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Shock Interference Prediction Using Direct Simulation Monte Carlo

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The direct simulation Monte Carlo (DSMC) method is used to model the flowfield produced when an incident shock impinges on an inlet cowl lip of 0.1-in. radius for flight conditions of approximately Mach 15 and 35-km altitude. The shock interaction results in a supersonic jet which can impinge on the cowl lip surface and cause extremes in surface heat transfer and pressure. Although this is a nonstandard application, DSMC offers two major advantages to the computational modeling of this problem over other schemes. The basic flow physics is simulated without the imposition of the continuum assumption, and the modeling of finite-rate chemistry is straightforward with a relatively small computational time penalty. The details of the simulation are presented with preliminary results for surface properties.

Nomenclature

d = typical dimension
Kn = Knudsen number
Kn' = local Knudsen number
M = Mach number
P = pressure
q = heat transfer
T = temperature
x, y = linear dimensions
α = macroscopic flow property
Θ = angular position measured clockwise from centerline
λ = mean free path
ρ = density

Subscript

0 = undisturbed case stagnation value

Introduction

THE application of advanced solution techniques to the most stubborn viscous-inviscid interaction problems has done much in recent years to advance the hypersonic flight vehicle on its path from a concept to a reality. One such problem, the shock-interference heating on the surface of a cowl lip in the presence of an incident shock, has received considerable attention in the literature.[1-3] This paper presents the modeling of the flowfield around the cowl lip for a generic flight case using direct simulation Monte Carlo (DSMC). This method allows accurate modeling of the flow physics, including nonequilibrium chemistry, and does not rely on the continuum assumptions inherent in the Navier-Stokes equations which may not be valid for all portions of the flowfield.

The interaction of an impinging shock and the cowl lip bow shock can lead to surface heat transfer rates which are higher than the undisturbed cowl lip stagnation heating by more than an order of magnitude. The most severe heating occurs for the interaction pattern known as type IV (Fig. 1), using Edney's system of classification.[4] This type of interaction, with the incident shock generated by the vehicle nose or forebody compression surfaces, cannot be avoided for the hypersonic vehicle designs currently under consideration.[2] The design of the cooling system for the cowl leading edge will be driven by the prediction of this heating for the expected flight conditions. Therefore, it is necessary that this prediction be as accurate as possible.

The degree of departure of a flow from the continuum is indicated by the value of the flow Knudsen number

$$Kn = \lambda/d \tag{1}$$

A precise assessment of the validity of the continuum equations in any portion of the flow can be based on the local Knudsen number

$$Kn' = (\lambda/\alpha)(\partial\alpha/\partial x) \tag{2}$$

where α is a macroscopic flow variable such as the density, velocity, or temperature. In general, errors associated with continuum calculations become significant when the local Knudsen number exceeds 0.1.[5] These errors occur because the strength of the viscous-inviscid interactions tend to be weaker and occur over larger distances in noncontinuum flows. In the current calculations, some portions of the flow have been shown to have local Knudsen numbers in the range 0.1 to 0.2. Therefore, it is possible that the accurate prediction of the flowfield and surface heating depends on the use of a solution technique which models the discrete nature of the gas, such as DSMC.

The ability to calculate nonequilibrium chemistry with DSMC is important for this problem. The high temperatures involved in the problem indicate that the perfect-gas assump-

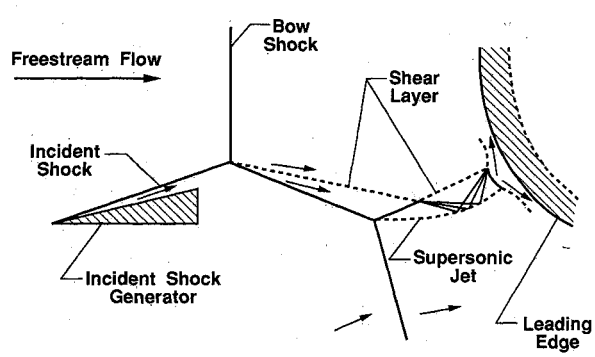

Fig. 1 Type IV supersonic jet interference pattern.

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tion is inappropriate, and the quick convection of high-temperature gas to the surface in the supersonic jet suggests that the equilibrium chemistry assumption is also unsuitable. Earlier work by one of the authors[6] demonstrated the usefulness of DSMC for the analysis of complex viscous-inviscid interactions relevant to inlet-type geometries at relatively low densities. The application of DSMC to the current problem further demonstrates the usefulness of DSMC for the analysis of complex hypersonic flow problems under more continuum-like conditions.

Obtaining a DSMC solution of such a shock interaction is not, however, an easy task. DSMC is ordinarily used to solve low-density problems, typically at altitudes of 80 km or greater. The much higher density of the 35-km case severely limits the physical size of the flow region which can be simulated, given the current constraints on computer memory and speed. To minimize memory requirements and computation time, the problem was calculated in two portions—the generation of the incident shock and the shock interaction. To illustrate the requirements, the shock-interaction calculation required 400,000 simulated molecules and about 800 h of CPU time on a Sun SPARCstation-2 with 64 megabytes memory. The undisturbed cowl shock was also investigated.

Computational Method

Direct simulation Monte Carlo (DSMC) is a discrete particle method used to obtain a numerical simulation of the flow of gases in the transition regime. (The transition regime is the category of flow which falls between the continuum regime, where the Navier-Stokes equations are valid, and the free-molecule regime, which is the limit of infinite Knudsen number.) The simultaneous trajectories of many thousands of simulated molecules are computed along with their appropriate collisions and boundary interactions. Each simulated molecule represents a very much larger number of real molecules. The molecular motion and intermolecular collisions are uncoupled over the small timestep used to advance the simulation. The physical space is divided into a number of discrete cells by a grid. The exact position coordinates are stored for each simulated molecule and the grid is used only to determine collision partners and for the sampling of macroscopic properties. Position, velocity, and internal state information is stored for each molecule and modified with time as the molecules are followed through representative collisions and boundary interactions The Variable Hard Sphere model is used for molecular interactions, the Larsen-Borgnakke method for partitioning of internal energy, and a 5-species and 23-reaction model was chosen for the nonequilibrium chemical kinetics. The program is the general two-dimensional/axisymmetric (G2) code of Bird,[5,7,8] who has documented the details of the above models. Boundaries can be a surface, a vacuum outflow, a specified uniform flow, or a molecule input/output boundary. The initial condition is either a vacuum or a specified uniform flow. The simulation is always treated as unsteady, but a steady flow solution is obtained as the large time state of the simulation.

The computational approximations inherent in the above model give rise to certain conditions which must be met to ensure an accurate solution. The timestep over which collisions are uncoupled from molecular motion should be less than the local mean collision time. The dimensions of the cells must be such that the change in flow properties across each cell is small. In particular, cell size in regions of significant flow property gradients (such as density or temperature gradients) are traditionally chosen to be about one-half to one-third of the local mean free path. If the length scale over which the flow property changes is much larger than the mean free path, this requirement can be relaxed. Also, the number of simulated molecules in a cell should be on the order of 10–20 to avoid distortion of the collision rates between the various species. Representing a very large number of real molecules by a single computational molecule causes the fluctuations in flow properties to be enhanced. Although no evidence of any instability associated with these fluctuations has been observed, a large sample through time averaging is required to obtain convergence to the correct value.

Analysis and Results

With the goal of obtaining a nominal design heat load, the work presented in this paper was performed for the generic flight condition described below. The cowl lip radius is 0.1 in. and surface temperature is 811 K. The surface was assumed to be noncatalytic. The freestream velocity is 4610 m/s, density is 0.00922 kg/m^3, and temperature is 241 K (corresponding to approximately Mach 15 and 35 km). The incident shock is two-dimensional flow over a 6-deg wedge, resulting in a shock angle of approximately 9 deg.

The computational modeling of this complex problem was performed in a series of steps. The undisturbed cowl bow shock was first computed with DSMC. Then the incident shock was generated with DSMC and the properties across the shock investigated. A relatively crude grid was used for preliminary investigations of the shock-interference phenomena and for several positions of incident shock impingement relative to the cowl lip centerline. From these preliminary results, an incident shock location representing what appeared to be the worst heating case was selected for further study. For this case, the grid was refined in enough detail to make a reasonable first calculation of the surface heat transfer. When more results from continuum analyses become available for the same flow conditions, comparisons of the solutions will answer questions about the importance of modeling rarefied and nonequilibrium chemistry effects in the simulations.

Undisturbed Cowl Bow Shock

The computational grid for the cowl bow shock simulation consisted of 9000 cells and 360,000 simulated molecules. The boundaries of the computational space and its division into regions are shown in Fig. 2. A small portion of the grid is shown to illustrate the typical mesh density for the DSMC calculations of this paper. Region 1 is fitted to the surface of the cowl lip and encompasses the boundary layer. Region 3 has been fitted to the cowl bow shock (an iterative process). The normal cell dimension next to the surface in region 1 is less than one mean free path in order to accurately resolve the flow gradients, and is also small in region 3. In region 2, behind the shock, the cells are larger since the properties are fairly constant. Similarly, in region 4 the cells are large because the flow is freestream. The vacuum boundary condition at the edge of the computational region is used because the flow is fully supersonic at this boundary except very near the surface. The error near the surface resulting from imposing this condition is not considered significant because the region of interest is the stagnation point on the cowl lip, several

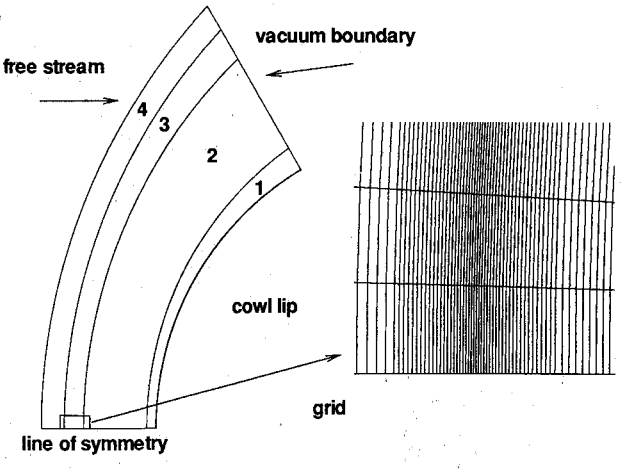

Fig. 2 Undisturbed cowl lip bow shock geometry.

thousand mean free paths from the boundary. The grid-refinement requirements for the undisturbed case were within the capability of the available computers and the grid used was sufficient to obtain a value for surface heat transfer which should be accurate to within 5–10%.

Mach contours and temperature contours for the undisturbed cowl bow shock are shown in Figs. 3 and 4. As can be seen from the sonic line in Fig. 3, the vacuum boundary is well into the supersonic region except very close to the surface. The peak temperature in the shock is approximately 8000 K, temperatures behind the shock but outside the boundary layer are between 5000–6500 K and in the boundary layer they reduce gradually to about 850 K. The stagnation-point heating is approximately 16 MW/m^2, and stagnation-point surface pressure is 1.9×10^5 Pa.

Incident Shock

A feature of the G2 code, the ability to write a molecule output file across a region boundary, was exploited in this study to separate the generation of the incident shock from the prediction of the shock interaction. This was accomplished without any loss of detail of the properties across the width of the incident shock. The shock is generated as two-dimensional flow over a 6-deg wedge (Fig. 5). The wedge surface is modeled as a specular reflector to prevent the formation of a

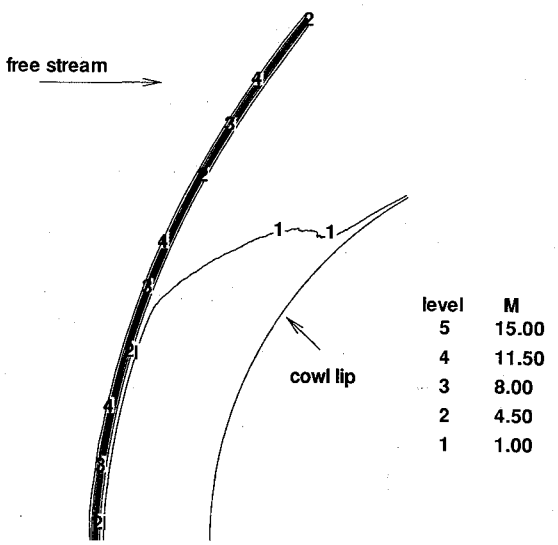

Fig. 3 Mach contours for undisturbed case.

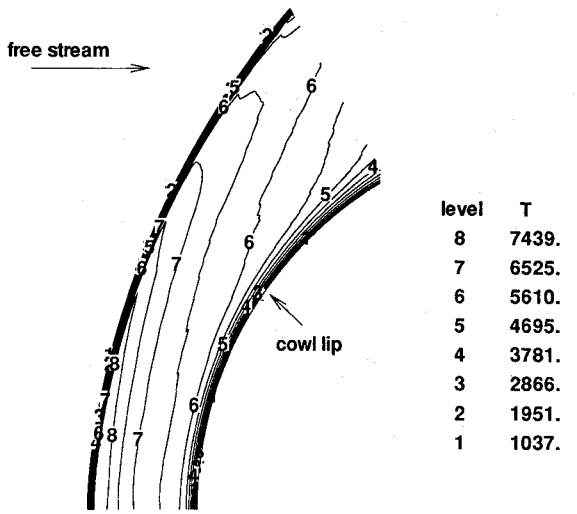

Fig. 4 Temperature contours for undisturbed case.

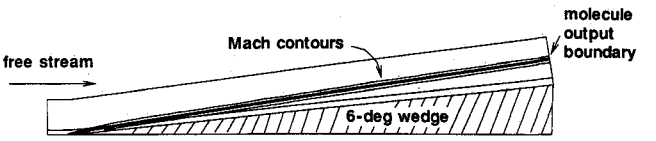

Fig. 5 Incident-shock geometry and Mach contours.

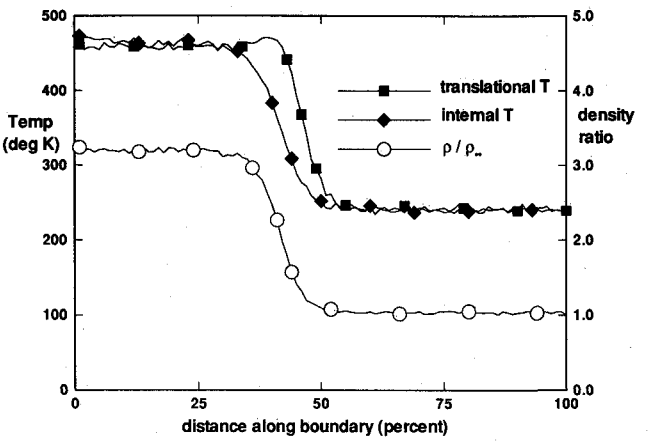

Fig. 6 Properties across the molecule output boundary.

boundary layer which might produce an unrealistic influence on the interaction at the cowl lip. The region outflow boundary perpendicular to the shock is defined as the molecule output boundary. The distance along the wedge which is required for the computational region is a function of the desired size of the molecule output boundary. The length of this boundary was selected to be approximately six shock thicknesses, with the shock placed near the center. After steady flow is established, all simulated molecules which exit this boundary are written into a file called the molecule output file. No molecules enter at this boundary. The position, velocity components, species identity, and internal state of each exiting molecule are written to the file along with certain simulation parameters. These parameters are used later by the program which reads the molecule input file to relate the conditions of the two simulations. A region near the surface of the wedge is excluded from the region which contains the molecule output file to prevent small disturbances near the surface from being passed to the shock-interaction calculation.

The incident-shock computation required 5000 cells and 150,000 molecules. A molecule output file containing 1000 records each with 1000 molecules was produced. Translational temperature, internal temperature, and density ratio are plotted as a function of the percentage distance along the molecule output boundary, starting from the lower edge, in Fig. 6. A compromise has been made between the amount of storage required for the file and the level of scatter in the data, which goes as the square root of the number of samples.

Effect of Position of Incident Shock

To investigate the effect of the incident-shock positioning, a grid similar to that for the undisturbed cowl bow shock was used. Differences are that the problem is no longer symmetric about the cowl lip and a region boundary which exactly matches the geometry of the incident-shock molecule output boundary must be included for the incident-shock molecule input. Several cases were run with varying locations of the incident shock. For these cases (Fig. 7) only three regions were used and advantage was taken of mesh clustering ability in the G2 code to concentrate the cells in the boundary layer and at the predicted shock locations. The location of the incident

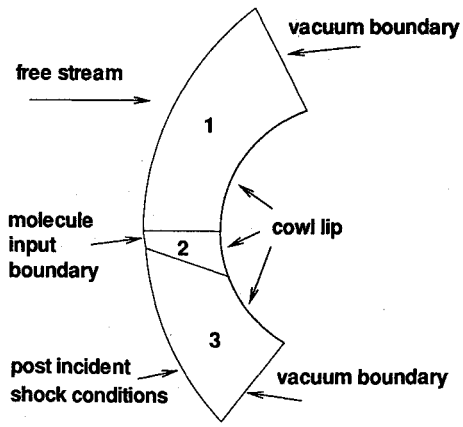

Fig. 7 Geometry for shock interaction.

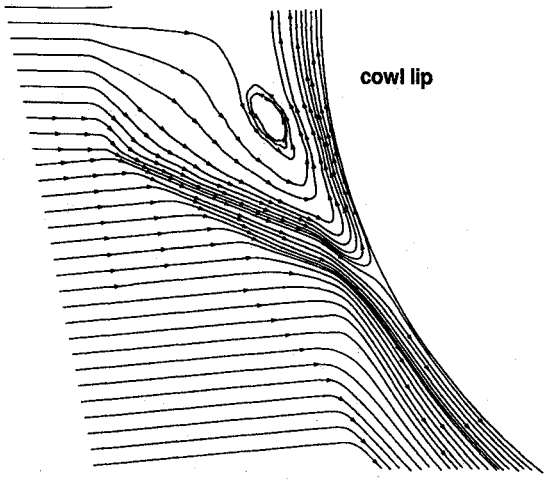

Fig. 8 Streamlines with location of incident shock below worst heating case.

shock was varied by translating the molecule input boundary up or down in the direction normal to the cowl lip , with the corresponding change in shape of the three regions.

In these cases there are two vacuum boundary conditions at the limits of the computational region. There is a freestream boundary condition in region 1. The molecule input file for region 2 exactly duplicates the incident shock. Molecules are read from a randomly selected record in the input file and in a random order. After half of the molecules in a particular record have been read, another record is selected. This procedure preserves the statistical nature of the incident-shock simulation. The stream boundary in region 3 is specified as the uniform conditions behind the incident shock. The calculations were performed with approximately 15,000 cells and 350,000 molecules.

Although the computational grid used in these cases was too coarse to provide surface heat transfer information, experience has shown that even a coarse grid will give reasonably accurate flow patterns. These patterns were investigated to determine which location gave most nearly the classic type IV interaction and appeared to be the worst case for surface heat transfer. Streamlines, separated by the same physical distance at the incident shock boundary in each case, are plotted for three of the cases in Figs. 8–10. Figure 9 is the location which was determined to be the most severe, with Fig. 8 a position of the incident shock below that in Fig. 9 and Fig. 10 a position above that in Fig. 9. It can be seen that the supersonic jet is more concentrated and impinges more nearly normal to the surface for the case of Fig. 9 than in either of the other cases.

Detailed Shock-Interaction Study

Using the flowfield solution from the coarse grid simulation described above, it was possible to adapt a grid (Fig. 11) to the worst-case problem which concentrated cells in the areas of primary interest. The cell dimensions are on the order of one to ten mean free paths near the surface (regions 1, 3, and 6) for reasonably accurate prediction of the surface heating and in the shock-interaction region (region 4) for resolution of the viscous interaction and dispersion of the supersonic jet. By adapting the grid specifically to these locations, a much improved simulation was possible with only a moderate increase in the required number of molecules and cells. Specifically, 17,200 cells and 450,000 molecules were used.

Mach and temperature contours are shown in Figs. 12 and 13 for the shock-interaction region and can be compared with those for the undisturbed cowl lip case in Figs. 3 and 4. The surface heat transfer and surface pressure, normalized by the undisturbed stagnation values, are plotted in Fig. 14 for the portion of the surface near the peak heating. Heat transfer is plotted against angular position on the cowl lip below the . The predicted dimensional value of peak surface heating is about 380 MW/m^2.

The only other numerical simulation of this generic flight case available in the open literature is that of Sobel.[2] His paper describes computational results for the flight case and for two wind-tunnel test cases of the same shock-interaction phenomena. Sobel assumes equilibrium chemistry and continuum flow throughout. His numerical method yields upper and lower bounds on the surface heat transfer at the shock-impingement

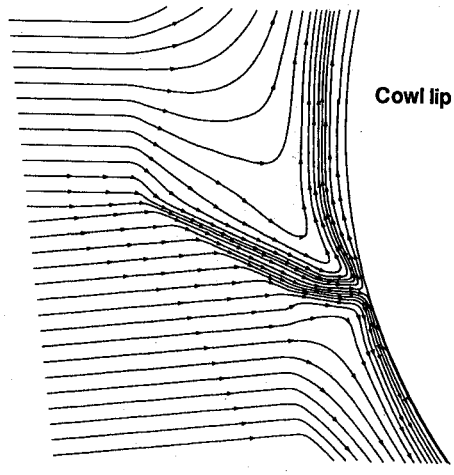

Fig. 9 Streamlines with location of incident shock at worst heating case.

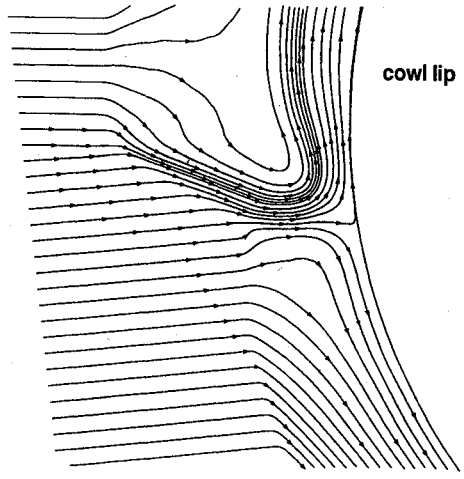

Fig. 10 Streamlines with location of incident shock above worst heating case.

location. For the two wind-tunnel tests, which were more fully in the continuum regime than the flight case, the experimental value lies between the limits predicted. The flight case surface heat transfer is predicted to be between 390 and 980 MW/m^2, if the values are extrapolated to an 811 K surface temperature as used in the current analysis. The DSMC result is near the lower limit and the agreement is as good as one would expect

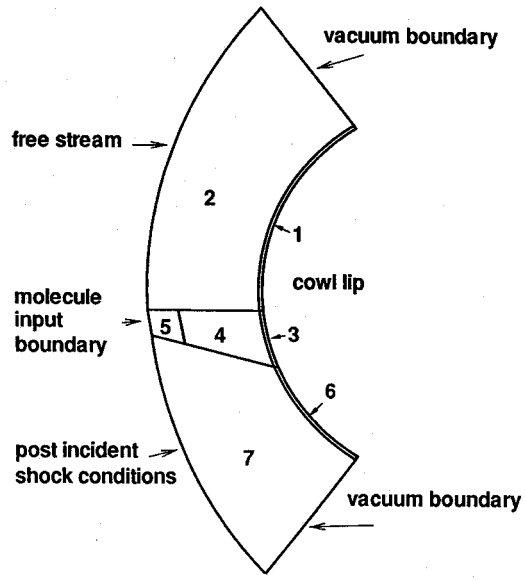

Fig. 11 Geometry for detailed shock-interaction study.

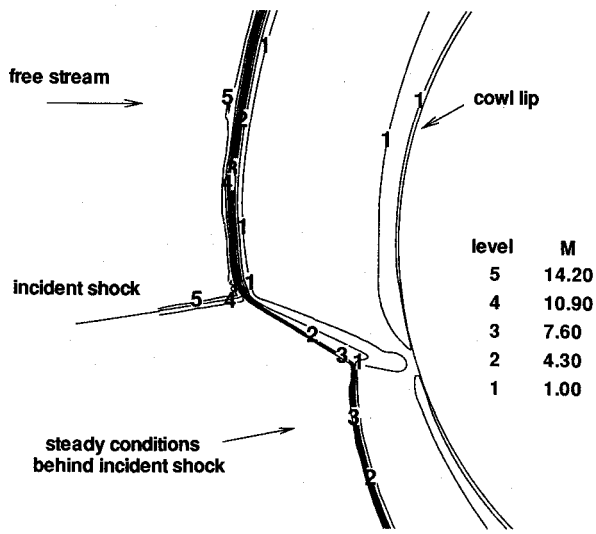

Fig. 12 Shock-interaction Mach contours.

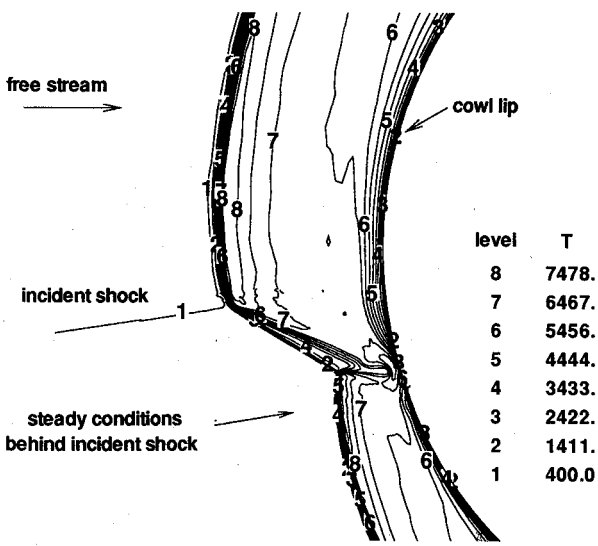

Fig. 13 Shock-interaction temperature contours.

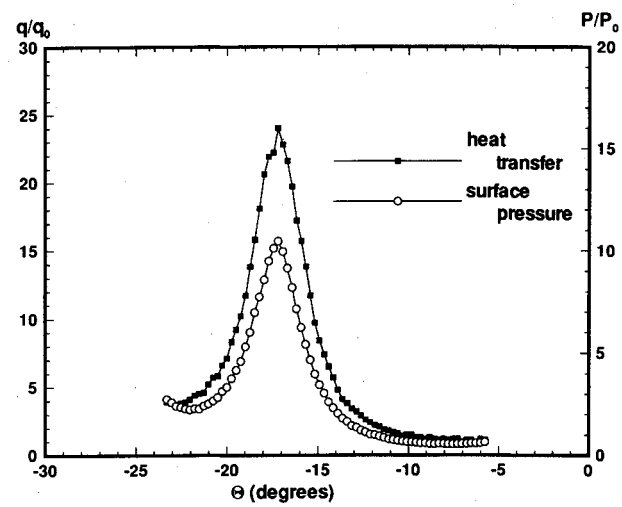

Fig. 14 Cowl surface properties in the region of peak heating (q_0 = 16 MW/m^2, P_0 = 1.9 × 10^5 Pa.

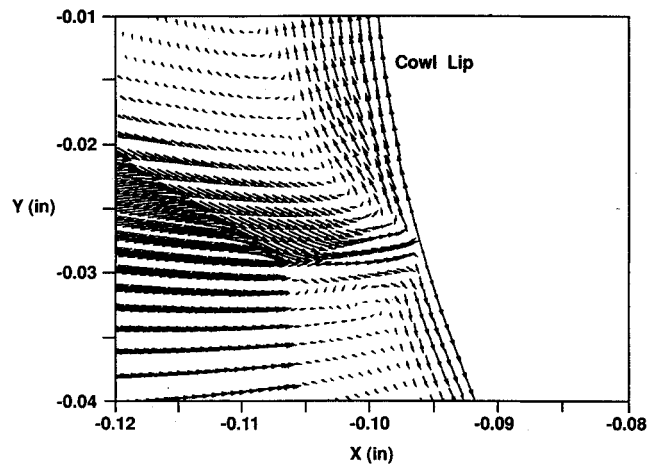

Fig. 15 Velocity vector field in the region of peak surface heating from the study of Ref. 2.

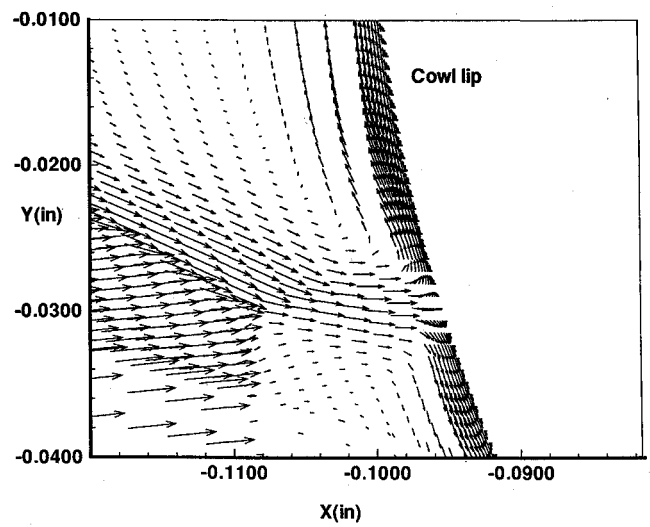

Fig. 16 Velocity vector field in region of peak surface heating from the present calculation.

given the differences in methods. A qualitative comparison between the two solutions in the region of the supersonic jet flow is presented in Figs. 15 and 16. Figure 15 is generated from the data of Sobel while Fig. 16 is the current calculation.

Because of the small lip radius and correspondingly large Knudsen number, noncontinuum effects may be significant for the flight case and Navier-Stokes solutions may not be adequate. The strength of interactions can be expected to be weaker in transitional flows and the use of a purely continuum based analysis typically leads to an overprediction of the local heating rates. Although the overall flowfield appears essentially continuum, a detailed investigation reveals that in the shock-interaction region, the shear layers, and in parts of the supersonic jet region the local Knudsen number based on density scale length

$$Kn' = (\lambda/\rho)(\partial\rho/\partial x) \tag{3}$$

is on the order of 0.1–0.2. Therefore, although the current comparison involves differences in chemical modeling which may account for some of the discrepancies, local rarefied flow effects may be expected to influence the results.

Concluding Remarks

The discrete particle technique of direct simulation Monte Carlo (DSMC) has been applied to the problem of incident-shock impingement on the engine cowl leading edge for a hypersonic flight vehicle at a generic Mach-15 flight condition. The combination of altitude and small characteristic dimensions for this problem indicates that portions of the resulting flowfield are characterized by transition rather than continuum flow. Accounting for noncontinuum effects is necessary because viscous-inviscid interactions may be expected to be weaker in transitional flows. The use of a purely continuum analysis for this problem could lead to overprediction of the local heating rate. Also, the modeling of finite-rate chemical processes in the flow is performed. High shock temperatures indicate that chemical reactions will be significant, and the rapid convection of gases toward the surface in the supersonic jet indicates that there may be a high degree of nonequilibrium which must be considered in the flow solution.

Both the undisturbed flow and the shock-interaction flow about the cowl lip were computed. The computation of the shock interaction was performed in two segments. The incident shock was generated separately and the result was merged with the simulation of the flow about the cowl lip. This separation of the problem into two parts made it relatively simple to investigate the effect of varying the position of incident-shock impingement relative to the cowl lip . A worst case interaction was selected for detailed study. Preliminary results from this case show a clear type IV interference pattern, Knudsen numbers above the continuum range through portions of the interaction region, and surface heat transfer augmentation of about 25 over the undisturbed cowl lip stagnation heating.

More detailed studies are in progress and comparisons with continuum solution methods are planned as those solutions become available. A DSMC calculation of the flight case with the chemical reactions suppressed is in progress. This solution will be compared to perfect-gas Navier-Stokes solutions, which may be more readily available in the literature than finite-rate chemistry solutions. It is also desirable to compare a DSMC calculation directly with test data. If tests could be performed at lower densities or with smaller models, such comparisons might be possible. Further advances in computer speed and memory, advanced grid-adaptation techniques, and adapting the code to utilize parallel processing are all improvements which are expected to significantly extend the range of conditions which can be modeled.

Acknowledgments

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