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Extensive Validation of a Monte Carlo Model for Hydrogen Arcjet Flowfields

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A particle-based Monte Carlo numerical method is applied for the first time to model the nozzle and plume flows of a low-thrust hydrogen arcjet. Starting from a continuum solution of the flow just downstream of the constrictor, the present analysis employs the direct simulation Monte Carlo technique to compute the nonequilibrium fluid mechanics and thermochemical relaxation. Simulation of plasma field effects is included at a simple level using charge neutrality. A model is implemented to include ohmic heating in the simulation. Results are presented for two different arcjet flow conditions. Comparisons of Monte Carlo results with experimental measurements for a variety of flowfield properties are made in the nozzle interior, the nozzle exit plane, and the near-field plume flow. Comparison of prediction with measurement is also made for thruster performance. For almost all flow properties, good agreement is obtained between simulation and measurement. This indicates that the Monte Carlo model is a viable approach for optimization of arcjet performance, and for the prediction of spacecraft interaction effects.

Introduction

ARCJETS operated at a power level of about 1 kW are an attractive candidate for use as electric propulsion devices on spacecraft. They offer substantial increases in specific impulse compared with chemical rockets and resistojets. Unfortunately, the performance of arcjets remains poor with propulsion efficiencies in the range of 30–50%. There is a need for accurate numerical simulation of the flows generated by these devices, both for improving their performance and for the analysis of potential spacecraft interaction effects such as contamination. There are many coupled physical phenomena at work in an arcjet that makes numerical simulation difficult. Nonequilibrium kinetic processes include rotational and vibrational relaxation, and several chemical mechanisms including dissociation, recombination, and ionization. In addition, plasma effects are important.

A hydrazine arcjet has been developed and flown in space.[1] In terms of basic research, however, hydrogen arcjets have received considerable attention. Several experimental studies have been conducted on an arcjet designed and fabricated at NASA Lewis Research Center. The nozzle has a half-angle of 20 deg, an exit diameter of 9.525 mm, and an exit-to-throat area ratio of 225. A schematic diagram of this thruster is shown in Fig. 1. The NASA Lewis Research Center's hydrogen arcjet has been used in experimental investigations to determine its performance[2] and flowfields.[3,4] Of considerable importance is the fact that several different diagnostic techniques have been applied to these flows, yielding measurements that include translational and rotational temperature, velocity, and number densities of atomic and molecular hydrogen. These data offer excellent opportunities for detailed calibration of modeling efforts. Arcjet models based on continuum formulations have been developed by several groups.[5–8] There are two main problems with the continuum approach. First, there is a significant degree of thermal and chemical nonequilibrium in these flows that may not be simulated accurately using a continuum formulation. Second, it is difficult to extend the continuum simulations out to the plume produced by the arcjet, and so these methods are not well suited for the prediction of spacecraft interference effects.

This paper describes the first application of the direct simulation Monte Carlo method (DSMC) (Ref. 9) for computation of the flowfields of an arcjet. A continuum solution[5] of the arcjet is used to start the DSMC computation at a point just downstream of the nozzle throat. The DSMC computation proceeds through the nozzle and into the near-field plume expansion region for a hydrogen arcjet. The motivation in applying this technique to the nozzle flows, where existing continuum formulations are already well developed, is the availability of experimental data to allow verification of the DSMC models. In satellite propulsion, the DSMC technique has been applied and successfully verified to the plume of a hydrazine rocket,[10] and to the nozzle and plume flows of both a nitrogen resistojet[11] and a cold flow of hydrogen through an arcjet.[12] In this paper, a brief description is provided of the kinetic and plasma models developed for this application; more details may be found in Ref. 13. Extensive comparison of the Monte Carlo calculations with available experimental data is made in the nozzle interior, nozzle exit plane, and plume expansion flowfields. Comparison is also made with measurement for thruster performance.

Numerical Method

The DSMC (Ref. 9) uses the motions and collisions of particles to perform a direct simulation of nonequilibrium gasdynamics. Each particle has coordinates in physical space, three velocity components, and internal energies. A computational grid is employed to group together particles that are likely to collide. Collision selection is based on a probability model developed from basic concepts in kinetic theory. The method is widely used for rarefied nonequilibrium conditions and finds application in hypersonics, materials processing, and micromachine flows.

The extension of the technique for application to arcjet flows is described in detail by Boyd.[13] This required development of a number of new physical models. Deposition of energy by the arc into the gas flow is highly localized, giving temperatures of about 30,000 K and ionization fractions of 30% on the axis downstream of the constrictor. This small region of high-temperature plasma mixes with the main flow consisting of low-temperature, molecular hydrogen. In terms of intermolecular collisions, mechanisms must be included in the nu-

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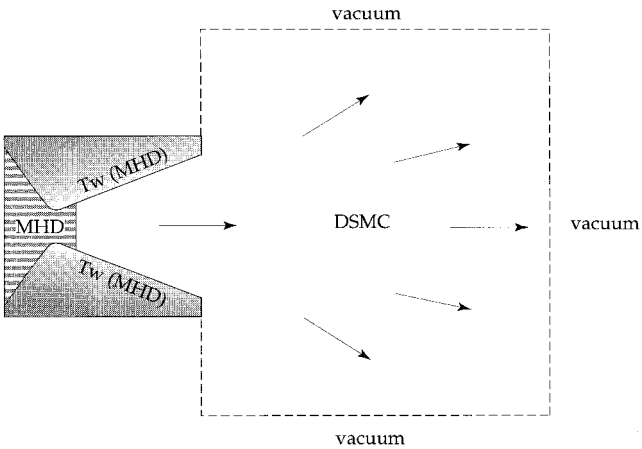

Fig. 1 Schematic diagram of the 1-kW hydrogen arcjet showing DSMC boundary conditions.

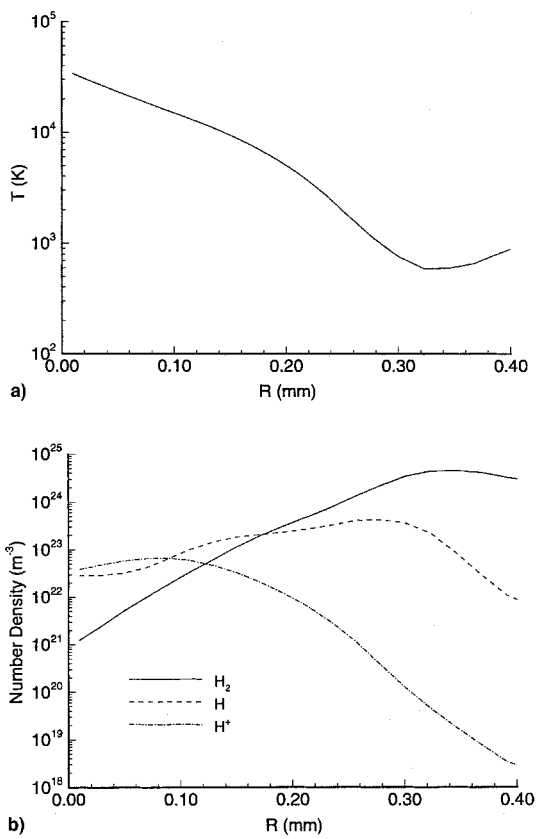

Fig. 2 Radial profile of a) temperature and b) species concentrations near the nozzle throat.

merical model to account for 1) momentum transfer, 2) rotational excitation, 3) vibrational excitation, 4) dissociation/recombination, and 5) ionization/recombination. The presence of charged species requires modeling of plasma effects at some level.

For a hydrogen arcjet, the four main species present are H_2, H, H^+, and e^-. In general, the most important collision types that determine the arcjet flowfield are H_2–H_2, H_2–H, H–H, H_2–e^-, and H–e^-. The widely used variable hard sphere (VHS) collision model of Bird[9] is employed in the present work. The total collision cross sections for the first three collision types are obtained from the momentum cross sections of Vanderslice et al.,[14] in which collision integrals were tabulated for the temperature range of 1000–15,000 K. The cross section for the H–e^- collision is determined using the experimental data of Crompton and Sutton.[15] The cross section for the H–e^- collision is determined using the simple analytical expression given by Yos.[16] The level of agreement between the models used in the DSMC code and the original sources is excellent. Other cross sections are much less important and are assigned values such that the results of hydrogen atoms are used for hydrogen ions. For example, the cross sections for H–H collisions are also used for H^+–H^+ collisions. While this results in some lack of accuracy, it is expected that the effect will be small because these collisions are relatively infrequent.

Molecular hydrogen is an interesting diatomic molecule because it has relatively large values for the characteristic temperatures of rotation and vibration. This results in long relaxation times for these modes. Previously, a rate model for determining the probability of translational–rotational energy transfer for hydrogen at low temperatures was developed and verified.[12] This same model is employed again here, although it is recognized that it may be inaccurate at the very high temperatures encountered in the arcjet. The probability of vibrational energy exchange employs the familiar Landau–Teller relaxation time with parameters obtained experimentally by Kiefer and Lutz.[17] Once again, it is recognized that this approach may be inaccurate at the very high temperatures found in the arcjet. There are only two chemical reactions implemented in the present study, they are the dissociation of molecular hydrogen and the ionization of atomic hydrogen. The rate coefficients are obtained from Refs. 18 and 19.

The DSMC technique has been combined directly with plasma simulation methods such as particle-in-cell in the electric propulsion and plasma processing communities.[20] In those cases, the peak electron number density is sufficiently small to make this computationally possible. That is not the case here, and so a very simple scheme is employed to simulate electric field effects. The electrons are constrained to move through the flowfield with the average ion velocity in each cell. In terms of electron motion, this means that the average electron velocity is equal to the average ion velocity. This approach

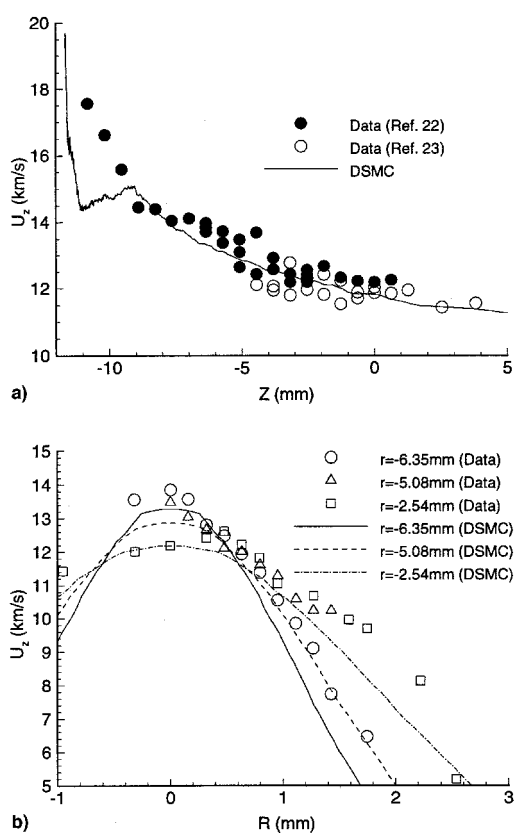

Fig. 3 a) Axial velocity component along the nozzle centerline and b) radial profiles of axial velocity component at different axial locations in the nozzle for P = 1.34 kW.

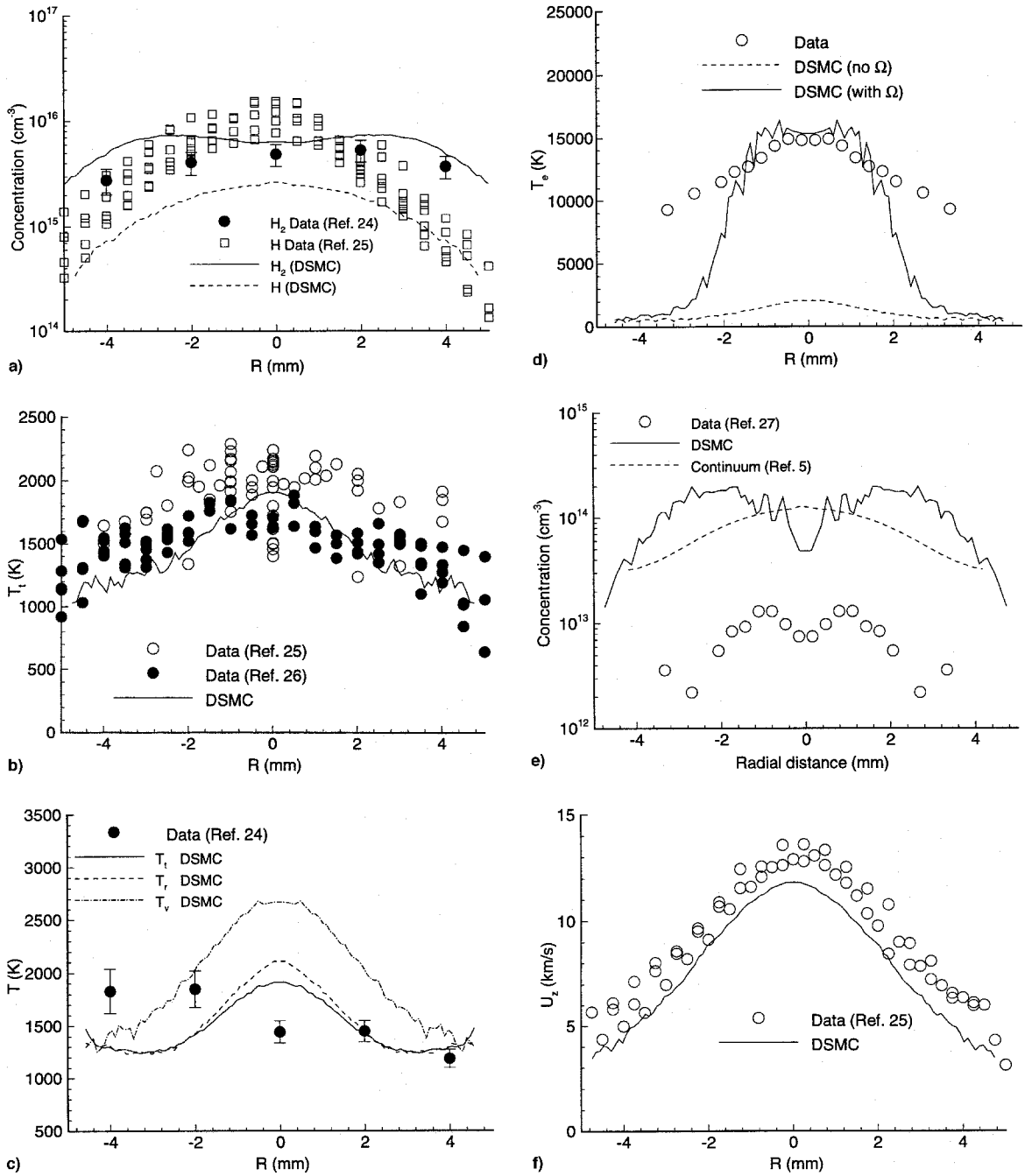

Fig. 4 a) Concentrations of neutral species, b) translational temperature of atomic hydrogen, c) thermal nonequilibrium of molecular hydrogen, d) electron temperature, e) electron concentration, and f) axial velocity component of atomic hydrogen in the nozzle exit plane for P = 1.34 kW.

ensures charge neutrality, but omits the effect of the electric field on the ions. A second important plasma effect that is included in the DSMC simulation is ohmic heating. This is an important source of energy that results from the current represented by the flux of charged species through the thruster. Using standard plasma physics theory, a source of energy is computed in each cell of the simulation caused by ohmic heating. This energy is added to the charged particles in each cell in each iteration of the calculation. This energy is eventually conveyed to the neutral particles through intermolecular collisions. The scheme is described in detail in Ref. 13.

The collision and plasma models are implemented in an existing DSMC code that is designed for efficient performance on vector supercomputers.[21] The DSMC computations are begun at a location downstream of the nozzle throat as shown in Fig. 1. The initial profiles of flow properties are obtained from continuum simulations provided by the magnetohydrodynamics code (MHD) of Butler.[5] This continuum code solves the Navier–Stokes equations using a single fluid hydrodynamic description of the flowfield. The code simulates the deposition of power into the fluid by the arc and computes a temperature profile along the nozzle wall based on energy transport to this surface. The DSMC code employs the continuum profiles of temperature, velocity, and species number densities to generate the appropriate numbers of particles with properties sampled from Boltzmann energy distributions using standard DSMC algorithms. The profiles of temperature and species number density used to begin the DSMC computations are shown in Figs. 2a and 2b, respectively. These profiles show that the arc deposits energy in a region very close to the axis, and that the degree of ionization falls off rapidly away from the flow centerline.

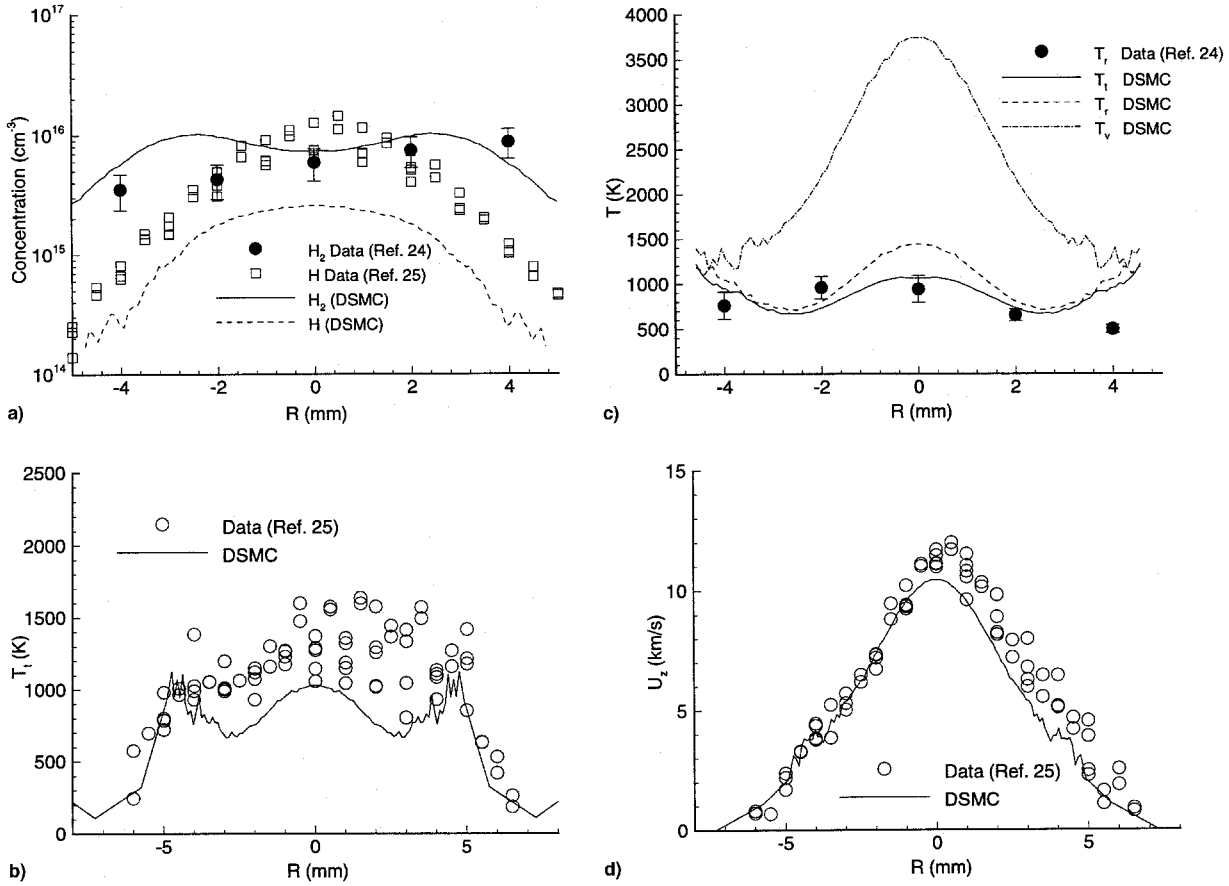

Fig. 5 a) Concentrations of neutral species, b) translational temperature of atomic hydrogen, c) thermal nonequilibrium of molecular hydrogen, and d) axial velocity component of atomic hydrogen in the nozzle exit plane for P = 0.80 kW.

The interaction of the gas with the wall of the nozzle is assumed to be diffuse with full energy accommodation to the wall temperature profile obtained from the continuum MHD simulation. Charged species are neutralized upon contact with the wall. The computations extend through the nozzle exit plane to a distance of 30 mm from the thruster along the axis. Expansion is assumed to occur into a perfect vacuum.

The grids employed typically consist of 500 by 55 cells. Because of the wide dynamic range in density for these flows, the cells are adapted to the local mean free path, and the time step in each cell is scaled by the local mean time between collisions. Despite the time step variation, the transient phase of the simulation remains long. Typically, it requires at least 15,000 iterations before steady state is reached. Steady state is assumed to occur in DSMC computations when there is no further change in the total number of particles in the system. Macroscopic results are then obtained by sampling properties over another 10,000 time steps. At steady state, there are at least 300,000 particles present in the simulation.

Results

Results are presented for a mass flow rate of 13.3 mg/s and power levels of 1.34 and 0.80 kW. These correspond very closely to conditions considered in a number of experimental investigations. Comparison of DSMC predictions with experimental data for various flowfield properties is made at the following locations: 1) in the interior of the nozzle, 2) in the nozzle exit plane, and 3) in the plume flowfield. In addition, comparison is made between measurement and prediction for specific impulse.

Nozzle Interior

In Fig. 3a, the variation of axial velocity component along the nozzle centerline is shown at 1.34 kW. The axis labeling is such that an axial coordinate of zero is located at the nozzle exit plane. The experimental data is from two different studies performed by Storm and Cappelli.[22,23] The DSMC simulation provides good agreement with the data. Far upstream, the measured data indicate velocities that are significantly higher than the computed values; however, this is the region of greatest experimental uncertainty. The minimum turning point shown in the DSMC calculations is a result of the diffusion of cold hydrogen molecules from the boundary layer into the hot core region where the plasma deposition of energy is greatest. The cold molecules have a smaller velocity than the hot plasma, and so at first, the diffusion leads to a rapid reduction in flow velocity. As the gas expands along the diverging nozzle, the flow on the axis is accelerated. Further along the nozzle, there is significant radial diffusion leading to a decrease of velocity on the axis accompanied by an increase in velocity away from the centerline.

Radial profiles of axial velocity component at three different axial locations inside the nozzle are shown in Fig. 3b, where the measurements are taken from Ref. 22. In general, the shapes of the measured and predicted profiles are in good agreement and are found to improve with increased downstream distance. In particular, the profile computed at a distance of just -2.54 mm from the nozzle exit plane shows the best agreement with the data.

Nozzle Exit Plane

In Fig. 4a, the concentrations of molecular and atomic hydrogen across the nozzle exit plane are shown. Experimental measurement of H_2 was performed by Beattie and Cappelli,[24] using Raman scattering. The measurements for H are those reported by Wysong et al.,[25] obtained using a two-photon laser-induced fluorescence technique. In general, the agreement between computation and measurement is better for H_2 than for

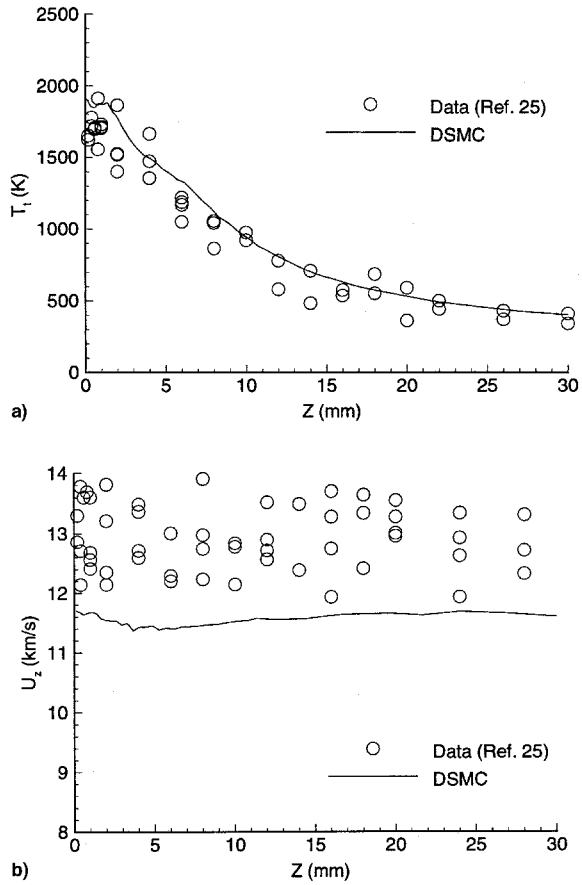

Fig. 6 Profiles of a) translational temperature and b) axial velocity component along the plume axis for P = 1.34 kW.

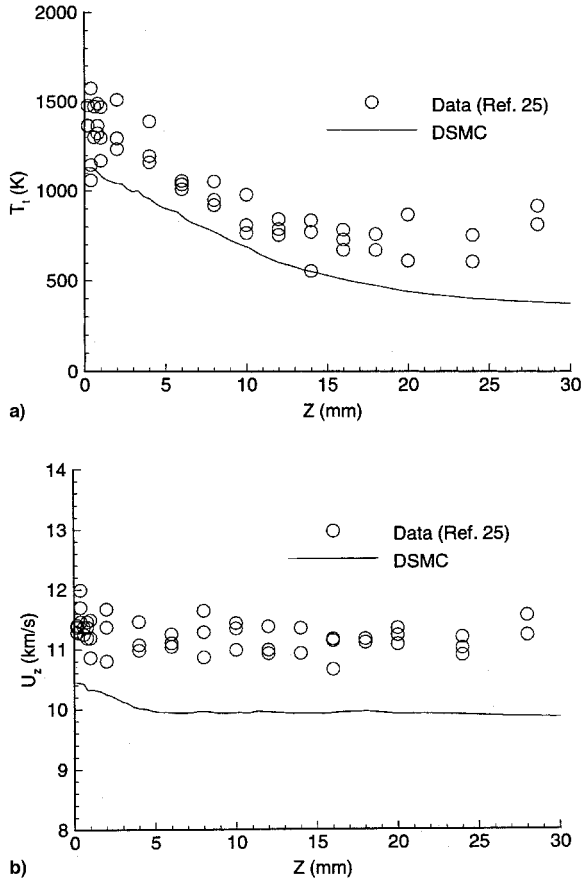

Fig. 7 Profiles of a) translational temperature and b) axial velocity component along the plume axis for P = 0.80 kW.

H. In particular, the simulations predict an atomic concentration on the axis that is a factor of 3 to 4 smaller than the experimental data. A further simulation performed with the dissociation rate for H_2–H collisions increased by a factor of 10, leads to an increase in H-atom concentration at the nozzle exit of just 10%. It is found on close examination that chemistry plays a minor role in the DSMC computation. The discrepancy between measurement and calculation for the hydrogen atom concentrations is therefore attributed either to too little dissociation in the continuum solution used to start the DSMC calculation, or (and) to experimental error.

In Fig. 4b, the translational temperature profile of atomic hydrogen across the nozzle exit plane is shown. Two sets of experimental data reported by Wysong et al.[25] and Storm and Cappelli[26] are shown. The DSMC results show excellent agreement within the scatter of the measured data. The degree of thermal nonequilibrium of the flow in the nozzle exit is illustrated in Fig. 4c. Here, the translational, rotational, and vibrational temperatures of molecular hydrogen predicted by the DSMC technique are compared with the rotational temperature measurements of Beattie and Cappelli.[24] The predicted rotational temperatures offer reasonable agreement with the measured data. Note that the peak vibrational temperature is about 1000 K higher than the peak translational temperature.

A further indication of the degree of thermal nonequilibrium in this flow is illustrated in Fig. 4d, in which the electron temperature at the nozzle exit plane is shown. The experimental data is from Storm and Cappelli.[27] There are two DSMC results shown in which the effect of including ohmic dissipation (Ω) is considered. With ohmic dissipation, there is good agreement obtained with the experimental data. By comparison, omission of Ω leads to significant underprediction of the electron temperature. Note that with ohmic heating, the peak electron temperature is an order of magnitude higher than the peak translational temperature, again illustrating the strong degree of thermal nonequilibrium in these flows. In Fig. 4e, the electron concentration across the nozzle exit plane is shown. The experimental data were also reported in Ref. 27. The agreement between simulation and measurement is very poor with the DSMC technique predicting concentrations that are an order of magnitude higher than the data. The continuum results for electron number density from Butler[5] are included and show remarkably good agreement with the DSMC profile. The agreement for the two numerical methods indicates that the simplified DSMC plasma modeling appears to be adequate. The lack of agreement between the predicted and measured data illustrates a need for further experimental measurement and computational analysis of the properties of the electrons.

Finally, the axial component of velocity in the nozzle exit plane is shown in Fig. 4f. The experimental data are that of Wysong et al.[25] While offering relatively good agreement, the DSMC results are consistently lower than the measured data across most of the exit plane. The shape of the velocity profile is captured very well by the simulation.

In Figs. 5a–5d, comparisons of simulation and data for a power level of 0.80 kW are shown for neutral species concentrations, translational temperature of hydrogen atoms, internal temperatures of hydrogen molecules, and axial velocity component of hydrogen atoms. Overall, the same observations hold at this power level as for the 1.34 kW case. The agreement between simulation and measurement is generally very good, except for the hydrogen atom concentrations in which the DSMC technique predicts densities that are a factor of about 4 lower than the experimental data.

Plume Flowfield

Of the many experimental investigations of hydrogen arcjet flows, Ref. 25 is unique in that data taken in the plume are

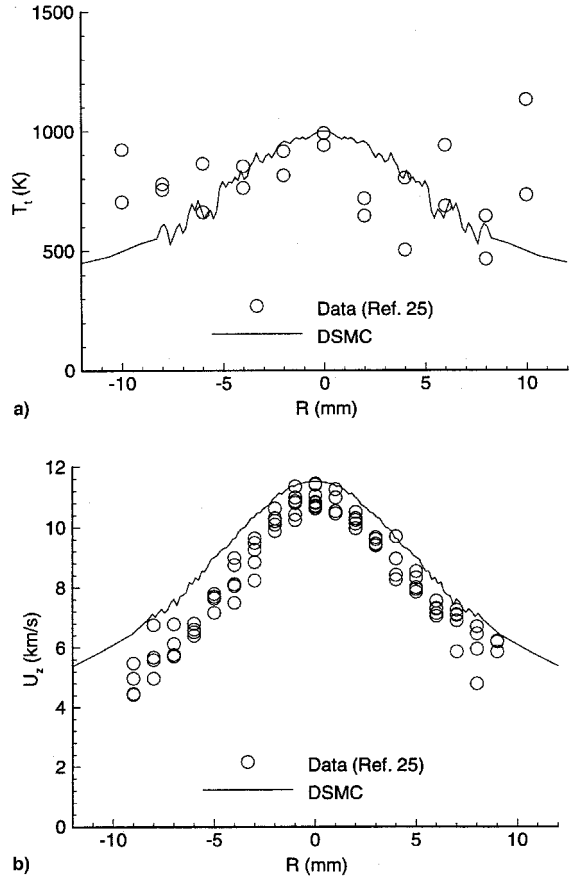

Fig. 8 Radial profiles of a) translational temperature and b) axial velocity component at 10 mm from the nozzle exit for P = 1.34 kW.

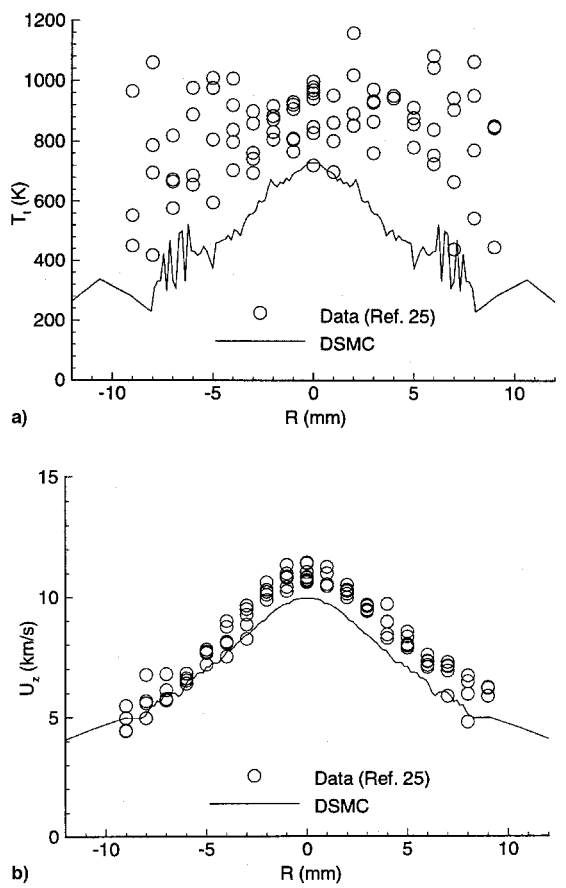

Fig. 9 Radial profiles of a) translational temperature and b) axial velocity component at 10 mm from the nozzle exit for P = 0.80 kW.

reported that are unaffected by chamber effects. These data are compared in this section with the corresponding DSMC results out to a distance of 30 mm from the nozzle exit plane. Variation of translational temperature and axial velocity component for atomic hydrogen along the axis of the plume are shown in Figs. 6a and 6b for a power level of 1.34 kW. In these plots, the axis labeling is such that the nozzle exit plane is again located at zero. It should be noted that these are the first comparisons between simulation and measurement conducted in the plume of an arcjet thruster. As shown in Fig. 6a, the temperature profile predicted by the DSMC technique is in excellent agreement with the experimental data. In terms of velocity, the DSMC results lie consistently 1–2 km/s below the data. In the plume, the velocity predicted by DSMC is almost constant. This represents a balance of two mechanisms. Referring back to Fig. 3a, it is found that the velocity decreases throughout much of the nozzle flow. This continues into the plume, but is balanced by an increase in velocity because of the rapid expansion into vacuum. The scatter in the measured data makes it impossible to say for sure if this predicted behavior is realistic.

Axial plume profiles of translational temperature and axial velocity component at a power level of 0.80 kW are shown in Figs. 7a and 7b. In this case, the DSMC temperature predictions are slightly lower than the measured data. While the scatter in the data is large, it does appear that there is an increase in temperature far from the nozzle. This may indicate some effect of the finite back pressure of the experimental facility on the measured data leading to higher temperatures. The velocity predictions are again lower than the experimental results by 1–2 km/s.

In the experimental investigation of Wysong et al.,[25] radial profiles of plume properties were also measured at an axial distance 10 mm from the nozzle exit plane. In Figs. 8a and 8b, profiles of translational temperature and axial velocity component of atomic hydrogen are shown for a power of 1.34 kW. Within the large scatter exhibited by the measurements, the temperature profile predicted by the DSMC technique offers reasonable agreement. The velocity profiles are in excellent agreement.

In Figs. 9a and 9b, the temperature and velocity profiles for a power of 0.80 kW are shown. The DSMC method predicts slightly lower temperatures and velocities.

Axial and radial profiles of hydrogen atom concentration were also measured in Ref. 25. The comparisons of those data with the DSMC predictions are consistent with the behavior at the nozzle exit plane. Thus, the DSMC method predicts densities for hydrogen atoms throughout the plume that are a factor of 3 to 4 lower than the measured data.

Thruster Performance

Validation of DSMC predictions for flowfield properties is important for assessment of spacecraft interaction effects such as contamination. However, an equally important role for numerical simulations lies in the optimization of arcjet design. For computational methods to be taken seriously in this respect, it is essential that they are able to accurately predict overall thruster performance. A series of measurements of the thrust obtained from the hydrogen arcjet under different operating conditions and geometries was conducted several years ago at NASA Lewis Research Center.[2] The data employed here for comparison with the DSMC results are for the arcjet configuration that most closely resembled that employed in the flowfield measurements and simulations. In Fig. 10, variation of specific impulse with specific energy (power/flow rate) is shown. Experimental data are provided at two different flow rates that bound the condition considered in the simulations. Two sets of DSMC data are shown that indicate the effect of

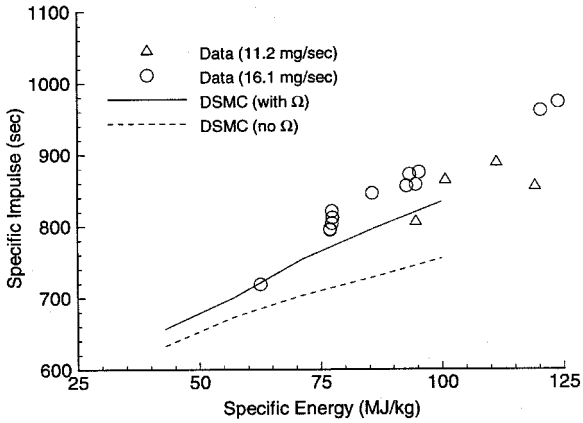

Fig. 10 Comparison of DSMC prediction and experimental measurement of specific impulse.

including ohmic dissipation in the simulation. As expected, with finite Ω, the specific impulse is increased, and the amount of the increase appears to grow with specific energy. Because of the scatter in the measurements and the fact that the flow rates are different from the simulation, it is difficult to make a definitive comparison. However, it does appear that the DSMC predictions that include ohmic heating agree with the measured data to within 5%.

Concluding Remarks

A Monte Carlo method has been developed and applied to simulate flow in the nozzle and plume of a hydrogen arcjet. The model includes detailed simulation of nonequilibrium collision and plasma phenomena. These models are implemented in a numerically efficient computer code. In this study, extensive comparisons between code predictions and a variety of experimental measurements were presented. The comparisons were made for two different arcjet power levels, and for several different aspects of the arcjet flowfields. In particular, predicted results were compared with measured data in the nozzle interior, at the nozzle exit plane, and in the plume expansion. Monte Carlo prediction of specific impulse was also compared with experimental measurement.

In terms of the arcjet flowfields, there was generally good agreement between prediction and measurement for both translational temperature and velocity. There was an overall tendency in the simulations to predict slightly lower values of temperature and velocity in comparison with the experimental results. The greatest discrepancy occurred for the concentration of atomic hydrogen for which the Monte Carlo approach predicted values that were a factor of 3 to 4 lower than those measured. This behavior was found to be consistent at the nozzle exit and throughout the plume flowfield. A significant increase in the hydrogen dissociation rate employed in the simulation did not increase the hydrogen atom concentration significantly. In the absence of chemical effects, the only way in the simulation that the atomic number densities could be increased is through use of a different continuum starting condition. One interpretation of the poor prediction of atomic number density is that the chemistry mechanism in the continuum code should be revised. This lies beyond the scope of the present investigation. It must also be recognized, however, that calibration for a radical species like atomic hydrogen is difficult in the two-photon laser-induced fluorescence technique used in Ref. 25.

At the nozzle exit plane, the nozzle expansion process has created a flow that is in a state of strong thermal nonequilibrium. The Monte Carlo simulation predicts different values of temperature for the translational, rotational, and vibrational energy modes, and for the electrons. In terms of the electrons, it is demonstrated that a model is required to simulate ohmic heating to accurately predict the electron temperature profiles measured experimentally. It was also found that the prediction of electron concentrations was too high by about an order of magnitude, and that this was consistent with a continuum solution.

For thruster performance, the Monte Carlo simulation was able to reproduce experimental measurements within about 5% when ohmic heating is included in the computation.

In summary, the generally successful comparisons between the prediction and measurement of flowfield properties indicates that the Monte Carlo method is capable of computing hydrogen arcjet flows with engineering accuracy. This has the significance of demonstrating that the numerical method may be used for the prediction of spacecraft interaction effects when arcjets are employed on real satellite configurations. The good agreement obtained between computation and measurement for specific impulse demonstrates that the Monte Carlo method may be employed for optimization of the performance of hydrogen arcjets.

Acknowledgments

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