DSMC Simulations in Support of the STS-107 Accident Investigation

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Abstract. Three-dimensional Direct Simulation Monte Carlo simulations of Columbia Shuttle Orbiter flight STS-107 are presented. The aim of this work is to determine the aerodynamic and heating behavior of the Orbiter during aerobraking maneuvers and to provide piecewise integration of key scenario events to assess the plausibility of the candidate failure scenarios. The flight of the Orbiter is examined at two altitudes: 350 kft and 300 kft. The flow field around the Orbiter and the heat transfer to it are calculated for the undamaged configuration. The flow inside the wing for an assumed damage to the leading edge in the form of a 10-inch hole is studied.

INTRODUCTION

On January 16, 2003, the Space Shuttle *Columbia* was launched from Kennedy Space Center to begin STS-107, the 113th mission in the Space Shuttle Program and Columbia's 28th flight. As it passed just northwest of Hawaii sixteen days later on Saturday, February 1, 2003, *Columbia* initiated a maneuver to return to earth for a landing at Kennedy Space Center in Florida. By the time it reached the US mainland and continued its descent over the western United States, people on the ground observed bright objects coming off of *Columbia*. *Columbia* broke apart at an altitude of approximately 200,000 feet near Dallas, Texas at approximately 8 AM CST, just 15 minutes before its scheduled landing at Kennedy Space Center in Florida.

The conclusion of the investigation [1] was that the physical cause of the loss of *Columbia* and its crew was a breach in the Thermal Protection System. At 81.7 seconds after the launch, a piece of insulating foam separated from the left bipod ramp section of the External Tank and struck the Orbiter, causing a breach on the leading edge of the left wing. During re-entry, this breach in the Thermal Protection System allowed superheated air to penetrate through the leading edge insulation and progressively melt the aluminum structure of the left wing, resulting in a weakening of the structure until increasing aerodynamic forces caused loss of control, failure of the wing, and break-up of the Orbiter. The investigation of this scenario involved numerous CFD [1] and Direct Simulation Monte Carlo (DSMC) [1,2] simulations to provide the heating and forces on the Orbiter and, in particular, on the leading edge of the left wing. In this paper, representative DSMC calculations conducted in support of the investigation of this particular failure scenario will be presented. It should be noted that at the time when this work was performed the conclusion of the investigation was not available. The purpose of the simulations presented herein was to assist the work of the investigation committee, especially in an area where forensic and physical data were not available.

In the first part of the paper, the undamaged full 3-D geometry is studied and the flow field characteristics analyzed. In the second part of the paper, boundary conditions are extracted from the full body simulations to be used in examining the wing leading edge with an assumed 10-inch diameter hole. It is interesting to note that

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after this analysis was completed, an experimental reproduction of the impact on the wing leading edge indicated that the size of the hole might have been even greater than 10 inches and possibly as large as 16 inches.

METHODOLOGY USED

For the purposes of this work, the "DAC" DSMC [2] implementation of LeBeau [3] was used. Since the DSMC algorithm is well established on physical arguments, DSMC implementations differ mostly in the flow field discretization methods and the way they represent the modeled geometry. The DAC software employs a two-level embedded Cartesian grid system. Thus the computational domain is a rectangular box, aligned with the Cartesian axes. Embedded within the flow field grid is the surface geometry. DAC represents the surface geometry as a collection of unstructured triangular elements, which also act as sampling zones for surface properties.

The rectangular bounding box for the computational domain is specified by the user, as is the discretization in each of the three Cartesian directions. The cells created by this uniform Cartesian grid are referred to as Level-I Cartesian cells. Each of these Level-I Cartesian cells can be further refined by its own embedded Cartesian grid. These embedded Cartesian grids form Level-II Cartesian cells. The two-level embedded Cartesian grid system permits variable refinement throughout the computational domain, which is essential for meeting the local mean-free-path cell size requirement. To model chemical reactions, Bird's Total Collision Energy model (TCE) model was used. The chemical reaction data used in the simulations are those proposed by Park [4].

SHUTTLE ORBITER MODEL DEVELOPMENT

The model of the Shuttle Orbiter was based on a detailed CAD design provided by Boeing Huntington Beach. From this, a surface grid of approximately 32,000 triangular elements was constructed. A Cartesian gas-phase grid of more than 5,000,000 elements (after the adaptation) was used for the computational domain. Every possible effort was made to ensure that all these parameters complied with Bird's criteria [2] for a successful DSMC simulation. The time step was such that molecules, on average, did not move more than a cell per time step, and cells were smaller than the local mean free path. For the gas-phase grid adaptation, the "Level-II cell" procedure (outlined in LeBeau [3]) was used. The adaptation procedure allowed up to 20 Level-II cells in each Level-I cell.

The solution was run fully diffuse, and the surface wall temperatures used for the simulations were estimated to be 525 K for the 350-kft case and 950 K for the 300-kft case. A chemistry model for high-temperature reacting air was used that contained six molecular species: O_2, N_2, O, N, NO, and Ar. The mole fractions of these species were obtained from the 1976 Standard Atmosphere Model [5]. Number density, velocity, and free stream temperature were obtained from STS-107 flight data.

FLOW FIELD CALCULATIONS OF THE UNDAMAGED GEOMETRY

For the purposes of the investigation, two cases were examined. The first one was in the rarefied regime and the second the transitional regime. The conditions of the two instances are given in Table 1. For these conditions no CFD calculations were performed. The times corresponding to the two cases are measured in seconds from "Entry Interface" (EI), an arbitrarily determined altitude of 400 kft, where the Orbiter begins to experience the effects of Earth's atmosphere. Entry Interface for STS-107 occurred at 8:44:09 AM (EST) on February 1st, 2003. The first abnormal indication occurred 270 seconds after Entry Interface, i.e. approximately 70 seconds after the second instance (300 kft) occurred. This fact was known to neither the crew nor Mission Control since sensor data were recorded and stored onboard the Orbiter.

Figures 1 and 2 present the average temperature (average flow energy) profiles around the Orbiter for the 350-kft and the 300-kft cases, respectively. The flow travels from right to left. In the 350-kft case, as the first free stream molecules hit the surface of the vehicle, they are slowed down, and, as a result, a large compression region is formed. This compression region is an extended Knudsen/boundary layer. Diffusion of air molecules upstream (due to the density gradient) gives rise to head-on collisions between these molecules and the free-stream-air incoming molecules. These highly energetic collisions lead to an increase of the temperature of the flow that is clearly shown as the extended high-temperature area. The thickness of this area

is of the order of ten local mean free paths. As the flow moves closer to the surface of the vehicle, the temperature of the flow decreases since for the simulation, the temperature of the vehicle was kept constant for each instant.

TABLE 1. Flight conditions for the DSMC cases examined during the STS-107 investigation

Properties	350 kft	300 kft
Time from Entry Interface (s)	91	197
Mach Number	25.1	27.0
Altitude (km)	106.7	91.4
Altitude (ft)	350,274	300,003
Angle of Attack (deg)	41	40
Knudsen number	0.02	0.001

In Figure 2, the temperature profile is shown for the 300-kft case. A distinct shock layer is developed starting from the nose of the vehicle and expanding along it. The temperature reaches almost 15,000 K. It is worth noting that, although the shock layer is much thinner in this case due to the shorter mean free path, the temperatures achieved are similar to those in the previous case. The higher density of this case (by almost one order of magnitude) resulted in a heat flux greater than the 350-kft case by almost one order of magnitude.

In the wake of the vehicle, both the density (not shown here) and the temperature drop by one order of magnitude due to the rapid expansion. More details about these flow fields can be found in Reference [6].

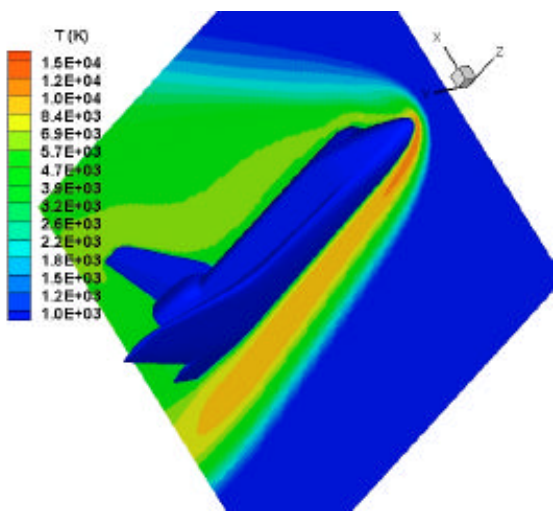

FIGURE 1. Temperature profile (350-kft case)

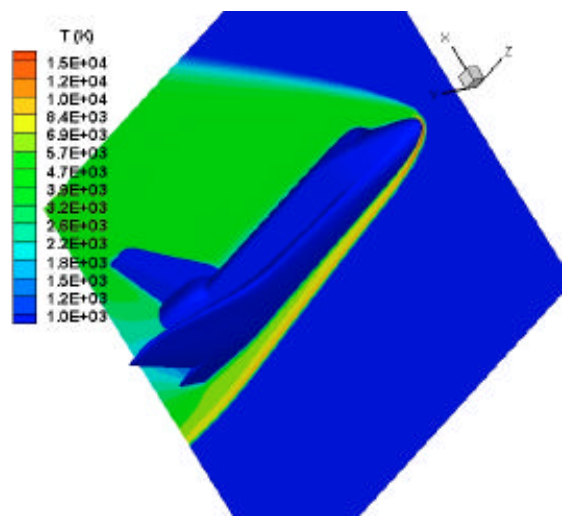

FIGURE 2. Temperature profile (300-kft case)

FLOW THROUGH A 10-INCH HOLE IN THE LEADING EDGE

In the second part of the analysis, the internal flow behind the Re-enforced Carbon-Carbon (RCC) panels 7, 8, and 9 due to a 10-inch hole in RCC panel 8 was simulated. For the simulation of the internal-flow cases, the inflow boundary conditions were extracted from the previously run DSMC external flow solutions. Vents were also applied to each side of the geometry with a total area equivalent to 66 in^2 to emulate the venting holes along the upper surface of the wing.

A heritage CAD definition for the RCC cavity was obtained from Jim Greathouse [7]. This definition includes wing geometry from the leading edge back to the wing spar and includes a definition for the earmuffs between panels. The geometry used in this case was developed using the GridGen grid generation tool. After importing the CAD into GridGen, a 10-inch hole was generated in RCC panel 8 at a location of X = 1065 inches, Y = -219 inches, and Z = 286 inches in the Orbiter coordinate system. Vent holes were included on each side of the geometry. It was assumed that the RCC thickness was uniform at ¼ inch, so the 10-inch hole in RCC panel 8 was given a thickness of approximately ¼ inch.

Since DSMC solutions had already been obtained for the undamaged cases, it was felt that it was not necessary for a full-length shuttle case to be run for this failure scenario. Instead, an external-flow field box-like "geometry" was created that connected to the hole from the external flow side. Great care was taken to create an external flow field geometry large enough so that the geometry of the hole would not significantly affect the flow at the upstream boundary but small enough so that the case would run in a timely manner. The external flow field geometry was created to connect to a corresponding portion of the outer RCC surface which, in turn, connected to the surface representing the thickness of the hole.

In DAC, the surface geometry is represented as a collection of unstructured triangular elements and the entire surface geometry must be created to be "watertight" and possess continuous connectivity among triangles. In this case, the surface geometry contained approximately 53,000 surface triangles. Each individual surface triangle has specific boundary conditions associated with it. The triangles representing the surfaces of the wing were given the "solid wall" boundary condition, which means that no molecules are produced at the wall and none pass through. The triangles representing the vents were given the "outflow" boundary condition, which means that any molecules that hit the surface will disappear. Finally, the triangles representing the external flow field surface were given the "inflow" boundary condition. An inflow boundary creates molecules on the flow field side of the triangle, but any molecules that hit the surface will disappear.

The computational domain was specified to encompass the surface geometry created in this case and the boundary conditions of the computational domain were specified as vacuum. For the 300-kft case, the Level-I discretization employed cells of 0.0015 meters. The total number of cells after the adaptation was in excess of 10 million (grids up to 40 million cells were also used). For the 350-kft case, the Level-I cells were sized at 0.033 meters. The total number of cells after the adaptation was approximately 1 million.

The wall temperature was assumed to be 300 K. The chemistry model used was the same as for the external- flow cases.

Internal Flow Results

Figure 3 displays a Y-slice of the flow field number density for the internal flow case at 350 kft. In this figure the streamlines shown depict the movement of the flow as it enters the hole in panel 8 and begins recirculating inside the cavity. The exact location of these panels along the leading edge of the vehicle is given in Reference 1. In this simulation, the flow is allowed to escape through the exits at panels 7 and 9; however, the total area provided was not enough for the flow to exit and as a result the recirculation zone shown in Figure 3 is formed. A result of the formation of a recirculation zone in the leading edge cavity is that the heat transfer to the wing spar is increased. Another undesirable result of the existence of flow in the wing cavity is to weaken the integrity of the wing spar by removing layers of material from it.

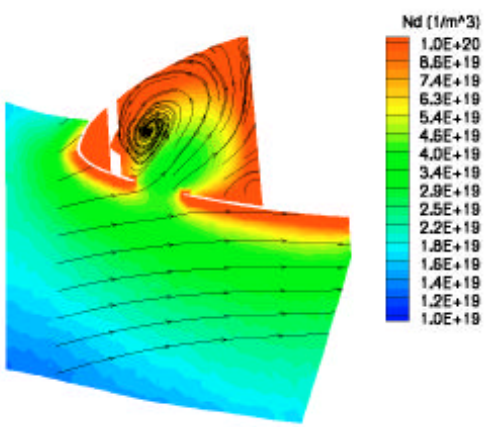

FIGURE 3. Number density and streamlines for the 350-kft internal-flow case

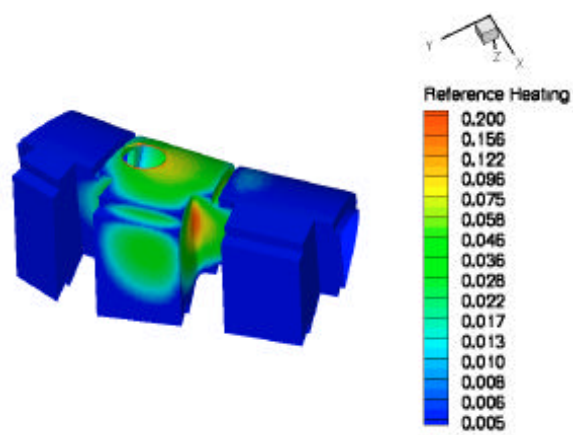

FIGURE 4. Reference heating for the 350-kft internal-flow case

Figure 4 shows the normalized (by the stagnation point heat flux) heating distribution in the RCC cavity for the 350-kft case. The heating values shown in the legends on the right side of the figure have been normalized

by reference heating values based on the free-stream properties. From these figures, it is evident that the area of highest heating due to the breach is near the area between panels 8 and 9. As the flow hits the corner of the earmuff, a shock is formed and the flow is seen to splash onto the spar. Elevated heating levels are also seen between panels 7 and 8.

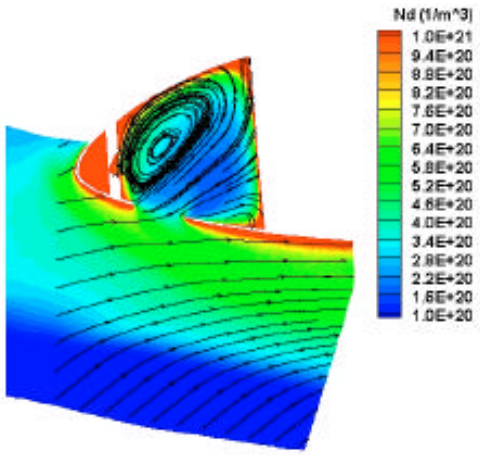

FIGURE 5. Number density and streamlines for the 300-kft internal-flow case

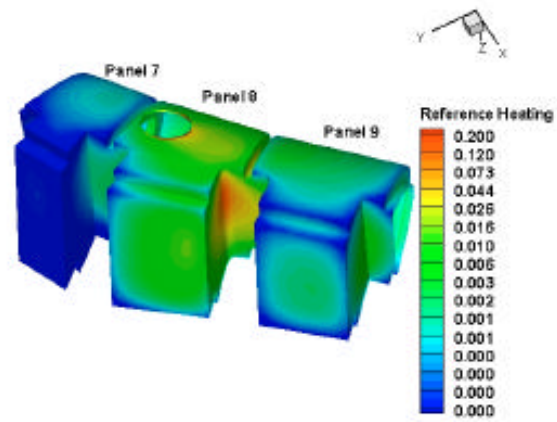

FIGURE 6. Reference heating for the 300-kft internal-flow case

Figures 5 and 6 show the number density and normalized heating profiles for the 300-kft case. In harmony with the 350-kft case, the initial free-stream conditions were extracted from the 300-kft simulation. Figure 5 shows the density and flow streamlines. In a similar fashion as the 350-kft case, a recirculation region is formed inside the wing cavity. The normalized surface heating is given in Figure 6. The actual levels of heating in this case are about one order of magnitude greater than in the previous case. However, the position of the maximum heating point is the same for both simulations. This should not be a surprise since the angle of attack is nearly the same in both cases.

Comparison between DSMC Results and Plume Heating Methodology

During the STS-107 investigation, a three-dimensional plume heating methodology was developed based on very limited CFD results and represented a "highly engineered" environment for thermal analysis. It was desired to compare the engineering methodology to high-fidelity DSMC and CFD results for STS-107 types of geometries and assess the quality of the engineering predictions used for the subsequent thermal analysis. Given the complexity of the problem, the comparisons represent more of an independent assessment than a validation of the methodology, primarily since time did not allow a second loop through the process to incorporate lessons learned. Rather, the comparisons focused on gross fluid dynamic features and qualitative assessments.

Two types of comparisons with the DSMC results at 350-kft are displayed in Figure 7. On the left side of the figure, both sets of data have been normalized by the peak impingement heating values on the panel 8/9 earmuff. The DSMC results provide additional support for the predicted internal jet direction since both methodologies predict peak heating values in the same location. DSMC results also provide an independent source for secondary splash heating to the spar region behind panel 8, again in line with the engineering methodology. Shadowing of the panel 9 spar region and some enhanced heating to the panel 9/10 earmuff are also predicted by the DSMC results, in line with engineering assumptions. The right side of the figure provides a comparison of predicted heating magnitudes with the STS-107 engineering methodology. The engineering method predicts higher heating by roughly a factor of two. However, the engineering methodology is based on continuum assumptions and the calculations are made at rarefied conditions so the conservatism is not surprising.

CONCLUSIONS

DSMC simulations of Columbia Shuttle Orbiter flight STS-107 for the prime candidate accident scenario are presented. The analysis identifies instances where the localized heat flux to the Orbiter was in the proximity of the damaged leading edge. Calculations of the flow inside the leading edge also indicate the development of a recirculation area enhancing the heat flux to the walls. The DSMC results compare well with the plume engineering methodology used in the investigation.

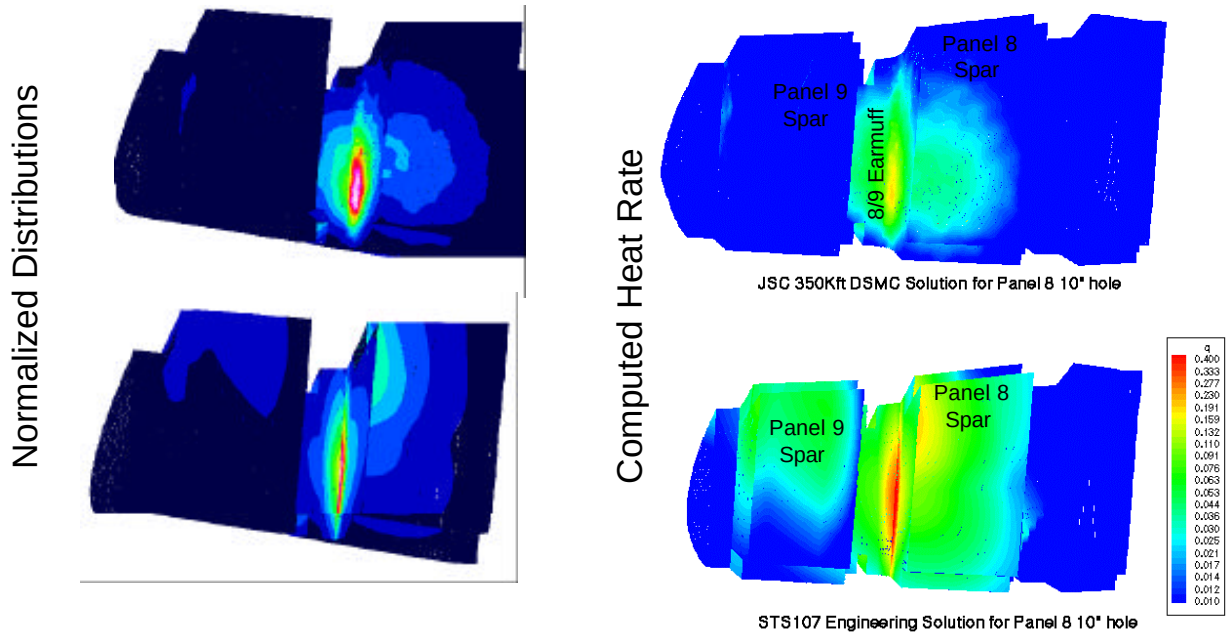

FIGURE 7. Qualitative comparison of engineering methodology with DSMC calculations at 350 kft

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