AXISYMMETRIC PLUME SIMULATIONS WITH NASA'S DSMC ANALYSIS CODE

B. D. Stewart and F. E. Lumpkin III
NASA JSC – Applied Aeroscience and CFD Branch (EG3)
Houston, Texas

ABSTRACT

A comparison of axisymmetric Direct Simulation Monte Carlo (DSMC) Analysis Code (DAC) results to analytic and Computational Fluid Dynamics (CFD) solutions in the near continuum regime and to 3D DAC solutions in the rarefied regime for expansion plumes into a vacuum is performed to investigate the validity of the newest DAC axisymmetric implementation. This new implementation, based on the standard DSMC axisymmetric approach where the representative molecules are allowed to move in all three dimensions but are rotated back to the plane of symmetry by the end of the move step, has been fully integrated into the 3D-based DAC code and therefore retains all of DAC's features, such as being able to compute flow over complex geometries and to model chemistry. Axisymmetric DAC results for a spherically symmetric isentropic expansion are in very good agreement with a source flow analytic solution in the continuum regime and show departure from equilibrium downstream of the estimated breakdown location. Axisymmetric density contours also compare favorably against CFD results for the R1E thruster while temperature contours depart from equilibrium very rapidly away from the estimated breakdown surface. Finally, axisymmetric and 3D DAC results are in very good agreement over the entire plume region and, as expected, this new axisymmetric implementation shows a significant reduction in computer resources required to achieve accurate simulations for this problem over the 3D simulations.

INTRODUCTION

At high altitudes, plume impingement problems cannot be modeled using Computational Fluid Dynamics (CFD) solvers because the continuum assumption becomes invalid as the flow expands into a near vacuum. The Direct Simulation Monte Carlo (DSMC) method[1], which models gas at the molecular level, is the method of choice to simulate such flows. Even at the low densities encountered in high altitude plume impingement problems, the actual number of molecules in the gas remains very large and cannot be simulated directly. Instead of simulating the actual gas molecules, the DSMC method uses representative molecules, usually between several millions to hundreds of millions, to model the gas flow. Representative molecules are tracked in space and time inside a meshed domain and the DSMC method assumes that the transport and collision phases can be modeled in two distinct computational steps. A network of computational cells is used to group neighboring molecules with possible collision partners and individual or groups of computational cells are also used to statistically sample the molecular data to produce macroscopic properties such a density and temperature.

The main requirements to obtain an accurate solution using the DSMC method are threefold. First, the timestep size must be smaller than the local mean collision time to enable the decoupling of the transport and collision phases. Next the collision cell size must be smaller than the local mean free path, or mean distance travelled by a molecule between two successive collisions. This requirement ensures that artificial viscosity isn't introduced into the solution by colliding molecules separated by more than one mean free path. Finally, each computational cell should contain a large enough number of representative molecules per cell to ensure an accurate statistical representation of the gas during the collision phase.

The DSMC method is well suited to solve plume expansions into a vacuum as it can theoretically model flows that span continuum, transitional and free molecular regimes. Unfortunately, based on the fundamental constraints of the method, accurate computations of the continuum regions of the flow with the DSMC method are prohibitively expensive. Additionally, the far field regions of the plume that are in the rarefied regime cannot be modeled using a continuum approach. Therefore, plume expansion problems are usually solved using a sequential approach. The near-field region of the expansion plume is usually computed using either a source flow model or using a CFD solver. Then, at a prescribed interface, the necessary data is extracted from the continuum solution and is provided as input to the DSMC code. Even when only modeling the far field region of the plumes the computational cost of the DSMC simulation may still be prohibitive, therefore, cost savings approaches, such as taking advantage of the symmetry of the problem, whenever possible, must be considered. Examples of plume impingement problems solved using the DAC code include Space Shuttle's airlock venting gas on the Hubble Space Telescope (HST) solar array[2], high fidelity plume impingement on the International Space Station (ISS)[3], and Orion self-impinging plumes during re-entry[4].

The purpose of the present analysis is to validate the axisymmetric approach that has recently been implemented in NASA's DSMC Analysis Code (DAC) for the simulation of high altitude plumes. Axisymmetric results are compared to an analytic solution for a spherically symmetric gas expansion into a vacuum and to CFD and to 3D DAC results for the R1E thruster plume.

SIMULATION METHOD

One of the primary objectives in developing NASA's DAC code[5] was to provide a high fidelity modeling tool for vacuum plume impingement on spacecrafts and satellites.

PLUME SIMULATIONS

Simulating plume expansions into a vacuum can be a challenging problem as no single computational approach can accurately and/or efficiently model the gas from the combustion chamber to the far field region where the gas impinges on a given surface. Instead, a multi step approach is generally chosen where different methods appropriate for different regimes of the gas flow are used sequentially. For a given thruster, a CFD approach is used to model the flow inside the nozzle and into the near field region of the thruster. At some distance from the nozzle exit plane, the gas is sufficiently expanded that the continuum assumption breaks down and the CFD solution becomes invalid. The limit between continuum and non-continuum regions of the flow is usually described using a Bird breakdown parameter, B, equal to 0.05, where B is given by[6]:

$$B = \frac{-\lambda \vec{V} \nabla \rho}{\rho \bar{c}} \tag{1}$$

where λ is the mean free path and $\bar{c}$ is the average molecular speed of the gas.

The computed interface is generally smoothed out and is connected to the nozzle exit lip to form the inflow surface that will be used in the DSMC computation. The last step of this process is to interpolate the CFD results to the inflow surface such that required input, such as density, temperature and gas velocity, can be provided to the DSMC code.

DAC AXISYMMETRIC IMPLEMENTATION

The DAC code is a fully three dimensional parallel DSMC code that has been used over the years to solve a wide range of rarefied problems from high altitude re-entry flows to plume

impingement studies. In order to solve flows around complex geometries, the surfaces are represented in DAC by triangulated, topologically water tight meshes that are then embedded inside a two-level Cartesian grid system. The grid system can be refined following the DSMC requirements on cell size and timestep size using an iterative adaptation process. The DAC code models the relevant energy exchange between the translation, vibrational and chemical modes of the molecules and has been designed to support fully three dimensional, two dimensional, and axisymmetric simulations.

While inherently three-dimensional, due to the random movement of the molecules, the standard DSMC method can be modified to solve axisymmetric problems. The most common axisymmetric implementation allows molecules to move in all three dimensions but forces them back to the symmetry plane by the end of the transport phase. One drawback of this approach is that, depending on the actual implementation, this approach may produce depleted density and pressure contours near the axis of symmetry due to the fact that the cell volumes are very small in that region of the domain[7]. The original DAC axisymmetric implementation used a different approach that employs a physical wedge to constrain molecules to a small region of space around the symmetry plane. Unfortunately, this approach could not guarantee that the cell size was smaller than the mean free path everywhere in the domain, more specifically in the regions far away from the axis of symmetry. The new DAC axisymmetric implementation which is a hybrid between the original method used in DAC and the most common method is presented in more detail in the present section.

Because DAC was initially implemented as a 3D code, the present approach requires the input of a 3D surface geometry (Figure 1). For a plume simulation, the outline in the symmetry plane of the breakdown surface for the CFD solution is extruded in the third direction to create a triangulated inflow surface where molecules will be input to the DSMC simulation. This surface is integrated with other walls, modeled as outflow surfaces for plume simulations, that will help define the computational domain as shown in Figure 1. As long as the extracted surfaces extend outside of the domain limits for the Cartesian mesh, the surface geometry is no longer required to be water tight. This approach provides a way to save on memory usage as fewer triangles are required to define the surface geometry.

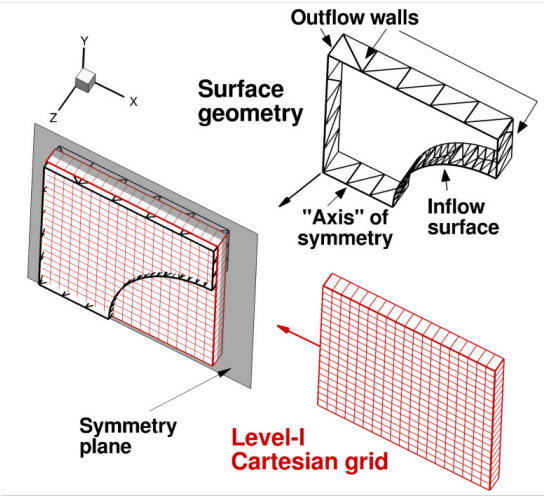


Figure 1: Schematic of the surface geometry for a DAC axisymmetric simulation of a spherically symmetric expansion plume into a vacuum.

Because the surface geometry and the Cartesian grid no longer model the actual symmetry of the problem, a pre-processing step has been added to the DAC code to accurately model the axisymmetric problems. First, the current approach computes the cell volumes in three dimensions and prost-processes them to obtain the actual axisymmetric cell volumes. For both computational cells with and without intersecting surfaces, the present approach computes the axisymmetric volumes to within a few percent of the actual values. Next, the surface triangles are intersected with the symmetry plane in order to produce inflow and solid line segments. Because of the symmetry of the problem, each line segment may represent a different rotated shape and this has to be taken into account during both the creation and the move phases. The vertical segments represent flat rings, the horizontal segments represent cylinders, while all other segments represent conical sections. Molecules are created from the inflow line segments and enter the domain inside the symmetry plane. Next, the molecules are moved in all three dimensions. Because DAC allows variations in timestep and ratio of real to simulated molecules from one Level-I cell to another, the code first computes the time it takes a molecule to reach the edge of the cell. The main difference from the 3D solver is that in the direction perpendicular to the axis of symmetry, the code must compute the time it takes the molecule to reach the cell edge *after* it has been rotated back to the symmetry plane. If the molecule crosses to another cell, the timestep size required to reach the edge is computed and the molecule is moved by that timestep. Next, the code checks if the 3D molecule path intersects any of the surfaces represented by the solid line segments and, if it does, the code computes the time it takes the molecule to reach the surface and models the surface interaction. At the end of this sub-step, the molecule is rotated back to the symmetry plane. This process is repeated until the molecule has been moved by the full timestep. The other steps in the DSMC method, such as the molecular collision and sampling phases, remain similar to the 3D implementation. Once the simulation is over, surface properties can be computed and are output in line plot format after being possibly smoothed out or interpolated to uniform segments.

RESULTS

SPHERICALLY SYMMETRIC ISENTROPIC EXPANSION INTO A VACUUM

A spherically symmetric flow that isentropically expands into a vacuum is an example of a self-similar flow because the gas properties only depend on the radial distance from the point of origin. Using the isentropic relationships and number density, n^*, and temperature, T^*, at the sonic radius, r^*, the gas properties at radius r are given by:

$$\frac{r}{r^*} = \sqrt{\frac{1}{M}\sqrt{\left[\frac{2+(\gamma-1)M^2}{\gamma+1}\right]^{\frac{\gamma+1}{\gamma-1}}}}$$

$$T = \frac{(\gamma+1)T^*}{2+(\gamma-1)M^2} \qquad (2)$$

$$V = M\sqrt{\gamma RT}$$

$$n = n^*\left[\frac{\gamma+1}{2+(\gamma-1)M^2}\right]^{\frac{1}{\gamma-1}}$$

where γ is the ratio of specific heat, R is the ratio of the ideal gas constant by the gas molecular weight, and M, T, V, and n are the Mach number, temperature, velocity and number density at radius r, respectively.

Unfortunately, this analytic solution is only valid in the near field region of the expansion because, as the gas expands, the flow becomes rarefied and the continuum assumption used to produce Equation (2) breaks down. The objective of the present simulations is to show that the DAC axisymmetric implementation correctly models the physics of the expansion in the continuum regime while also accurately modeling the departure from equilibrium as the flow becomes rarefied. Therefore, the interface at which the analytic solution is passed as input to the DAC simulation is chosen to be in the continuum region of the flow and instead of specifying the number density at the sonic radius, the Bird breakdown parameter is used.

For the present self-similar flow, the Bird breakdown parameter at radius r can be rewritten as:

$$B = 2\frac{V\lambda}{\bar{c}r} \tag{3}$$

Replacing the mean molecular speed and using the hard sphere approximation for the mean free path, the number density can be expressed as function of the Bird breakdown parameter as:

$$n = \frac{1}{2}\sqrt{\frac{\gamma}{\pi}}\frac{M}{Bd^2r} \tag{4}$$

where d is the molecular diameter.

The present simulation models the expansion of an argon perfect gas with a ratio of specific heats of 5/3, a molecular weight of 39.948 g/mol and a collision diameter, d, of $4.17e^{-10}$ m. The sonic conditions occur at a radius of 1 m from the point of origin of the expansion with a gas temperature of 1000 K and a Bird breakdown parameter of 0.0025. The inflow surface where molecules are created in the DAC domain is located at a radius of 1.05 m. As shown in Figure 2, the flow conditions at the inflow surface are still in the continuum regime and the continuum assumptions are expected to break down at a radius of about 2.5 m. The DAC simulation is started on a uniform grid with a cell size of the order of the mean free path for a gas at a number density one order of magnitude smaller than the gas at the inflow surface. Because this grid under-resolves the flow near the inflow surface, the simulation uses virtual sub-cells in order to reduce the effective collision cell size[8]. The total number of molecules in the domain is approximately 175 million and cells near the inflow surface have as many as 10,000 molecules. This simulation took less than one hour to run using 120 processors. Based on this initial simulation, an adapted grid is created with a grid size everywhere in the domain of the order of the local mean free path. Because the number density in the entire domain is actually much lower than the value used to create the uniform grid the adapted simulation uses a lot fewer cells and therefore molecules, only approximately 4 million, while still following the basic DSMC constraints on cell size, timestep size and number of molecules per cell. As a consequence, the adapted case is much faster than the uniform case and takes only five minutes to complete when using 120 processors.

Axisymmetric implementations in DSMC codes have been shown in the past to have problems simulating the gas flow near the axis of symmetry because the cell sizes in that region of the domain become very small[7]. The present axisymmetric number density contours (Figure 2), however, show no depletion near the axis of symmetry and the contours are concentric over the entire domain. In order to directly compare the DAC axisymmetric and the analytic solutions, data have been extracted along the white lines shown in Figure 2. The three different lines, in the +X direction, in the +Y direction and along the Y = -X direction, were chosen in order to validate the solution over the entire domain. The non-dimensional number density DAC line plots as function of radial distance from the point of origin (Figure 3a) are in very good agreement over the entire domain with the analytic solution. The non-dimensional temperature line plots, however, show that for radial distances greater than around 5 m, the DAC temperatures depart from the equilibrium temperature obtained with the analytic solution. As the gas becomes more and more rarefied, the local collision rate decreases to the point where there is no longer enough collisions for the gas to remain in local thermal equilibrium. The temperature freezes and therefore departs further and further from the analytic temperature which continues to decrease with radial distance. This departure from equilibrium happens downstream of the location at which the Bird

breakdown parameter is equal to 0.05 which means that for this case the initial assumption that the continuum assumption breaks down at that location is conservative.

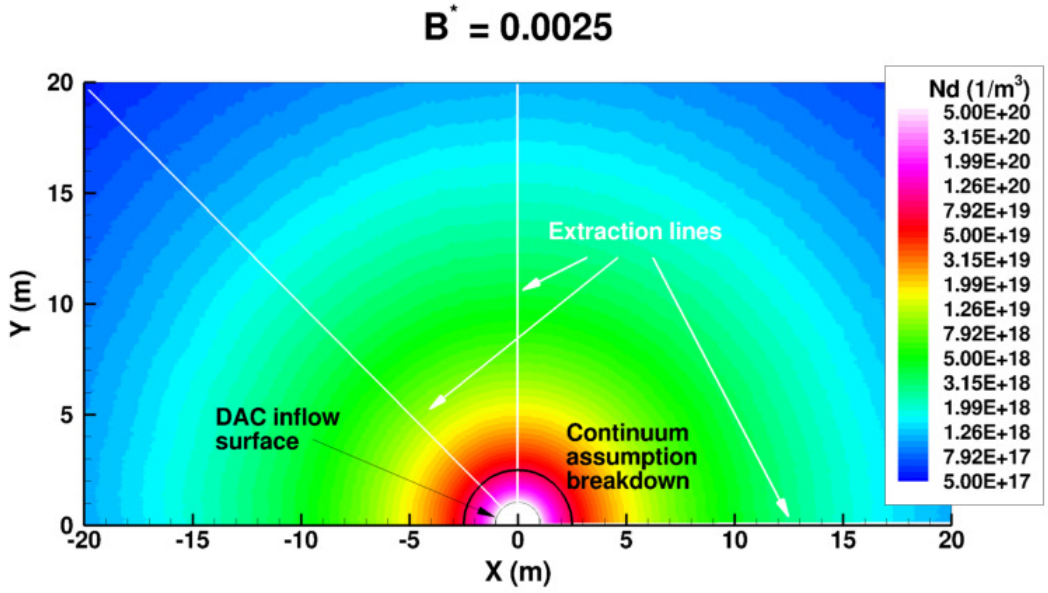
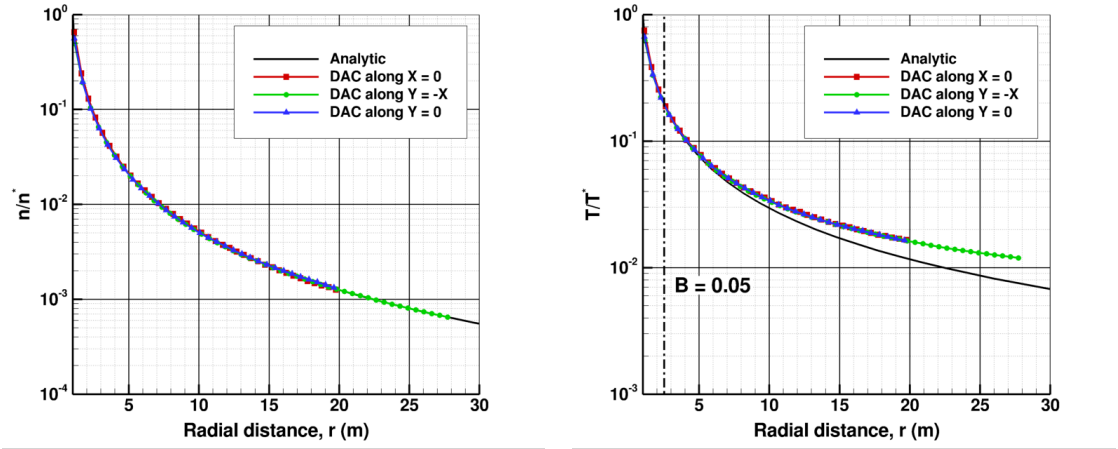


Figure 2: DAC axisymmetric number density contours for a spherically symmetric expansion into a vacuum.



(a) **(b)**

Figure 3: DAC and analytic non-dimensional number density and temperature line plots as function of radial distance.

R1E THRUSTER PLUME

A more realistic test of the new axisymmetric implementation is to simulate an actual thruster plume expansion into a vacuum. The R1E thruster is used in the present simulations to compare the axisymmetric DAC results to both 3D DAC results and a CFD solution. The nozzle section of the thruster and the near field region of the plume have been computed using a CFD solver. Figure 4 shows the Bird breakdown parameter contours for the CFD solution. Please note that the contours are not matching at the boundaries between the CFD sub-domains because gradients aren't computed based on data located on both sides of the boundaries. The inflow surfaces for the axisymmetric and 3D solutions are created based on the contour line where the Bird breakdown parameter is equal to 0.05 and by respectively extruding the line in the Z direction or rotating the line 360 degrees. For reference, the outline of the inflow surface in the symmetry plane used in the DAC simulations is also shown in Figure 4. Once the inflow surface has been created, the CFD solution is interpolated to each surface. In the present DAC simulations, the thruster gas is assumed to be a single species with a molecular weight equal to the average molecular weight in the CFD solution at the interface near the centerline of the plume. The axisymmetric simulation ran under thirty minutes on 48 processors and an iterative adaptation process was again used in order to properly refine the mesh and timestep size everywhere inside the computational domain. For the adapted grid simulation, the grid resolved the local mean free path everywhere in the domain and the number of molecules decreased to 7 million from the 8 million used in the uniform grid simulation. The 3D run took about nine hours to run on 180 processors and required 90 million molecules for the simulation on the uniform grid and 630 million molecules for the simulation on the adapted grid. The simulation on the adapted grid was also resolved to mean free path resolution by using virtual sub-cells for selecting the collision pairs[8].

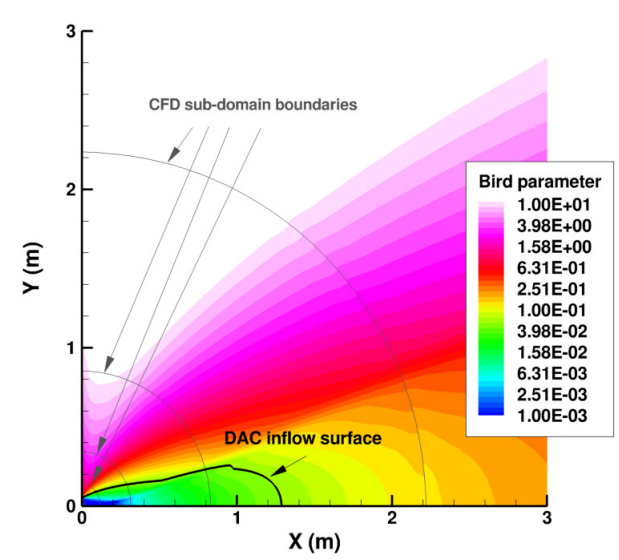


Figure 4: CFD Bird parameter contours in the symmetry plane for the R1E thruster.

Non-dimensional density and temperature contours are shown in Figure 5. Overall, the 3D and axisymmetric DAC density and temperature contours are in very good agreement over the entire domain. The DAC density contours also compare favorably to the CFD solution except very near the left boundary of the domain. In the CFD solver, the region near the nozzle lip is simulated as a viscous wall. In the DAC simulation, however, there is no physical wall there and the gas is allowed to freely expand. This difference in the modeling of the boundary can be seen

in the density increase near the wall for the CFD solution. As with the expansion, when comparing the DAC solutions to the CFD results, non-equilibrium effects are mostly apparent in the temperature contours. The non-dimensional DAC temperature contours are very different from the CFD contours except very near the axis of symmetry, near the inflow surface. Therefore, for this case, the departure from equilibrium occurs near the location at which the Bird breakdown parameter is equal to 0.05. Similar to the expansion flow, the temperature computed in the DSMC simulations freezes as the gas expands and is therefore higher in most of the domain than the temperature computed in the CFD simulation.

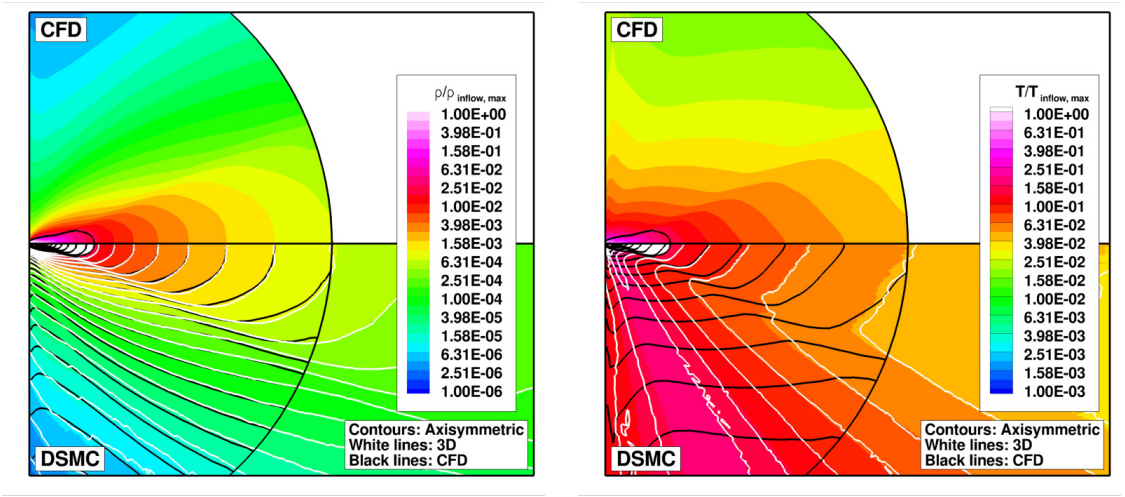


Figure 5: Non-dimensional density (left) and temperature (right) contours in the symmetry plane for the R1E thruster.

SUMMARY AND CONCLUSIONS

Axisymmetric DAC results have been compared to an analytic solution for a simple spherically symmetric expansion. The results are in very good agreement with the analytic solution in the continuum region of the domain and show the expected departure from equilibrium in the temperature line plots downstream of the estimated continuum breakdown location. Axisymmetric results have also been compared to CFD and 3D DAC solutions for the R1E thruster. For this case, the density contours are in very good agreement with the CFD contours except very near the left boundary of the domain and freezing of the temperature is observed everywhere in the DSMC domain. Finally, the axisymmetric and 3D DAC solutions are in very good agreement over the entire domain and as expected the axisymmetric results were generated faster than the 3D results by more than one order of magnitude.

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