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Validation of Hypersonic Flow Simulations via Molecular-Scale Physics

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14. ABSTRACT

The numerical simulation of hypersonic flows is a well-developed capability. It is now possible to simulate full vehicles, resolving relevant geometric details and including effects of finite-rate chemical kinetics and gas surface interactions. However, there are known deficiencies in the governing equations, models, and numerical methods that are used to represent these flows. Thus, the overall goal of the research program was to use fundamental molecular-scale data to validate, improve, and extend the existing numerical simulation approaches for hypersonic and high-temperature flows. This work has resulted in the ability to perform more accurate and reliable simulations of Air Force relevant hypersonic flows. The research leveraged extensive prior work on the development of computational chemistry data and an array of numerical simulation method to achieve this goal. The Boltzmann equation is the most basic description of a flowing gas, and the compressible Navier-Stokes equations for a mixture of non-reacting gases can be derived from this equation. This derivation requires that the velocity distribution function is not far from equilibrium, however there is no such fully complete derivation available for a reacting gas. Kinetic theory provides expressions for the mixture viscosity and mass diffusivity of the gas mixture. It is computationally intensive use the complete kinetic theory results, and significant simplifications are made in all simulation codes.

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Final Report

Validation of Hypersonic Flow Simulations via Molecular-Scale Physics

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Objectives of the Research Program

The numerical simulation of hypersonic flows is a well-developed capability. It is now possible to simulate full vehicles, resolving relevant geometric details and including effects of finite-rate chemical kinetics and gas surface interactions. However, there are known deficiencies in the governing equations, models, and numerical methods that are used to represent these flows. Thus, the overall goal of the research program was to use fundamental molecular-scale data to validate, improve, and extend the existing numerical simulation approaches for hypersonic and high-temperature flows. This work has resulted in the ability to perform more accurate and reliable simulations of Air Force relevant hypersonic flows. The research leveraged extensive prior work on the development of computational chemistry data and an array of numerical simulation method to achieve this goal.

The Boltzmann equation is the most basic description of a flowing gas, and the compressible Navier-Stokes equations for a mixture of non-reacting gases can be derived from this equation. This derivation requires that the velocity distribution function is not far from equilibrium, however there is no such fully complete derivation available for a reacting gas. Kinetic theory provides expressions for the mixture viscosity and mass diffusivity of the gas mixture. It is computationally intensive use the complete kinetic theory results, and significant simplifications are made in all simulation codes. Furthermore, there is no theory-based model for the thermal conductivity of a non-trivial reacting gas mixture. The present research has begun to unravel the coupling between internal energy modes and dissociation; ongoing work is shedding light on the recombination process.

The research made use of advanced computational methods developed at the University of Minnesota under previous AFOSR support. These methods include a parallelized quasi-classical trajectory (QCT) code and Direct Molecular Simulation (DMS) code, an advanced Direct Simulation Monte Carlo (DSMC) code, and a state-of-the-art computational fluid dynamics (CFD) code. In addition, fundamental physical chemistry data for air has been computed from the potential energy surfaces (PESs) developed under the AFOSR MURI program. The combination of these computational methods has made it possible to validate continuum-level simulations with first-principles molecular-scale data.

The specific objectives that we sought to accomplish were:

- Use potential energy surfaces to develop accurate collision cross-section data for use in DSMC calculations of hypersonic flows. Use DMS to fully characterize the dissociation process.
- Make detailed comparisons between DSMC and CFD at increasing degrees of difficulty. Simulations were performed to target key modeling uncertainties, including diffusion, thermal conductivity in non-reacting and reacting mixtures, vibrational relaxation, and nonequilibrium dissociation.
- Validate numerical methods through careful comparisons between CFD and DSMC at conditions that stress particular aspects of current numerical flux functions.
- Based on the results of the comparisons, extend and improve models and numerical methods for practical hypersonic flow simulations.

- Use quasi-classical trajectory analyses to study the recombination process for air reactions; develop models to represent this process at relevant conditions.
- Make comparisons with existing and forthcoming experimental data and help design future experiments to be sensitive to modeling uncertainties.
- Implement the resulting models and methods in the University of Minnesota US3D CFD code for use by the US hypersonics community; support the DoD CREATE program for hypersonic CFD development.

In addition to these goals, we responded to requests to analyze the Boundary Layer Transition (BOLT) flight test experiment. This work involved the application of high-fidelity simulation tools to the BOLT flow field to characterize the boundary layer transition process on this relatively complex configuration.

Introduction

Background and Technical Issues

Hypersonic and re-entry flows are characterized by extreme gradients in key flow quantities, nonequilibrium internal energy and chemical state, and highly coupled convective and diffusive effects. For example, a re-entry vehicle has a shock layer that is only a few millimeters thick, with temperatures that can exceed 20,000 K. Over the past several decades, it has become possible to accurately solve the equations that describe these flows on very large and complex grids. However, all of these computational fluid dynamics (CFD) and Direct Simulation Monte Carlo (DSMC) codes use the *same* models, based on the *same* sets of assumptions. There has never been a rigorous evaluation of these models, and there are known deficiencies in their formulation.

A comparison between the best available CFD codes for aerothermal flows and experimental data was conducted by CUBRC Inc. during the Summer 2014 AIAA Fluid Dynamics Conference. Two configurations were studied in the LENS-XX expansion tunnel: a hollow-cylinder-flare and a double-cone. Free-stream conditions were published prior to the conference, and the computational data were submitted without knowledge of the experimental measurements. Figure 1 plots two typical comparisons from this study.

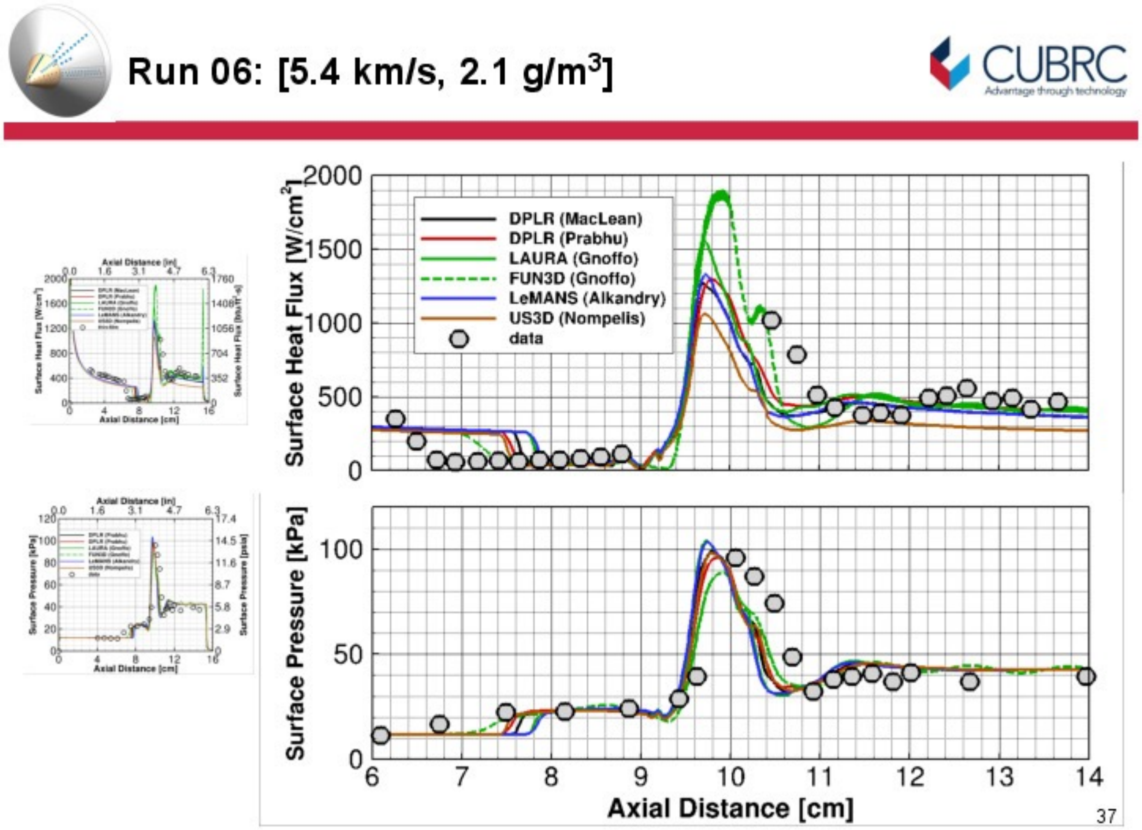

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Figure 1. Typical results from the 2014 CUBRC code validation study.

Both of these flows involve laminar shock / boundary-layer interactions, and a complex coupling between pressure gradients, flow separation, and chemical reactions. The large pressure and heat flux peak is caused by a shock wave impinging on the flare or second cone; this separates the boundary layer flow, as can be seen by the reduced levels of heat flux upstream of the interaction. In general, the CFD methods over-predict the strength of the interaction, and do not correctly capture the length of separated flow. Also note that there is more correspondence between the CFD results than with the experimental data. This occurs for all test cases considered. Previous comparisons in the CUBRC LENS-I reflected shock tunnel show similar poor agreement for high-enthalpy double-cone flows in air. No cross-facility comparisons have been made to quantify experimental data variation and sensitivity to facility type.

These flows are modeled using extensions to the compressible Navier-Stokes equations. Species conservation equations are solved to represent finite-rate chemical kinetics, and a separate internal energy equation is solved to account for possible thermal nonequilibrium effects. The coupling between the vibrational energy state and the dissociation rate is modeled. In addition, models for transport properties at high temperature are required, as well as to account for diffusive mass transport in a multi-species gas mixture. These models are built on assumptions that have not been tested at relevant conditions.

Prior to the present research, we identified some potential weaknesses of the modeling approach used by all CFD codes for aerothermal flows. These include:

- Transport property models are suspect, and in particular the thermal conductivity of a mixture of reacting gases relies on a simple assumption that has never been tested at relevant conditions.
- The full multi-component transport expression, which includes mass diffusion due to pressure and temperature gradients, is not used in present state-of-the-art CFD codes. This is in spite of the obvious fact that there are extreme pressure and temperature gradients in all hypersonic flows.
- The modeling of vibrational relaxation and its coupling to dissociation is simple and is based on an *ad hoc* approach dreamed up by its inventor (the Park TT_v model).
- There are no credible models for the redistribution of internal energy due to chemical reactions, even though this is the primary mechanism that affects the rate of these reactions.
- The physics of molecular recombination at relevant conditions is completely unexplored, and as a result, models have been fabricated based on intuition rather than factual data.
- All CFD methods use similar numerical methods and numerical flux functions; no rigorous validation has been conducted for aerothermal flows.
- The electronically excited states of atoms and molecules are assumed to not play a role in the chemical kinetics models.

The research used several recent advances that make it possible to examine and address these potential modeling weaknesses. Under a previous AFOSR MURI program, a nearly complete set of potential energy surfaces (PES) was been generated for the main ground-state air interactions (these include N_2-N_2, N_2-O_2, and O_2-O_2) [1, 22, 29, 41]. This development is profoundly important because it has made it possible to compute accurate collision cross-sections for individual interactions. For example, the momentum transfer rate can be computed directly from the PES and used to construct accurate viscosity and thermal conductivity models. Furthermore, with the Direct

Molecular Simulation (DMS) method it is possible to use the PESs to study critical high-temperature processes with exquisite detail [42, 43]. See also [20, 21, 23].

In addition, a new extremely powerful Direct Simulation Monte Carlo code has been developed at the University of Minnesota [9, 25, 30-34, 46]. Properly done (sufficient grid resolution, choice of time step, and correct physical models), DSMC is a statistically exact solution of the Boltzmann equation. With high-performance computing and scaling to massive numbers of computational cores, it is possible to run DSMC on relevant problems at the continuum limit. Thus, DSMC can be used to provide reference solutions for the continuum CFD simulations to validate models and numerical methods. This is an exciting development and we exploited it in the research program.

Commonly Used Continuum Transport Models

In the limit of near equilibrium (specifically as the local distribution functions approach equilibrium Maxwell-Boltzmann distributions), the mass diffusion, shear stress, and heat flux reduce almost exactly to the common transport models employed in hypersonic flow simulations. However, a number assumptions are employed and a number of terms are neglected. The procedure is referred to as Chapman-Enskog theory (see [7, 14] for full details), and uses a first-order perturbation to an equilibrium Maxwell-Boltzmann distribution. The form of the perturbation can be determined, and analytical expressions for the shear-stress and heat flux in the limit of near-equilibrium are obtained:

$$\tau_{ij} = \mu_{\text{mix}} \left(\frac{\partial C_{0_i}}{\partial x_j} + \frac{\partial C_{0_j}}{\partial x_i} \right) - \frac{2}{3} \mu_{\text{mix}} \frac{\partial C_{0_k}}{\partial x_k} \delta_{ij}$$

$$q_i = -\kappa_{\text{mix}} \frac{\partial T}{\partial x_i} + \sum_s n_s h_s \langle C_i' \rangle_s + \underbrace{\frac{kT}{n} \sum_s \sum_{t \neq s} \frac{n_t D_s^T}{m_s \mathcal{D}_{st}} \left(\langle C_i' \rangle_s - \langle C_i' \rangle_t \right)}_{\text{commonly neglected}} + q_i^{\text{rot}} + q_i^{\text{vib}}$$

Since diffusion velocities are defined relative to the mixture mass velocity, there is inherent coupling between species. The result of Chapman-Enskog analysis is that the set of diffusion velocities must be determined by solving the following system of equations, often referred to as the Stefan-Maxwell equations,

$$\sum_t \frac{n_s n_t}{n^2 \mathcal{D}_{st}} \left(\langle C_i' \rangle_t - \langle C_i' \rangle_s \right) = \mathbf{G_s}$$

Here, we have defined the mixture mass velocity, C_{0i} and the species s diffusion velocity as

$$\rho C_{0_i} \equiv \sum_s \rho_s \langle C_i \rangle_s \ , \qquad \langle C_i' \rangle_s = \langle C_i \rangle_s - C_{0_i}$$

These expressions for the transport properties are analytically exact, and each term results from a first-order perturbation from equilibrium. Therefore, each term should be accounted for in continuum hypersonic simulations. However, solving these equations presents significant challenges and as far as we know the full set of equations has never been used in hypersonic CFD simulations. The shear-stress expression is identical to that used in most CFD calculations and requires the mixture viscosity (μ_{mix}). The first two terms in the heat flux expression represent the standard Fourier model (with a mixture thermal conductivity κ_{mix}) and the transport of species enthalpy due to species diffusion velocities, both of which are typically used in CFD calculations.

In addition, the set of binary diffusion coefficients D_{st} defined for each species pair s,t, and the coefficient of thermal diffusion D_s^T defined for each species s, now appear in the above expressions.

The transport of energy due to thermal diffusion is not typically included in hypersonic CFD calculations. Furthermore, the pressure and temperature gradient terms that drive species diffusion are also neglected. Since hypersonic flows involve strong pressure gradients due to shock waves, and extreme temperature gradients in thin boundary layers, the assumption to neglect these terms needs validation. To make matters worse, the Stefan-Maxwell equations are not solved in standard hypersonic CFD simulations, due to computational cost. Instead, approximate models are used to calculate the diffusion velocities. A final complication is that species diffusion is inherently coupled to energy transport. As a result, the mixture thermal conductivity, κ_{mix} depends on the species diffusion velocities, which in turn require solution of the Stefan-Maxwell equations. In the present work, we have collaborated with the von Karman Institute for Fluid Dynamics to couple the MUTATION++ code to the University of Minnesota US3D code [6] to include the solution of the full Stefan-Maxwell equations.

The important point is that, even under continuum conditions, there are a number of first-order terms that are commonly neglected in hypersonic CFD simulations. Furthermore, the terms that are included, often employ simplifying assumptions, are discussed in the next section. However, since DSMC provides solutions to the Boltzmann equation, we can directly compare all terms in the governing equations. While it is well-known that these transport terms break down as the flow becomes locally rarefied, with highly parallel DSMC and CFD codes, we can now perform such term-by-term validation for continuum flows and geometries of practical interest to the Air Force. This was a major focus of the research; it has led to important new understanding of the role of thermal diffusion in hypersonic high-enthalpy flows. In particular, it has been found that it is not valid to neglect this transport term under many flight-relevant conditions.

Internal Energy Transfer and Chemical Reactions

DSMC can in principle simulate the Boltzmann equation including all internal energy transfer and chemistry physics with no empiricism. However, this requires that all state-transition probabilities are provided, which is impossible due to the huge number of possible collisional processes in high-temperature air 16, 17, 27]. DSMC simulations therefore employ simplified collision models that introduce empiricism.

In the present research, we relied on a recent development from Schwartzentruber's group: the Direct Molecular Simulation (DMS) method, which replaces the stochastic collision models used in DSMC with collisions integrated using a potential energy surface or surfaces. This method was originally proposed by Koura [20, 21, 23] and only in the past few years has Schwartzentruber's group fully extended the method to rotating, vibrating, and reacting molecules using ab-initio PESs. As described in [42, 43], since the DMS method performs collisions “on-the-fly” within a flow simulation, it only computes the state-transitions that occur with meaningful frequency, instead of pre-computing all possible transition probabilities as done for the conventional state-resolved approach. The Schwartzentruber and Candler groups demonstrated that DMS is capable of directly simulating rovibrational excitation and dissociation in nitrogen (both N-N_2 and N_2-N_2 collisions), revealing all relevant nonequilibrium physics, using the PES developed by the Truhlar group. Since state-resolved analysis for diatom-diatom collisions is intractable, DMS is the only method capable of producing such benchmark results. The present work has extended the use of DMS to the full reacting air system.

For example, consider N_2 molecules initially at 3000 K suddenly heated to 30,000 K. Figure 2 shows how the nitrogen molecules rotationally and vibrationally excite toward the fixed translational temperature of 30,000 K. N_2 immediately begins to dissociate; as a result, although average rotational and vibrational energy in the system (characterized by T_r and T_v) is increasing due to translational-rotational and translational-vibrational energy transfer, dissociation is removing internal energy from the system. Thus, the system reaches a Quasi-Steady-State (QSS) where T_r and T_v are lower than T_t. This effect was not correctly captured by any hypersonic CFD simulations prior to the current work.

Furthermore, Fig. 2 shows the evolution of the vibrational energy distribution function during the excitation phase and during the QSS. At early times the high-energy tail is overpopulated (red symbols) compared to an equilibrium Boltzmann Distribution (BD) based on the average vibrational energy (red line). This trend persists during the excitation (blue line and blue symbols). However, once high vibrational energy levels become populated, they begin to rapidly dissociate. The high energy tail during QSS is therefore depleted compared to an equilibrium Boltzmann distribution based on the average vibrational energy. These trends have also been found in studies of N-N_2 and O-O_2 systems. Since dissociation is strongly coupled to the vibrational energy of colliding molecules, accurately modeling the non-Boltzmann behavior could be very important for predicting dissociation in hypersonic flows. Although significant prior research has investigated dissociation processes, standard CFD model formulations for vibration-dissociation coupling remain empirical (the Park TT_v model [28]) and are incapable of modeling non-Boltzmann effects. The present research has developed a new model that captures these effects and is based on the fundamental data embodied by the potential energy surfaces [8-11, 35-37].

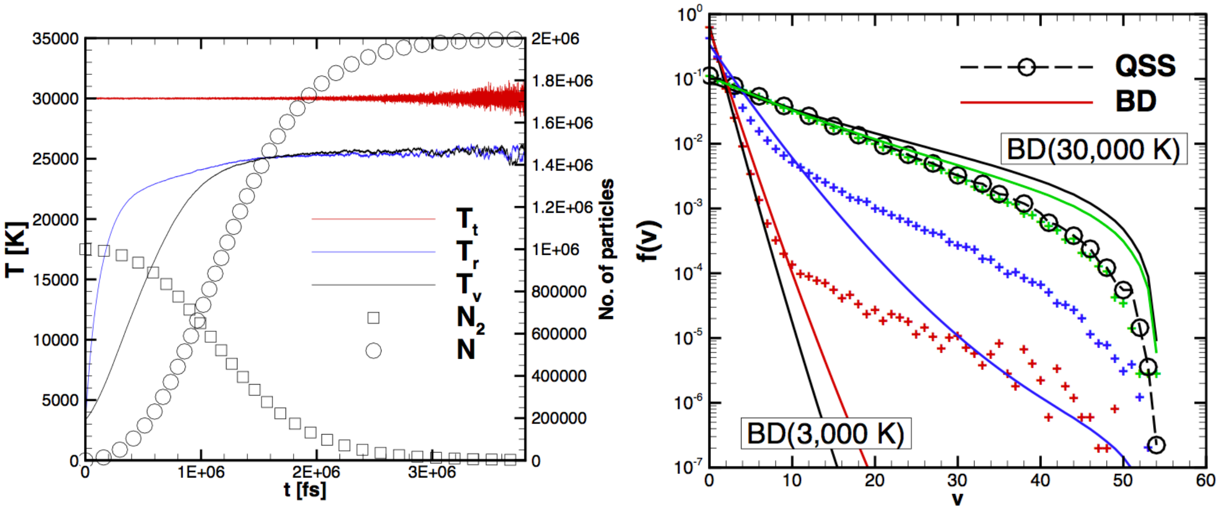


Figure 2. DMS solution for rovibrational excitation to 30,000 K and dissociation.

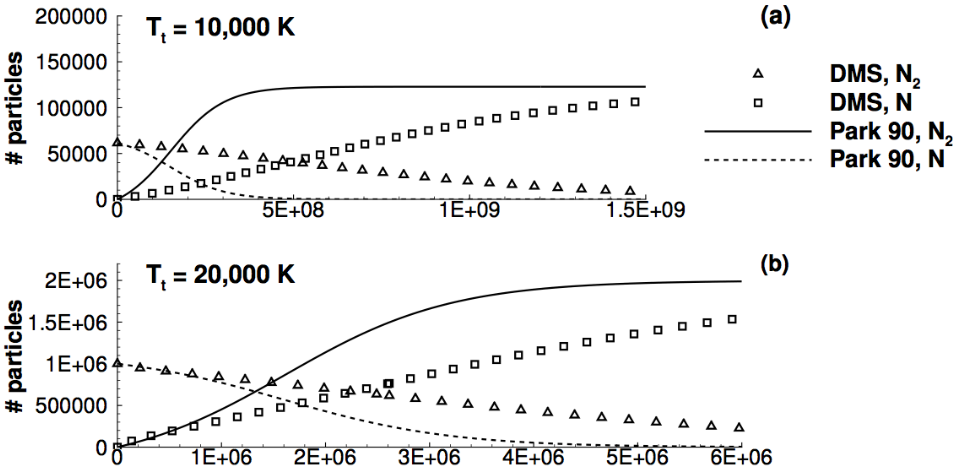


Figure 3. DMS results compared to the Park TT_v model with the Millikan-White vibrational relaxation model.

Since DMS is now capable of solving a full nitrogen system (both N-N_2 and N_2-N_2 collisions), we are able to compare these ab-initio based results (essentially a solution to the Boltzmann equation using only a PES) to a CFD solution using the standard Park TT_v model combined with the Millikan-White (MW) vibrational energy exchange model. The results are shown in Fig. 3. Clearly there are significant differences in dissociation rates at temperatures below 20,000 K, whereas the results begin to agree at higher temperatures.

Finally, Fig. 2 highlights perhaps the most significant challenge in developing a hybrid DSMC-CFD simulation capability. The vibrational nonequilibrium and coupling to dissociation occurs under continuum flow conditions. High-temperature chemically reacting flows are inherently nonequilibrium, with non-Boltzmann energy distributions present throughout the flow field. DSMC naturally simulates non-Boltzmann distributions, but current CFD models do not account for such physics. Therefore, passing information between DSMC and CFD within a hybrid simulation is problematic for reacting flows, even if such information transfer occurs in regions of continuum flow.

Hybrid DSMC-CFD capability has progressed over the past decade [12, 30, 38, 44], however, hybrid DSMC-CFD capability for hypersonic reacting flows has not yet been demonstrated. Holman and Boyd [15] performed matching DSMC and CFD simulations for reacting flow over a sphere. The study focused only on surface properties (heat flux and shear stress) and showed close agreement under near-equilibrium continuum conditions and quantified the disagreement under more rarefied conditions. Further research is needed to evaluate consistency between CFD and DSMC within the entire flow field including the diffusive flux to the surface and also for practical vehicle geometries. In the current research, we have been working to ensure full consistency between DSMC and CFD models and simulations, for transport properties, internal energy transfer, and coupling to chemical reactions. Significant progress has been made and we are now close to having a complete approach to develop a hybrid DSMC-CFD.

Overview of the Research Program

The research had the goal of improving the accuracy and reliability of hypersonic flow simulations through the use of detailed molecular-scale data. As discussed above, prior CFD codes solve the multispecies Navier-Stokes equations with extensions for finite-rate internal energy relaxation and chemical reactions. Certain aspects of these equations are well founded in theory, but the limitations of the complete set of equations and associated models is not well characterized. For example, it is not possible to determine if the differences between simulation and experiment shown in Fig. 1 are due to failure of the equations and models, problems with the numerical methods, or issues with the experimental measurements. The research program sought to systematically address these questions and develop fully consistent DSMC and CFD models for hypersonic flows.

Modeling Framework Weaknesses

As discussed above, there are several possible failure modes of the conventional simulation framework:

- The governing equations themselves may break down under the extreme conditions of hypersonic flight [2, 3, 45]. We know the Navier-Stokes equations fail when there are bimodal velocity distributions because the basic assumption of the Chapman-Enskog analysis is violated. For example, the flow inside a shock wave cannot be represented by conventional continuum equations (including the higher-order Chapman-Enskog solutions of the Boltzmann equation, e.g. the Burnett and super-Burnett equations) [4, 5].

- The approximations and assumptions made to deal with a mixture of reacting gases may not be valid. As discussed above, there is no perturbation solution of the Boltzmann equation for a complex reacting mixture of gases. Of course, the law of mass action must be valid because it is a statement of mass conservation, but its integration with the conservation equations for a nonequilibrium flowing gas is not completely straight-forward.

- Transport models and transport properties, and their implementation are not complete for mixtures of reacting gases. All CFD codes presently neglect pressure and thermal diffusion, and little has been done to verify that this is valid for Air Force relevant flows. Simple models for the mass diffusivity are used without careful validation. In addition, the Eucken relation for the mixture thermal conductivity is a particular weakness in the standard formulation.

- Internal energy relaxation and coupling to dissociation is a long-standing problem in high-enthalpy flow modeling. Current codes use the Park TT_v model and do not account for internal energy redistribution due to dissociation, which results in the QSS distribution discussed above.

- Numerical methods may be suspect at extreme conditions. There are a number of choices that are made in the construction of numerical flux functions, including the numerical scheme itself, the way in which the state is reconstructed at the cell face, how limiting is performed, and how dissipation is added. All of these choices can affect the simulation results.

Under the research program, significant progress has been made in understanding these potential issues.

Metrics for Comparison Between DSMC and CFD

We have made detailed comparisons between DSMC and CFD simulations of Air Force relevant flows. The DSMC was run at continuum conditions where any differences in the computed results must be caused by the governing equations, transport modeling, and/or numerical methods. As discussed in the next subsection, these comparisons can only be valid if there is complete consistency between the physical models used in both DSMC and CFD. This has never been attempted, and all previous comparisons between DSMC and CFD have either used inconsistent models for many aspects of the flow, were performed at rarefied conditions where the Navier-Stokes equations may not be valid, or investigated only certain results such as heat flux and shear stress. Thus, differences between the simulations are observed, but it is not possible to determine the root cause of those differences.

Simulations were designed to systematically stress individual components of the models and numerical methods. We started with simple flows and added physical complexity as we tested and validated components of the models. Large-scale DSMC simulations were performed to provide reference solutions for each test case.

Metrics for comparison of DSMC and CFD simulations used the following criteria:

- Complete consistency of all transport coefficients based on fundamental PES data.
- Each term in the mass diffusion and energy transport equations is verified by comparing to DSMC results.
- Detailed comparisons between the rates of internal energy relaxation and chemical reactions have been made.
- The velocity distribution functions obtained from DSMC and implied by the local state of stress, heat flux, and concentration gradients in the continuum simulations were to be compared; this has not yet been completed.
- The key variables of interest for practical application were compared: pressure and heat flux distributions, mass diffusion fluxes at the surface, and rates of surface catalytic processes and reactions.
- Numerical fluxes computed with DSMC and CFD are compared to validate the numerics.

Of course, under rarefied conditions, the continuum CFD results should and will differ from DSMC. The simulations and detailed comparisons highlight key differences in the modeling approaches. To further validate the simulations, we are currently working with experimentalists to design experiments to test critical aspects of the models and the simulation framework.

Consistency Between DSMC and CFD Flow Models

A major part of the proposed research was to develop transport property models and chemical reaction models that are completely consistent between DSMC and CFD. This work relied on the recently-developed potential energy surfaces for the main air interactions. For DSMC, collision cross sections have been computed for all relevant processes, and for CFD these were averaged appropriately to obtain the corresponding continuum models. Thus, all models were built on common fundamental data.

A key element of this modeling effort was to address the uncertainties associated with the Eucken relation used for the thermal conductivity. As discussed above, this is an ad hoc approach for relating viscosity to thermal conductivity and the internal energy state of the gas. With DSMC, it is possible to design flows that will directly test the validity of the Eucken relation with varying levels of gas complexity. For example, we performed one-dimensional box simulations between walls held at different temperatures for a range of gas mixtures. We then directly tested the results of CFD relative to the exact results obtained with DSMC to validate (or invalidate) the Eucken relation.

Assuring consistency between the DSMC and CFD models is relatively straight-forward for some aspects of the gas modeling. However, the vibrational relaxation and dissociation process is extremely complicated and inherently involves internal energy distributions. DSMC captures the non-Boltzmann vibrational distributions and the suppression of the upper level vibrational population, but CFD cannot because it must assume a form for the vibrational energy distribution. However, progress has been made to represent this effect, as discussed below.

The source term for the vibrational energy equation for a flow of reacting N_2 and N can be written as [24]:

$$\frac{d\epsilon_v}{dt} = \frac{\epsilon_v^* - \epsilon_v}{\tau_v} - k_{N_4}^d \left(\epsilon_v^d - \epsilon_v\right) [N_2] - k_{N_3}^d \left(\epsilon_v^d - \epsilon_v\right) [N]$$

The first term represents the Landau-Teller translational-vibrational energy relaxation corresponding to a time constant, τ_v. The second and third terms correspond to the vibrational energy lost due to dissociation ($\varepsilon_v{}^d$) relative to the mean vibrational energy of the gas (ε_v). Typically, these terms are not included in hypersonic CFD simulations and the assumption is that vibrational energy removed due to dissociation corresponds to the mean vibrational energy of the gas. DMS results can be used to accurately parameterize the terms in this equation for use in CFD simulations. Of course, the dissociation rate, k^d, must be accurately modeled along with its coupling to vibrational energy. We have recently figured out how to use DMS and QCT results to formulate a new dissociation model that is a candidate to replace the Park TT_v model. This model has the form [11, 35-37]:

$$k^d = A\, h\left(T_t, T_v\right)\, T_t^\eta \exp(-\frac{\epsilon_D}{k_B T_t})$$

Here, A is a constant determined from molecular properties and $h(T_t,T_v)$ is a pre-factor that increases or decreases the dissociation rate when the vibrational energy distribution function is overpopulated or depleted. This model is based on DMS results using an ab-initio PES, and can be implemented in DSMC and CFD in a consistent manner.

In summary, we can now ensure that DSMC and CFD simulations use consistent transport models (viscosity, thermal conductivity, and diffusivity). In addition, we now have a means to ensure consistency for the internal energy relaxation model and coupling to chemical reactions. All models can be based on ab-initio PESs. Such research is a significant advance in the field of CFD, DSMC, and hybrid CFD-DSMC.

Support for the BOLT-I Flight Experiment

A major emphasis during the research project concerned the analysis of the AFOSR Boundary Layer Transition (BOLT) flight experiment. Extensive CFD simulations of BOLT were made to provide support to the wind tunnel campaign, direct numerical simulations (DNS) of BOLT at Mach 6 quiet tunnel conditions were performed, and transient thermal analyses were run to provide data to the Applied Physics Laboratory. In order to perform the DNS, a new shock detection switch had to be developed; the standard shock detector produces spurious fluctuations in the flow field and it was not possible to obtain accurate low-disturbance results with that shock wave sensor. This approach enables new “quiet DNS” to be performed of transitional hypersonic flows to support and augment boundary layer stability analyses. Details of this novel approach are provided in [18, 39, 40] and are summarized below.

Key Accomplishments of the Research Program

The primary accomplishments achieved in the research program were:

- A new Modified Marrone-Treanor (MMT) vibration-dissociation coupling model was developed based on the detailed potential energy surfaces developed in the prior MURI project. The MMT model is designed to replace the ad hoc Park TT_v model in CFD codes.
- A new model for the effects of vibrational nonequilibrium and non-Boltzmann vibrational energy distributions was developed for the Direct Simulation Monte Carlo approach; this model captures the same effects as the MMT model, but is designed for DSMC.
- Detailed comparisons between DSMC and CFD at continuum conditions were performed and notable differences were identified; this has led to improvements in the CFD modeling approach for hypersonic flows.
- Based on the DSMC/CFD comparisons, thermal diffusion effects were added to the US3D code to improve near-surface modeling for strongly cooled surfaces. Work continues to quantify the effect of thermal diffusion for realistic flight conditions; however, it is clear that term cannot be neglected for many hypersonic flows.
- Extensive simulations of the BOLT-I flight experiment were carried out, and a new approach for the direct simulation of laminar-turbulent transition was developed. It is now possible to perform detailed simulations of instability growth in complex geometry boundary layers to expose multi-dimensional instability mechanisms and predict transition on realistic flight vehicles.
- The von Karman Institute for Fluid Dynamics MUTATION++ code was coupled to the US3D code; MUTATION++ provides extensive modeling capability for mixtures of reacting gases, including the solution of the Stefan-Maxwell equations for species mass and thermal diffusion.

More details are available in the cited papers. Here we summarize the primary results of the research program.

Modified Marrone-Treanor Model for Air Dissociation

A key development of the research program was the development and implementation of the Modified Marrone and Treanor (MMT) model for air dissociation in the US3D computational fluid dynamics code [6]. The MMT model captures the key physical processes that govern dissociation of oxygen and nitrogen at conditions relevant to hypersonic flight. The model was developed to be consistent with the quasi-classical trajectory analysis performed on the high-quality potential energy surfaces generated by the Truhlar group under a previous AFOSR MURI and subsequent AFOSR funding. The model represents three critical effects, while not being excessively complicated to implement and computationally expensive. The three key effects that must be captured correctly are: (1) vibrational excitation in the presence of molecular and atomic species; (2) dissociation rates across the full range of relevant temperatures, including the effects of vibrational energy nonequilibrium and depletion of the upper vibrational states; and (3) the rate of vibrational energy depletion due to dissociation. Closed-form expressions for each of these quantities have been developed and implemented in US3D. See [11] for complete details of the model development and implementation.

The Modified Marrone-Treanor (MMT) model was recently developed by Chaudhry and Candler [11] using quasi-classical trajectory (QCT) analysis data for N_2+N_2, N_2+N, N_2+O_2, O_2+O_2, and O +O reactions [8-10, 26]. It is based on the Marrone-Treanor preferential dissociation model, modified to account for the effect of rotational energy. The forward reaction rate is defined as a product of a modified Arrhenius form and a nonequilibrium correction factor of the form

$$k_f(T_t, T_v) = k_{\text{arr}}(T_t)\, Z(T_t, T_v)$$

$$k_{\text{arr}} = C T_t^n \exp(-\theta_D / T_t)$$

$$Z(T_t, T_v) = \frac{Q(T_t) Q(T_F)}{Q(T_v) Q(-U)}$$

where Q is the approximate vibrational partition function and T_F and U are pseudo-temperatures of the form

$$Q(T) = \frac{1 - \exp(-\theta_D / T)}{1 - \exp(-\theta_v / T)}$$

$$\frac{1}{T_F} = \frac{1}{T_v} - \frac{1}{T_t} - \frac{1}{U}$$

$$\frac{1}{U} = \frac{a_U}{T_t} + \frac{1}{U^*}$$

The vibrational energy exchange per dissociation is defined as

$$-\frac{\langle \epsilon_{\text{vib}} \rangle_{\text{d}}}{k_B} = \frac{\theta_v}{\exp(\theta_v / T_F)} - \frac{\theta_D}{\exp(\theta_D / T_F)}$$

The parameters C, n, θ_D, θ_v, a_U, and U^* are specified for each dissociation reaction-collision partner pair. We use fitted θ_D values for all reactions except oxygen dissociation with partner N_2. In addition, a non-Boltzmann correction factor can be added, as described in [11].

The MMT model is more complex than the simple Park TT_v model, but it correlates all of the QCT data and provides a self-consistent model that accounts for the suppression of dissociation due to vibrational nonequilibrium and the effect of preferential energy removal due to dissociation that also suppresses the dissociation rate and leads to the quasi-steady state (QSS) distribution discussed above.

The MMT model has been compared to the standard Park TT_v model across a wide range of conditions. In general, it is found that the MMT model produces effective dissociation rates that are about 3 to 4 times slower than the TT_v model. This results in reduced levels of dissociation under most conditions relevant to hypersonic flight.

Figure 4 summarizes one set of results; plotted is the normalized stagnation point heat transfer rate as a function of the free-stream density for a 10 cm sphere at 5 km/sec flight speed. Two boundary conditions are used: a catalytic surface such that any atoms that diffuse to the surface recombine due to gas-surface reactions, and a non-catalytic surface that does not promote (or catalyze) gas-surface reactions. Note that the two models give essentially the same results for a catalytic surface, but there are significant differences for the non-catalytic surface boundary condition. This result is consistent with classic Fay-Riddell theory and is caused by the differences in effective reaction rates between the TT_v and MMT models. At low density, there is very little reaction in the flow field, and there is no catalytic effect. At high density, the shock layer and boundary layer are close to equilibrium, and there is little to no effect of the surface boundary condition. At intermediate densities, there is a competition between these two effects, which produces a partially-reacted shock layer and boundary layer. For the case of the MMT model, the largest reduction in the stagnation point heating occurs at higher densities than TT_v. This is due to the slower dissociation rates that occur in the MMT model.

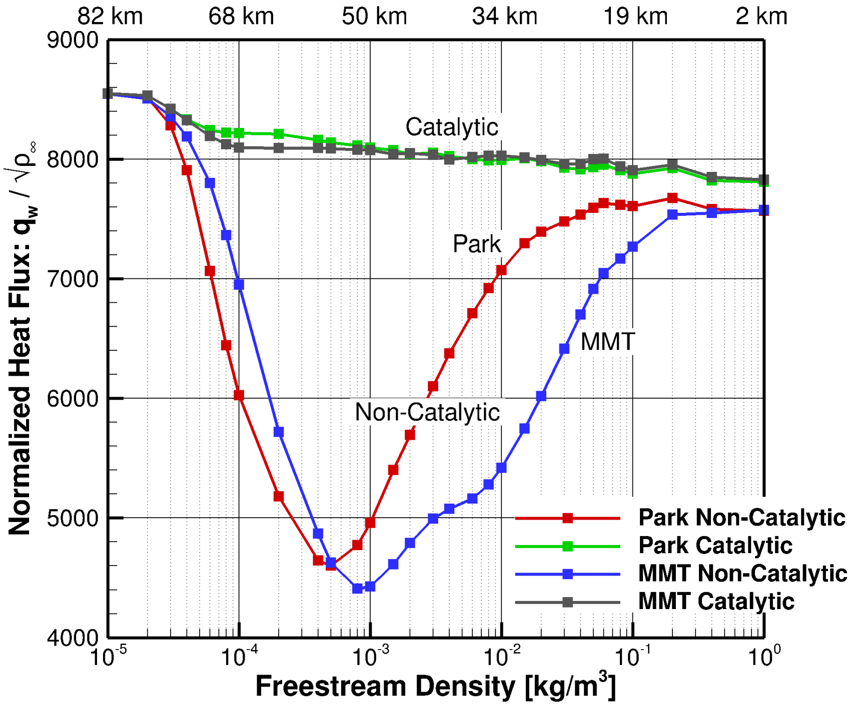


Figure 4. Comparison of Park TT_v and MMT models for the stagnation point heat transfer rate to a 10 cm radius sphere at 5 km/s; surface temperature is held fixed at 1000 K.

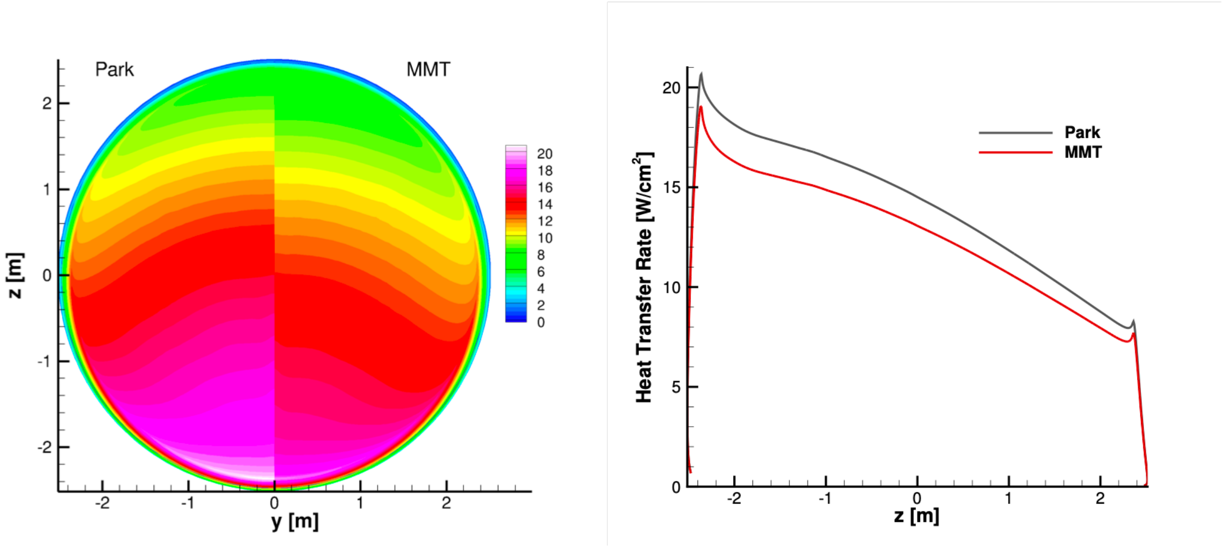


Figure 5. Wall heat flux, comparing MMT to Park TT_v for a blunt-body geometry.

Figure 5 shows that there can be an appreciable difference in heat transfer rate due to the differences in effective chemical reaction rates between the MMT and Park TT_v models. These results were obtained on a reference capsule geometry at typical re-entry conditions.

We are now working to fully validate the MMT model; in addition, we are developing an approach to correctly include the effects of recombination in the model. The model is fundamentally based on quantum computational chemistry results, detailed analysis of reactive collisions, and comparisons with Direct Molecular Simulations (DMS) carried out at the University of Minnesota. Thus, the MMT model is built on basic physics and each term is traceable to fundamental data. All comparisons made to date show that the model is consistent with experimental data and detailed simulations. Thus, objectively *the MMT model should replace the* TT_v *model in all hypersonic aerothermodynamics codes and flow field analysis methods*.

A current AFOSR grant with Caltech and Stanford is seeking to develop validation-quality data to fully evaluate the MMT model at conditions relevant to high-enthalpy hypersonic flight. The forthcoming validation studies will be augmented by a recent uncertainty quantification study with Sandia National Laboratories that rigorously assesses the uncertainty in CUBRC Inc. high-enthalpy shock tunnel measurements on double-cone geometries.

Detailed Comparisons Between CFD and DSMC

Under the research program, we made detailed comparisons between computational fluid dynamics methods that solve the Navier-Stokes equations and Direct Simulations Monte Carlo (DSMC) methods that statistically solve the Boltzmann equation (Knudsen number based on cylinder diameter and free-stream conditions of 10^{-3}). A key innovation and difference in the current work relative to past studies is that the DSMC simulations were run into the continuum regime where the Navier-Stokes equations should be valid. This type of accurate, high-fidelity, continuum or near-continuum DSMC simulations had never previously been performed.

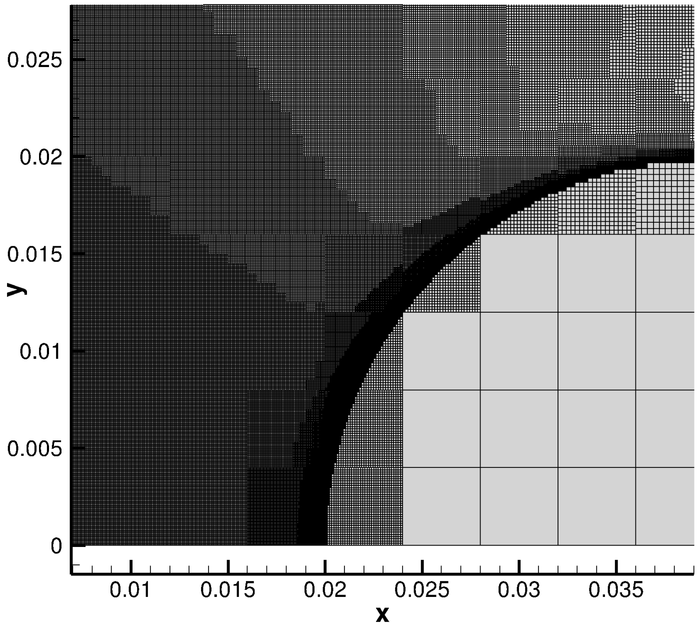


Figure 6. Adaptive mesh refinement in the MGDS DSMC code for a cold-wall hypersonic cylinder simulation showing several levels of grid refinement.

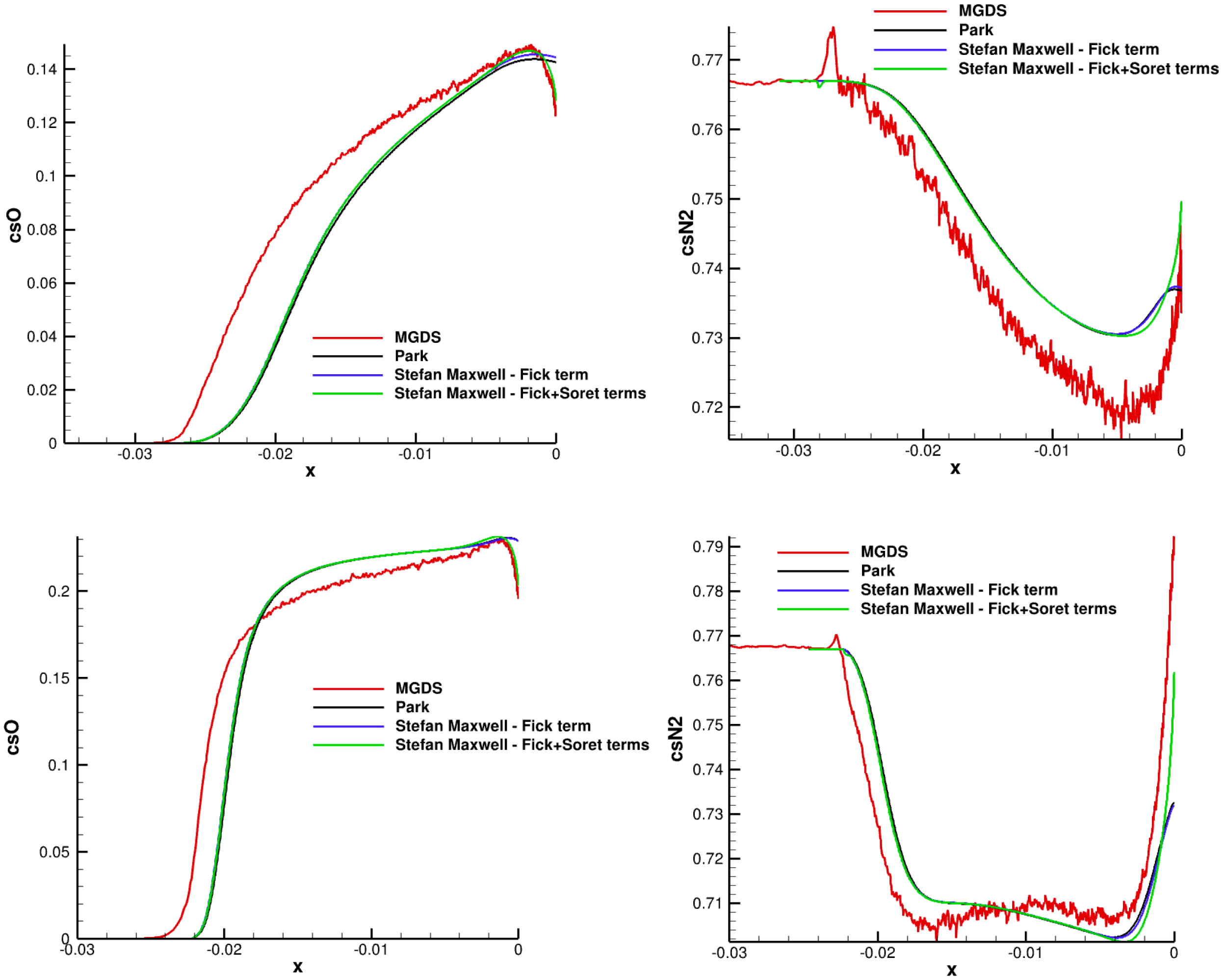


Figure 7. Stagnation streamline variation of oxygen atom mass fraction (left column) and nitrogen molecule mass fraction (right column) at 4 km/s (top) and 5 km/s (bottom). “MGDS” is the reference DSMC simulation, “Park” is the default CFD model with simple Fickian diffusion, “Stefan-Maxwell – Fick term” is a full multicomponent diffusion model, and “Stefan-Maxwell – Fick + Soret terms” includes the effects of thermal diffusion.

This aspect of the research was challenging because DSMC simulations must use grids with sub-mean-free-path resolution and time steps similar to the minimum collision time in the flow field. In order to perform these simulations, efficient adaptive mesh refinement (AMR) is essential. In addition, DSMC data handling, parallelization, and partitioning all must be performed with fully scalable methods. This work proceeded more slowly than expected due to bottlenecks in the DSMC method development. However, after key improvements to the AMR algorithms, it recently became possible to obtain fully-resolved continuum DSMC results. Figure 6 shows an adaptively-refined DSMC grid for a cylinder simulation; the method uses cut cells, so that the cylinder surface and boundary layer are represented by the clustered grid elements in the cylindrical region in the image. Cells within the cylinder are not used in the simulation.

Figure 7 summarizes the key result from the comparison between DSMC and CFD for the cylinder flow at 4 and 5 km/s flight conditions. These plots show the variation in oxygen atom and nitrogen molecule mass fractions along the stagnation streamline for this flow. Here, the surface temperature is fixed at 1000 K and the surface is assumed to be non-catalytic. There are some differences in the amount of chemical reactions in the inviscid shock layer due to differences in how the dissociation is modeled between the DSMC and CFD simulations. We are working to make this aspect of the models fully self-consistent as described above.

The near-surface behavior predicted by the DSMC is very interesting and unexpected. Note the large increase in N_2 mass fraction near the surface, and for the 5 km/s case the surface N_2 mass fraction level exceeds the free-stream value. There is also a deficit of O atoms near the surface in the DSMC. With a non-catalytic surface, the expectation is that the gradient of the mass fractions will be close to zero, since the surface is inert. Furthermore, it is completely unexpected that the N_2 mass fraction could exceed the free-stream. This means that diffusive processes are resulting in heavy diatomic species collecting at the surface, driving out the lighter atomic species.

Interestingly, the simple Fickian diffusion model (mass diffusion proportional to mass fraction gradients) and the full Stefan-Maxwell model do not produce significantly different results (comparison of the black and blue curves). However, including the thermal diffusion terms (the Soret terms, shown in green) makes significant differences in the near-surface part of the boundary layer. Note that that N_2 mass fraction increases significantly and that the O atom mass fraction decreases. It appears that the continuum modeling under-predicts the overall effect relative to DSMC, but *clearly the thermal diffusion terms are important here and cannot be neglected*. This is the first time that we know of that this effect has been seen in the literature.

We are now working to understand what effects thermal diffusion has on heat transfer rates; we do not expect much difference for non-catalytic surfaces, but there could be a significant effect for catalytic and ablative surfaces.

In addition to the cylinder simulations, an extensive study was conducted to compare CFD with DSMC on sharp leading-edge geometries. There has been a recent debate in the literature about the accuracy of the Navier-Stokes equations near the leading edge of sharp double-cone and hollow-cylinder-flare geometries. However, that previous work used the Navier-Stokes equations with a no-slip velocity and isothermal surface boundary condition. Such a boundary condition is fundamentally at odds with the Chapman-Enskog solution of the Boltzmann equation that results in the Navier-Stokes equations. The correct boundary condition that is consistent with this derivation is velocity and temperature slip with appropriate values for the accommodation coefficients.

The comparisons of the Navier-Stokes equations with a slip boundary condition and DSMC show that the continuum formulation is valid to much more rarefied conditions (larger Knudsen number) than if the no-slip surface boundary condition is used. This is not really a surprise, but it refutes a number of recent articles and assertions about the failure of the Navier-Stokes equations near sharp leading edges. These slip boundary conditions are implemented within the US3D CFD code and can be used for simulations on complex hypersonic flight systems.

Development of “Quiet Direct Numerical Simulations” for Transitional Flows

A major component of the research program involved the development of methods for quantifying instability growth in complex hypersonic flows. This work was motivated by the need to understand how the AFOSR BOLT-I flight experiment flow field amplifies instabilities that lead to boundary layer transition. Numerous papers have been published on this topic, and the reader is referred to additional details in the publications listed below.

The BOLT-I flow field is complicated due to the shape of the unswept nose and the highly-swept leading edge; in addition, the concave surface results in strong near-surface flow toward the centerline which lifts the boundary layer and promotes formation of large streamwise vortices. Figure 8 plots the predicted and measured heat transfer rate on BOLT-I at typical Mach 6 quiet wind tunnel conditions. Note the presence of streamwise heat transfer streaks due to the distortion of the boundary layer by shock curvature effects in the nose region. The comparison with the Texas A&M infrared imagery is excellent, with all features predicted by the CFD present in the experimental data. More quantitative comparisons show remarkable agreement between CFD and experiment. Note that the CFD simulations were obtained before the experimental measurements were made!

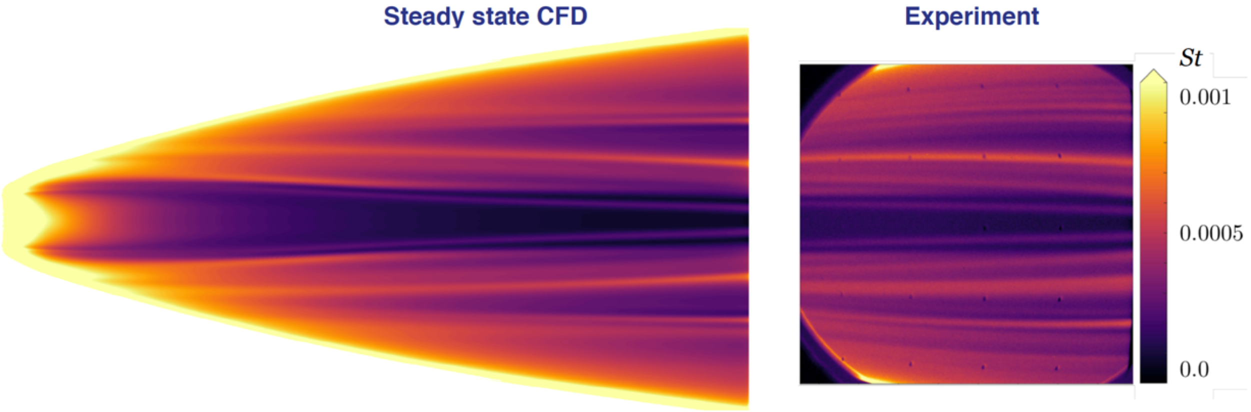


Figure 8. Comparison of heat transfer rate to BOLT-I at Mach 6 quiet tunnel conditions ($Re_L = 3.0 \times 10^6$); computed with a 4th-order accurate numerical method on a 160 million element grid (left) and infrared imagery obtained at Texas A&M University (right) [19].

In order to compute this flow, a number of improvements to standard numerical methods had to be developed and implemented in the US3D code. In addition, great care was required in the grid generation process to produce grids that correctly resolve the flow features and are aligned with the complex bow shock wave. The improvements to the numerical methods that were carried out over the past year include the following.

Development of a “quiet” shock sensor. The high-fidelity simulations use 4th-order and 6th-order low-dissipation numerical methods to obtain accurate solutions, typically requiring a factor of 10 fewer grid elements than conventional 2nd-order upwind methods. In order to control numerical error in the bow shock wave, dissipation must be added in a narrow region near the shock. We found that standard sensors used to detect where dissipation is needed (e.g. the Ducros sensor) typically add excess dissipation and also flicker on and off, resulting in numerical noise added to the simulation. This noise can activate instabilities in the flow, resulting in artificial transition to turbulence. Furthermore, the numerical noise interferes with the growth of the key boundary layer disturbances that lead to transition in the physical flow field. A new approach was developed to target the dissipation to a narrow region in the vicinity of the shock wave, and this dissipation is invariant in time to eliminate the flickering problem. It has been shown that it is possible to obtain machine-zero converged solutions on very large grids for BOLT-I. These simulations resolve all length scales of the flow field.

As part of this development, the high-order numerical methods were improved to make their formulation fully consistent with the thermodynamics. It was found that subtle changes in how the numerical fluxes are evaluated can affect the overall accuracy of the methods. Extensive testing was performed to optimize the accuracy and stability of the high-order, low-dissipation fluxes.

Related to the numerical flux development, the time-accuracy of the US3D code was rigorously assessed and it was found that it does not achieve 2nd-order (or higher) accuracy even though the numerical methods are formally of that accuracy. Extensions and improvements to the US3D implicit time integration have been made and validated. It is found that significantly improved time-varying results are obtained with the newly-developed 2nd-order accurate implicit time integration method. Even though this method is approximately two or three times more expensive per time step, it is possible to take significantly larger time steps, resulting in more accurate results with reduced computational time.

Finally, techniques were developed to produce high-accuracy grids with controlled alignment of the grid with the bow shock. This is essential to producing high-quality simulations because lack of grid alignment injects error into the flow field, contaminating the solution and overwhelming the growth of physical instabilities. This approach is particularly important for the BOLT-I geometry due to the complex curvature of the bow shock in the nose region. Poor shock alignment of the grid results in numerical error at the shock, which can corrupt the flow field. The grid generation process is still tedious and very time-consuming – this remains a significant issue where research investment could pay huge dividends.

The combination of these methods enables highly accurate flow field simulations on complex geometry hypersonic flight configurations. All length scales are resolved, and with sufficient grid resolution and accurate time integration, instabilities can be accurately computed in these flows. As demonstrated below, this allows multi-dimensional modal disturbances to be identified, and modal interactions can be quantified. This is a direct simulation of boundary layer instability growth, an approach we are calling "Quiet DNS," where the numerical flow field is quiet in the same sense as a low-disturbance quiet wind tunnel. *Quiet DNS has the potential to predict complex boundary layer transition mechanisms on realistic hypersonic flight vehicles.*

Analysis of Instability Growth in the BOLT-I Flow Field

The high-fidelity flow fields produced with the Quiet DNS approach can be used to study instability growth in complex flow fields such as BOLT. The approach is straight-forward: low levels of noise are added to the flow field and the simulation is integrated in time to allow the boundary layer to amplify the instabilities that are inherent to the flow state (see Fig. 9). Then, snapshots in time are extracted from the flow and a modal decomposition is performed to identify the key instability modes in the flow field. The process for this dynamic mode decomposition is given in Ref. [18].

Figure 9 shows a visualization of the instabilities predicted to be present in the BOLT-I flow field; here streamwise velocity perturbations (positive and negative) are used to visualize the primary instability modes. We have identified four main instabilities as denoted in the figure. Additional analysis quantifies the dominant frequencies of each mode and their growth rates may be computed directly from the simulation. Comparisons with experimental data show very good agreement with the location and frequency of the dominant instability modes.

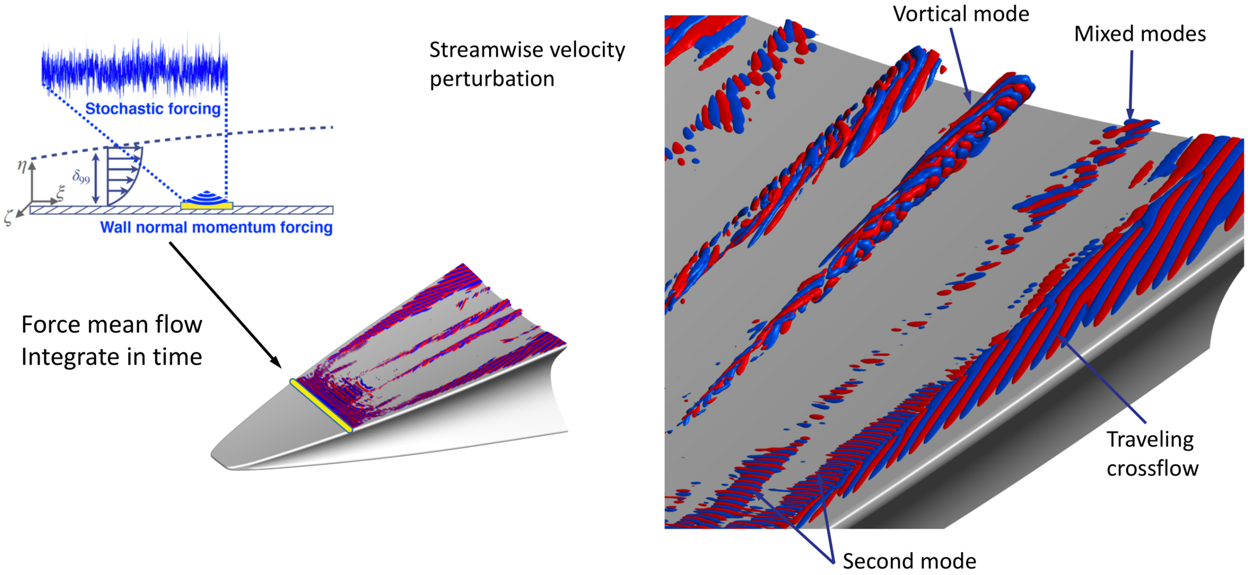


Figure 9. Forced DNS approach used to study the instabilities in the BOLT-I boundary layer (left) and isosurfaces of streamwise velocity perturbations to visualize growth of boundary layer instabilities in the BOLT flow field (right).

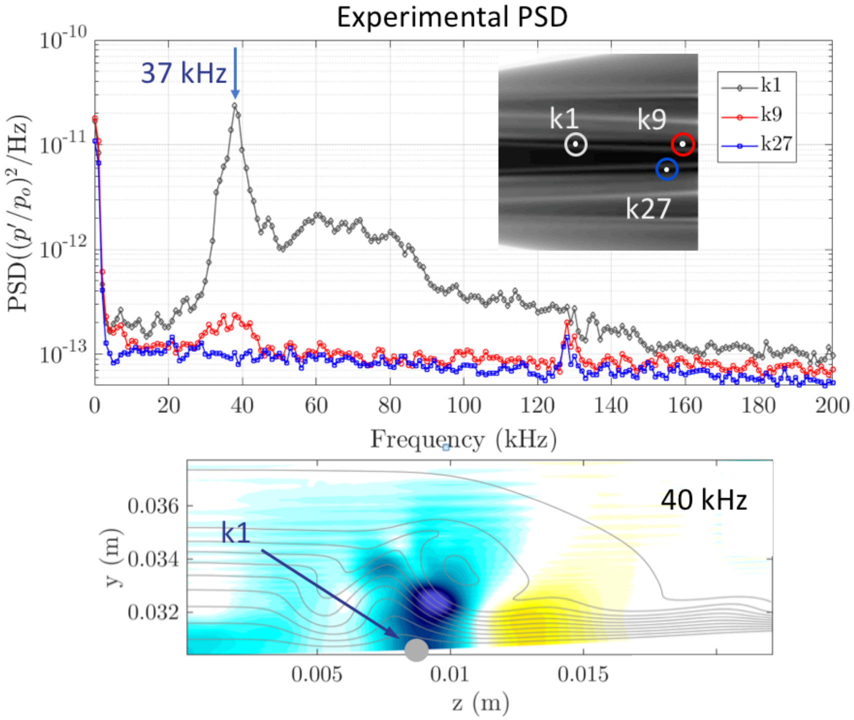


Figure 10. Power spectral density of the experimental surface pressure fluctuations at 3 sensor locations (top), and the Quiet DNS predicted 40 kHz pressure disturbance field near the k1 sensor (bottom).

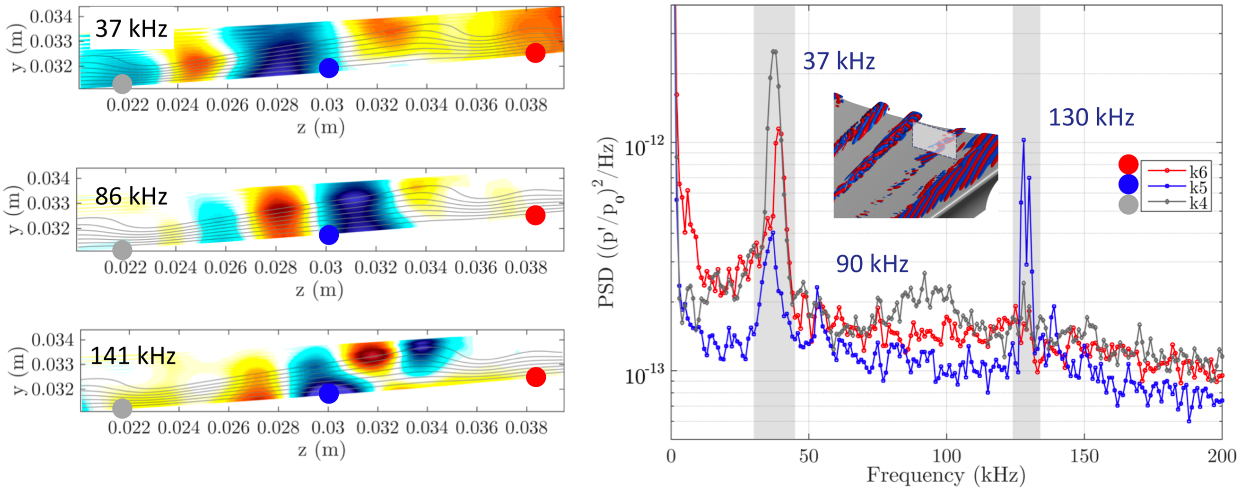
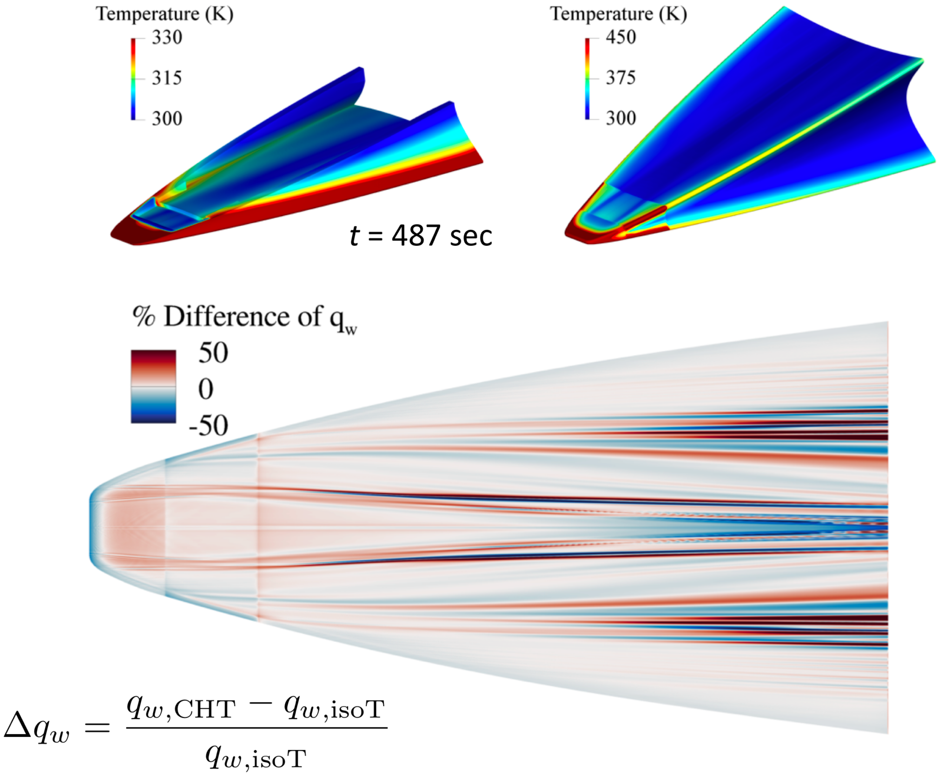


Figure 11. Sparsity-promoting dynamic mode decomposition analysis of the BOLT-I mixed mode instability: three dominant modes and location of kulite sensors (left) and experimental PSD for the three sensors (right).

For example, Figure 10 plots the power spectral density (PSD) of pressure fluctuations measured by three sensors in the Purdue Mach 6 Quiet Wind Tunnel and the primary pressure fluctuation mode identified from the present simulations. Note that the pressure sensor, k1, is located immediately underneath the maximum in the pressure mode, and that the frequency is close to the peak in the experimental PSD. This disturbance is due to the vortical mode illustrated in Figure 9. Figure 11 shows a similar analysis of the mixed mode; here there are three dominant energy-containing modes (pressure mode plotted on the left). The experimental PSD shows consistency with the predicted frequencies and localization of the pressure disturbances.

The advanced simulation methods are now being applied to BOLT-I to predict how the boundary layer will transition to turbulence at flight conditions. We are using a fully-coupled fluid / thermal response solution approach to predict the flight surface temperature and then use that as a boundary condition for the QDNS analysis. Figure 12 summarizes some of these results, showing the predicted surface and internal temperatures and the differences in heat transfer rate to the surface between the initially assumed isothermal condition and the predicted wall temperature distribution from the coupled fluid/thermal analysis.



$$\Delta q_w = \frac{q_{w,\mathrm{CHT}} - q_{w,\mathrm{isoT}}}{q_{w,\mathrm{isoT}}}$$

Figure 12. Predictions of BOLT-I temperature distribution at the nominal trajectory time of 487 sec (top) and the difference in surface heat transfer rate between an assume isothermal wall (T = 300 K) and the predicted flight surface temperature.

The Quiet DNS approach has great potential for identifying key boundary layer instabilities for realistic complex hypersonic flight configurations. The approach will have particular utility when used in conjunction with conventional multi-dimensional instability methods (e.g. bi-global methods) and emerging linear system theory approaches (such as input/output methods). We are continuing to develop this approach and make more detailed comparisons with theory and experimental data. The use of implicit methods that are higher-order in time is also critical, and this is being extensively studied and documented. We are currently working with the Applied Physics Laboratory transition the QDNS approach so that they can apply it to practical flows.

Summary of Key Findings

The research program produced the following tangible results and over-arching conclusions:

- The MMT model should replace the TT_v model in all hypersonic aerothermodynamics codes and flow field analysis methods. Further validation is required, but to date all indications are that it is significantly more accurate than prior models.
- The comparisons of the Navier-Stokes equations with a slip boundary condition and DSMC show that the continuum formulation is significantly rarefied conditions (larger Knudsen number) than if the no-slip surface boundary condition is used.
- Thermal diffusion terms may be significant in high-enthalpy flows with strong heat transfer.
- The Quiet DNS approach has great potential for identifying key boundary layer instabilities for realistic complex hypersonic flight configurations. QDNS has exposed a number of instability mechanisms in the BOLT flow field.

Publications Resulting from the Research Program

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