Thermochemical and Particulate Interfacing for Hybrid High-Altitude Plume and Control Jet Simulations

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Abstract. A hybrid modeling capability has been developed by coupling a CFD code to a DSMC code using a one-way coupled interface surface. Using a unique toolkit, named AEGIS, these surfaces can be generated for complex, arbitrary 3D shapes. The status of this technology development is described. Modifications that include non-equilibrium internal energy modeling in the CFD code and solid particulates for DSMC have extended these capabilities. Application to axisymmetric plumes at high altitude indicates proper coupling across the interface boundary. However, resolution of the low vibrational temperature found in expanding flows presents a computational challenge that must be addressed. Particulate modeling shows good agreement between CFD and DMC. For these high altitudes, the drag forces on the particulates are mostly negligible with thermal radiation being the dominant physics.

Keywords: Hybrid CFD/DSMC, Plume flows, Non-equilibrium flows
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INTRODUCTION

Computational modeling of rocket and missile exhaust plumes requires accurate physical models and sophisticated numerical methods. The nearfield plume can be modeled using conventional continuum-based CFD codes. As this flow expands, it becomes more rarefied. At high altitudes, the interaction of this plume with a rarefied freestream requires modeling the intermolecular interactions more directly. In this region, the direct simulation Monte Carlo (DSMC) [1] method is appropriate. Hybrid CFD-DSMC simulations of the plume flowfield typically consist of a continuum nearfield simulated using continuum-based CFD methods while the rarefied farfield is treated using DSMC methodology.

A hybrid modeling capability for high-altitude plumes, divert jets, and re-entry vehicles has been developed by combining the features of the CRAFT CFD® continuum code [2][3] and a modified version of the DAC97 [4] DSMC code called PDAC. Rarefied flow modifications are implemented into the continuum flow solver to extend its range of applicability to higher altitudes and more rarefied conditions in order to further reduce the computational effort on the non-continuum solver. The hybrid continuum-DSMC computations are performed by coupling the continuum and DSMC simulations along a breakdown surface, usually based on the Bird breakdown parameter.[1] Substantial progress has been made toward automating the coupling procedure.[5][6] The Automatic Efficient Generalized Interface Surface (AEGIS) Toolkit extracts three-dimensional iso-contours of the breakdown parameter and generates an optimal unstructured grid that approximates one of these iso-contours using an automated minimization and smoothing algorithm. Complex, and multiple, 3D interface surfaces can be constructed using the AEGIS Toolkit.

This paper presents the status of this hybrid technology, including the code extensions and AEGIS Toolkit with applications to high altitude plumes. Emphasis is placed on the propagation of flow properties, such as thermal non-equilibrium and particulate properties, across the interface boundaries. Thus, axisymmetric calculations are used in order to focus on these details.

HYBRID STATUS

Modifications to both the CFD and DSMC codes have extended their overall capabilities. For example, non-local thermodynamic equilibrium (NLTE) model additions to CRAFT CFD® coupled with modifications to PDAC's source specification allow non-equilibrium gas properties to be propagated across the interface boundary. For plume applications, these additions permit the continuum solver to be applied to a larger region which allows the coupling boundary to have a lower density than it would have otherwise. Two-phase flow capabilities already contained in the CRAFT CFD® continuum codes have also been incorporated into the PDAC DSMC code using one-way coupling. The particulate thermodynamic properties at the interface surface for PDAC are provided by CRAFT CFD® using movement procedures similar to those used for gas properties. However, collisions between solid particles are ignored and the effects of gas-solid collisions are specified using empirical drag and heat-transfer methodologies.

AEGIS

A unique Automatic Efficient Generalized Interface Surface Toolkit (AEGIS Toolkit) has been developed to automatically generate an interface surface that separates the continuum and rarefied non-continuum regions. AEGIS also generates a triangulated mesh and interpolates the necessary properties, ie. number densities, velocities, and temperatures, onto this triangulated surface. This toolkit is an extension of the Arbitrary Breakdown Surface Generation (ABSG) technique described previously [5] where it was applied to axisymmetric plumes. The AEGIS toolkit still uses a methodology based on Geometrically Deformed Model (GDM) theory.[7] This methodology employs a cost minimization algorithm based on an image parameter (such as the Bird breakdown parameter), smoothness (surface elasticity), and forcing function to produce an appropriate coupling boundary geometry from an often times complex and discontinuous field function. This coupling boundary approximates the breakdown iso-surface, although other more well-behaved flow parameters may be used to assist in defining the coupling boundary. Symbolically, the procedure can be thought of as a balloon expanding within a confined space that may have holes. As the balloon is inflated, it gradually takes on the shape of the confined space while the surface elasticity of the balloon prevents it from leaking out any of the holes until a point is reached where the balloon cannot expand unless broken.

The need to deal with complex interface surfaces and join them to bodies required additions and modifications to the original GDM methodology, and the software is now called AEGIS toolkit. One such improvement is the integration of the GNU Triangulated Surface (GTS) toolkit [8]. The GTS toolkit is Open Source Free Software that contains numerous features for triangulation of 2D and 3D surfaces and for performing geometrical and logical manipulation of these surfaces, such as determining unions, intersections, and differences. This methodology can be readily utilized to generate a body surface triangulation, remove the intersected regions between GDM surfaces, merge the body and GDM surface, etc., efficiently and, more importantly, automatically.

Figure 1 shows the interface surface generated by AEGIS for a generic 3D plume problem. Recently, a more complex 3D interface geometry was constructed for an Apollo re-entry flow at 85 km and 95 km. The Apollo command module geometry is shown in Figure 2a with the location of two reaction control (RCS) jets included. At these altitudes the wake is rarefied and a breakdown surface surrounding the body is generated which must be connected to the body. This surface is shown in Figure 2b. The two RCS plumes are modeled using the continuum solver until breakdown occurs. Figure 2c shows the breakdown surface where the two plumes merge which is then connected to the thruster exits on the vehicle afterbody. A separate simulation was also performed for a smaller value of the breakdown parameter for which the two plumes remain separate and are independently merged to the thrusters.

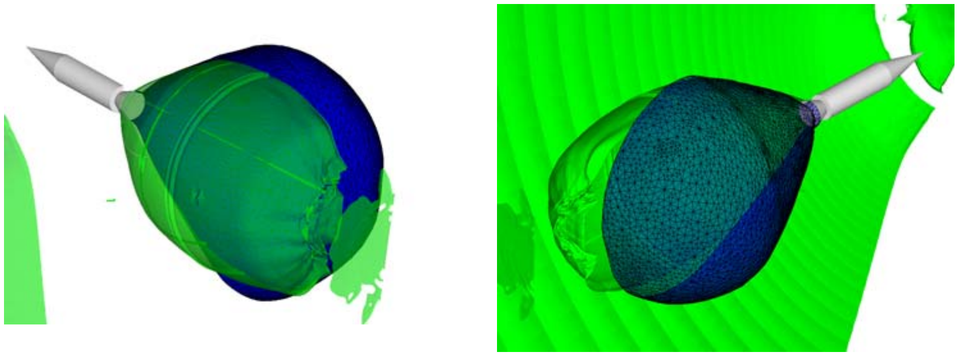
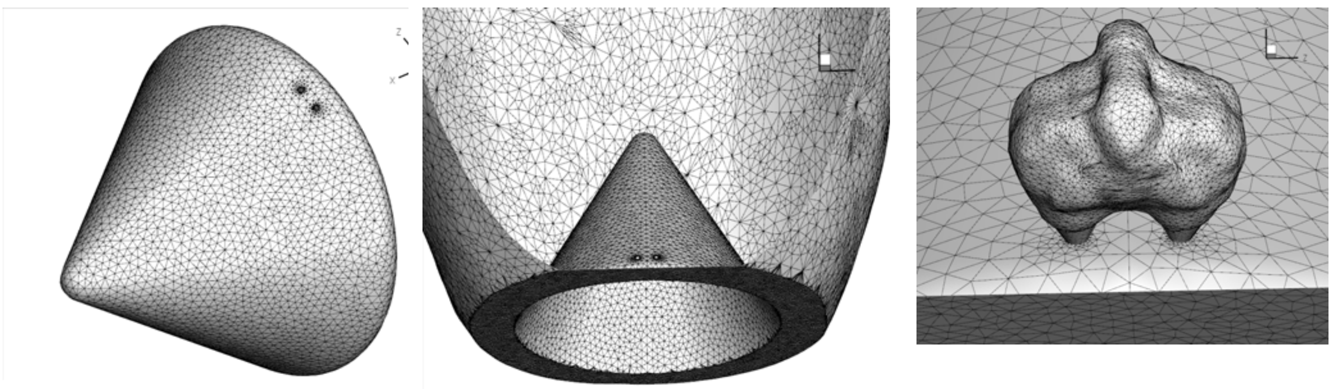


Figure 1: CFD-DSMC Plume Interface Surface.



a) Apollo command module

b) CFD-DSMC Interface merged with body

c) 2 RCS Plumes "Mixed"

Figure 2: CFD-DSMC Interface Surface for Re-entry Flow with RCS Jets.

NLTE

As plumes expand into a rarefied background, there are insufficient collisions to maintain thermal equilibrium between the various modes. For hybrid calculations, ignoring these effects in the continuum solver leads to either an unphysical discontinuity in internal mode temperature across the interface boundary or restricts the size of the continuum region. Various CFD codes have multiple temperature models to capture thermal non-equilibrium effects in hypersonic re-entry flows. CRAFT CFD® has a standard "two-temperature" model where only the species vibrational temperatures are assumed to be out of equilibrium. This model has been extended to include additional equations for modeling rotational relaxation. Refinements to the rotational relaxation rates were made to provide non-equilibrium behavior that is more consistent with that predicted by DSMC to facilitate better coupling for the hybrid framework. Separate temperatures can be maintained for each species, providing enhanced accuracy.

Vibrational and rotational non-equilibrium modeling introduces additional transport equations for each computed species assumed to be out of thermal equilibrium with its environment. If necessary, the formulation can be easily expanded to include each mode as a separate species. The general rate of non-equilibrium uses a Landau-Teller relaxation time formulation where the vibrational relaxation time is correlated from Millikan and White [9] and the rotational relaxation time is correlated from either Parker [10] or Lordi and Mates [11].

Earlier work tested these models for re-entry flow problems using the Apollo command module at moderate altitudes (85 – 95 km) and a CEV geometry as examples. Good agreement between CRAFT CFD® and PDAC was found for the Apollo case. The plume expansion problem presents a new challenge as the temperatures decay to values much lower than the characteristic vibrational temperatures. The intent is to be able to extend the CFD solution to a larger portion of the plume and thereby reduce the computational effort required for the DSMC simulation. The appropriate size of this inner plume region is likely altitude dependent.

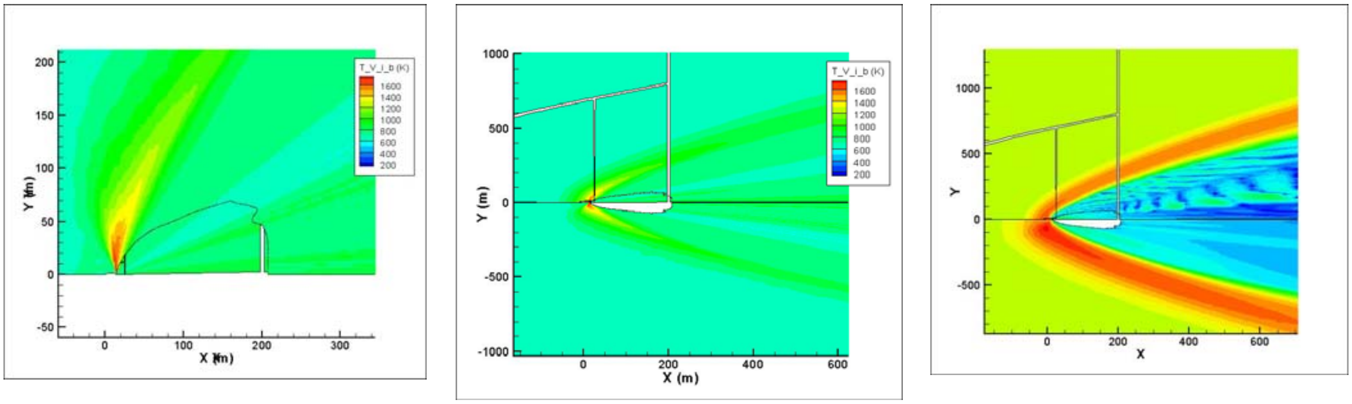
Particulates

Particulates (from solid motors) are also of interest for computing high-altitude plume flow characteristics and plume radiance. CRAFT Tech has developed extensive methodologies for multiphase modeling of both liquid and solid particulates in plumes and divert jets. The models have been implemented in our CRAFT CFD® code using both Eulerian and Lagrangian methodologies. A similar Lagrangian methodology has also been implemented in the PDAC DSMC code based on one-way coupling. In the one-way coupled, Lagrangian approach, the particle paths and temperatures are determined by integrating empirical drag and heat transfer equations to account for momentum and energy transfer from the gas to the particulates. The empirical equations used in PDAC are identical to those used in the continuum methodologies. PDAC also uses the same enthalpy-temperature curve fits and emissivity tables as the continuum codes, so that particle phase and radiative property changes occur seamlessly across the coupling boundary.

RESULTS

Thermal Non-equilibrium Simulations

The thermal non-equilibrium model was previously tested for Apollo re-entry. Here, the three temperature model is applied to a generic axisymmetric plume calculations performed at 150 km altitude and a freestream Mach number of 6.5. The rotational and translational temperature are still in equilibrium for this case, however it provides an opportunity to test the vibrational temperature model in CRAFT CFD®. Figure 3shows comparisons of the CRAFT CFD® solution with a hybrid solution generated using PDAC from an inner plume source provided by CRAFT CFD®. The vibrational temperature of N_2 is shown in Figure 3a. The interface surface is shown in black with the CFD solution inside and the DSMC outside. The flowfield properties appear to be properly propagated across the boundary. A comparison of the full CFD solution to the hybrid in Figure 3b shows good agreement for N_2. In both cases, the decaying vibrational temperature “freezes” during plume expansion. The comparison of translational temperature is also in good agreement as shown in Figure 3c. Further studies of the accuracy of the non-equilibrium internal energy modeling in the CFD codes are ongoing. For example, the accuracy of the model for complex multiple species systems has yet to be verified.

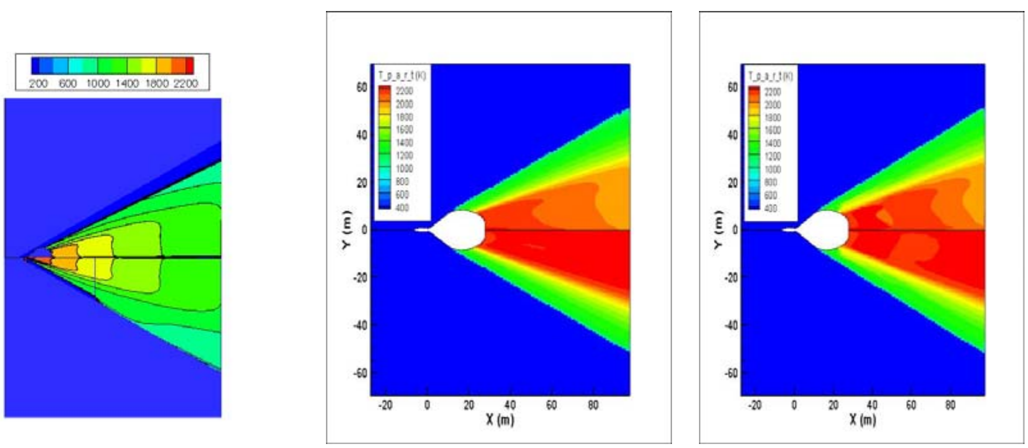


a) T_{vib}-N_2 at interface b) T_{vib}-N_2 CRAFT CFD (upper) & Hybrid (lower) c) T_{tr} CRAFT CFD (upper) & Hybrid (lower)

Figure 3: Comparison of CFD and Hybrid Calculations.

Particulate Simulations

Comparison of particle temperatures obtained with the CRAFT CFD® and PDAC one-way coupled approach is shown in Figure 4a for 1.7 micron-sized particles for a typical 120 km plume. Simulations at other particles sizes also demonstrate the level of consistency for the predictions in the nearfield plume expansion. For this particular problem, the convective heating and drag on the particles is relatively small, and particle temperatures are governed primarily by radiative cooling with phase changes occurring near the continuum breakdown surface. Figures 4b and 4c show the effect of thermal radiation on the PDAC solutions for two different particles sizes. Smaller particles (see Figure 4b) are affected more profoundly, as they are unable to store much heat. The seamless treatment of this behavior in the hybrid approach results in excellent agreement between CRAFT CFD® and PDAC particle temperatures near the axis downstream of the breakdown surface. Additional simulations varied the drag law modeled. Because the drag forces are mostly negligible at this altitude, no significant differences were found.



a) 1.7 micron b) 1.7 micron c) 3.2 micron

Figure 4: Nearfield predictions of particle temperatures: a) CRAFT CFD (lower) & PDAC (upper) b) With thermal radiation (upper) and without (lower) c) With thermal radiation (upper) and without (lower).

SUMMARY

A hybrid modeling capability has been developed by coupling a CFD code to a DSMC code using a coupled interface surface. The AEGIS Toolkit has been designed to generate arbitrarily shaped interface surfaces for highly complex 3D geometries and to simplify the surfaces where continuum breakdown iso-surfaces may exhibit complex behavior. This technology permits application-oriented engineering solutions for a variety of problems. Current work is focused on modifications such as non-equilibrium internal energy modeling in the CFD code and solid particulates for DSMC which have extended the overall capabilities of each code. Results from axisymmetric plume calculations at high altitude indicate proper coupling across the interface boundary. However, resolution of the low vibrational temperature found in rapidly-expanding flows presents a computational challenge, and additional work is planned for these applications. The tracking and properties of the particulates with the modified DSMC code agrees well with the CFD solutions. At these high altitudes, the drag forces on the particulates are mostly negligible with thermal radiation being the dominant physics.

ACKNOWLEDGMENTS

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