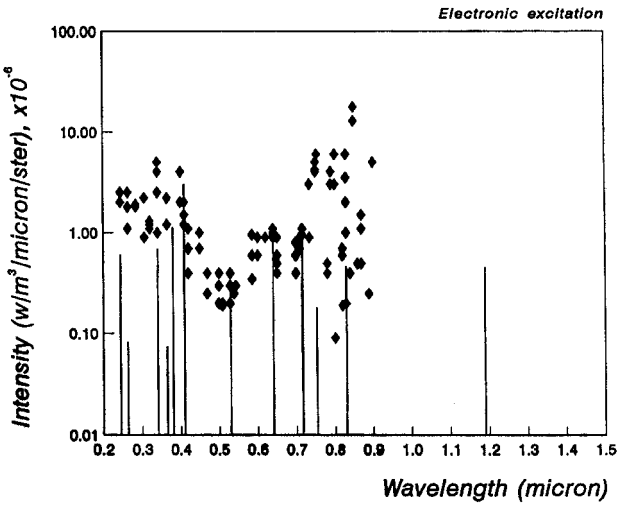

Fig. 26 Nonequilibrium DSMC spectral intensity prediction (Gallis and Harvey[38]), shown as lines, compared with an Avco-Everett experiment in air at Mach 29.

The expectation of predicting radiation accurately is poor, and the differences between calculation and experiment are often measured in orders of magnitude. This leaves the investigator to speculate which of many possible factors adversely influences the results. Within the codes there are many parameters that are not known with great certainty, and these can be adjusted to yield better results; hence, for truly objective validation of the codes, there is a pressing need to conduct blind contests. Before this is possible, suitable experimental data will have to be made available.

A further example where thermal radiation was predicted in the flow behind a shock wave is in a paper by Gallis and Harvey.[38] Here the authors show resolved spectra (Fig. 26) compared with laboratory measurements made in a nitrogen/oxygen mixture in a shock tube by Allen et al.[39] A maximum entropy formulation was used to model the chemical and ionizing reactions. Experimental and calculated cross sections were used to determine the excitation probabilities without assuming equilibrium of the excited states. Reasonably good agreement was achieved for the lines for which spectral data were available, especially in the nonequilibrium parts of the flow.

The somewhat circumstantial evidence from these thermal radiation test cases gives some credence that the DSMC method is capable of predicting thermal radiation with moderate accuracy and hence, presumably, the underlying chemistry. The degree of confidence is, however, significantly less than for the nonreacting flow cases.

There is one set of experimental data that has been obtained from ground-based facilities with the intention of extending the process of DSMC code validation. These data complement the information on the planetary probe just discussed by extending it into the high-enthalpy range. Experiments were conducted in the LENS facility at flow conditions of about 5 MJ/kg at which only moderate chemical activity takes place. Heat-transfer and surface-pressure measurements were made, but no flowfield data were taken. The density at which these tests were conducted was high for DSMC simulations, and unfortunately, so far, no fully converged solution has been produced although several have been attempted. Further tests have been carried out at higher enthalpies in HEG. The only statement that can be made about this series of tests is that, to date, the work is inconclusive principally because of the failure of the DSMC community to produce good solutions to this problem.

Reaction Rate and Cross-Section Evidence

The direct validation of the DSMC codes when applied to high-enthalpy reacting flow cannot proceed properly at the present because of a lack of good test-case experiments in which detailed

information on flowfield variables such as species number densities and molecular states has been measured. An alternative approach to establishing the validity of the code is to examine whether constituent parts of it perform correctly. In the case of the reacting flow codes, tests can be devised to see if the reaction part of the software tested on its own gives the correct chemical dynamics.

A problem that is encountered in doing this is that there is a scarcity of information about the reactions that occur at high enthalpies in air. What is really required is a set of detailed cross-sectional measurements for each reaction. But these are not generally available—even the Arrhenius reaction rates are often in dispute. Rates measured or theoretically predicted for other disciplines are commonly used without a clear indication that these data are applicable to the temperature regime of interest. Park[40] has compiled a set of the rates that are considered to be the most reliable for aerospace applications. This data set has been widely used, and it can be accepted that it contains the best available data. The first step in evaluating a DSMC code is to examine how well it reproduces the rates over a range of conditions. But by using these rates and assuming them to be correct, to validate the DSMC chemistry models we are obliged to compare equilibrium reaction rates, i.e., the integral instead of the integrand. Successful reproduction of these rates is a necessary but not sufficient condition for a chemistry model. Recently Wadsworth and Wysong[41] demonstrated that chemistry models having utterly different cross sections could successfully reproduce the same reaction rates.

For the case of ionized species, where the particles involved can readily be detected, the measurement of cross sections becomes much easier, and there is an extensive collection of data that is considered to be reliable. This is in marked contrast to their counterparts in nonionic chemistry. Gallis and Harvey[42] have used such cross-sectional data to support the appropriateness of their maximum entropy ionization model. Examples of such cross sections involving ionization of atmospheric species caused by electron and heavy particle impact are presented in Figs. 27 and 28. This theory predicts that the cross sections will vary according to an expression of the form

$$P = [1 - (E_{\text{ion}}/E)]^{\zeta_B} \exp(-aE_{\text{ion}}/E)$$

The ionization threshold is a known fixed quantity for each reaction. This leaves only one parameter that can be varied to fit the calculated cross sections to the measured values over the range of temperature or collision energy of interest. In practice very good agreement between the two is achieved, which gives credence to the fact that the theoretical model has captured the essential physics of the reaction and that it will represent the process correctly within a simulation even under conditions of severe nonequilibrium. Examples of these results are given in the two figures. Similar comparisons showing the same level of agreement can be obtained for virtually all of the

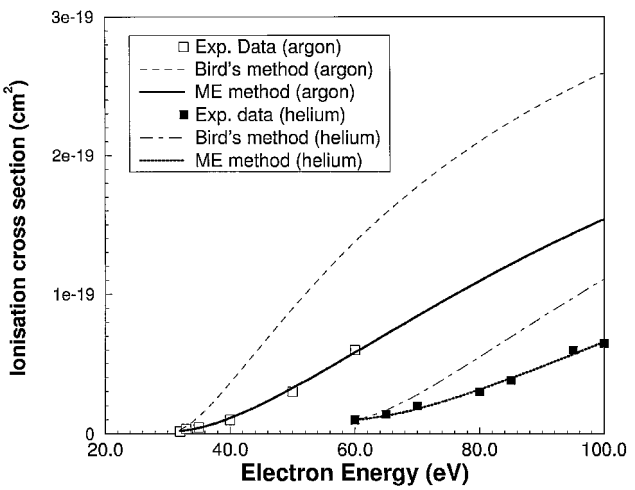

Fig. 27 Comparison of the measured and calculated cross sections for ionization of He and Ar, using a maximum entropy formulation (reproduced from Ref. 42).

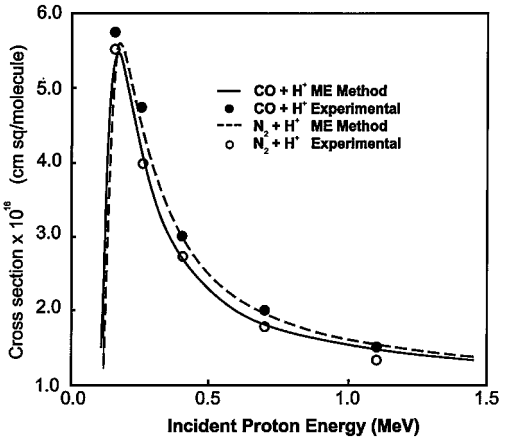

Fig. 28 Comparison of the measured and calculated cross sections for ionic reactions using a maximum entropy formulation (reproduced from Ref. 42).

relevant ionic reactions. The ability to match these cross sections is a far more stringent test of a model than simply producing the correct temperature dependence of the Arrhenius (i.e., near equilibrium) reaction rates.

Comparisons of the type just given provide vital insight into the performance of the chemistry models and enhance their credibility. It is accepted that there will be serious difficulties in performing wind-tunnel experiments to provide flow information for direct validation high-enthalpy data for DSMC codes. Perhaps as a less expensive alternative molecular beam experiments could be performed on individual reactions to obtain measurements that could be used to evaluate the chemistry models. If the chemistry model can be validated, one can reasonably assume that it will perform correctly if employed in a DSMC code.

Conclusion

There is overwhelming evidence that the DSMC method is capable of providing very accurate prediction of rarefied flows *where the only real-gas effect present is the exchange of internal energy, i.e., no chemical reactions or ionization take place.* Under these conditions the assertion can be made that there are a sufficient number of good quality computations and experiments that agree well and from this evidence the method can be said to have been validated beyond reasonable doubt. Furthermore it appears that the commonly used VSS and B–L molecular collision models perform adequately well for all engineering purposes. Most of the evidence to support this statement has, in fact, been obtained for hypersonic flows, but some also exists outside the scope of this paper that substantiate that the method works well for low-speed flows.

When it comes to reacting flows, the task of validating DSMC is not done. Circumstantial evidence suggests that the codes are working reasonably well. Much depends on how well the chemical reaction models perform under situations where considerable degrees of nonequilibrium exist. At this stage of the development of these models, it cannot be claimed that many of the models currently being employed have been shown to be capable of reproducing the correct cross sections. Only for the case of the ionizing reactions, where good data are available, has the behavior of the collision algorithms been shown to be correct.

Future validation of the prediction methods will have to be taken step by step. First, flows involving chemical reactions without ionization will have to be tackled. High-quality experimental data will be required. Before embarking on acquiring these data, it is essential that the research community involved carefully select appropriate problems to be studied. On the one hand, it is important to choose test cases that are sensitive to changes in the chemistry and to focus the experiments on measurements that pinpoint the differences in the codes and on the chemical reaction models used. On the other hand, it is important to decide on experiments that are practical to perform and where there is a very good chance that validation quality data will be forthcoming. It should not be forgotten that

accurate test condition characterization is an essential prerequisite for these studies. They will also involve the selection, and possibly even the development, of suitable measuring techniques to obtain data of direct value, such as species concentration, for the process of code validation. A shock/shock interaction with chemical reactions present may be a very interesting, exciting, and relevant problem, but it happens also to be extremely difficult to study experimentally and for this reason is unsuitable. An indented cone designed so that the flow is very sensitive to changes in the chemical activity within the flow—a problem that has already been suggested as a test case—would be a far more robust experiment and thus would be a more appropriate choice.

The importance of acquiring suitable data for meaningful code evaluation cannot be overemphasized. Pressures and forces are usually insensitive to chemical activity and so do little to assess the effectiveness of a code. Information that is really needed is flowfield number densities of individual species. Knowledge of the state of components would also be highly desirable, but generally acquiring this information is beyond the scope of present-day instrumentation in high-enthalpy facilities. On the other hand, being too ambitious and basing experiments on acquiring data that prove to be too difficult to measure with sufficient accuracy, even with state-of-the-art instruments, does little to further the cause of code validation.

Collaboration appears to have been a splendid catalyst in achieving results in the quest to validate codes. It is confidently hoped that the new NATO Research and Technology Organization Working Group 10, which grew from the AGARD WG18, will take on board this task of the next phase of validating DSMC methods, which inevitably will involve studying flows that are chemically active.

Beyond pure chemistry lies the area of higher-enthalpy flows that exhibit low levels of ionization. The task of providing precise experimental data for these flows appears even more daunting. But beyond this is the realm of highly ionized flow—real rarefied plasmas. Surprisingly these may well prove to be easier to investigate than even the nonreacting hypersonic flows, and they have already stimulated much interest for a variety of nonaerospace reasons. Some of the experiments to validate the codes can be conducted in low-speed flows under laboratory conditions, and the diagnostic methods are relatively much simpler. Once the DSMC method has been properly extended into this realm, it may well prove to be the regime where the various reaction models can be rigorously tested and from where a new series of validation tests as successful as the planetary probe will emerge.

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