Measurements for Validating DSMC and Navier Stokes Computations of Chemically Reacting Hypervelocity Flows

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Abstract. This paper gives details of a series of experiments that are being performed in the shock tunnels at the CUBRC Aerothermal and Aero-Optics Evaluation Center, Buffalo to derive validation data for high enthalpy rarefied flows that involve chemical reactions and real gas effects. The test series has been extended to include a range of leading edge and nosetip flows that are simpler to compute than the examples used in a previous phase of this study which involved shock/ boundary layer interaction. The importance of precise flow characterization is emphasized and a new laser spectroscopic absorption technique to measure species concentration and the free stream velocity and temperature is described. The complete results for this study will be published in the CUBDAT database.

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INTRODUCTION

Significant real gas and chemical reactions effects occur within the flow for many practical hypervelocity aerospace applications. Furthermore for many of these flows shock/shock and shock/boundary layer interactions play an important role, frequently resulting in intense localized heating of the vehicle's surface. Chemistry and flow complexity have persistently challenged the use of CFD and are well recognized as areas of uncertainties when employing Navier Stokes (N-S) methods for the denser flows. Although enormous strides have been made in developing particle simulation methods for rarefied flows, questions still remain about the accuracy of the solutions in high-enthalpy situations and there are aspects of the modeling of the molecular interactions where chemical reactions occur within the gas and on surfaces that remain to be substantiated.

In an attempt to address these problems, an extensive code validation activity has been conducted over the past decade in a combined American/European exercise that has sought to identify where the problems are and assesses the relative merits of different code strategies. Although only part way through, this program has already been successful in stimulating the development of CFD methods and in particular it has led to marked improvements in the accurate of DSMC solutions. A key element of this program was promoted by the NATO Research Technology Organization (RTO) under the auspices of its Working Group 10[1]. Of particular relevance is a group of experimental and numerical studies that have been conducted to examine the viscous/inviscid interaction regions developed over two closely related model configurations – a hollow cylinder flare and a double cone – under laminar hypersonic flow conditions. These provide well-posed and stringent tests for the numerical schemes and many groups collaborated in the exercise, producing high quality experimental and computational results. The test conditions for these flows spanned the rarefied and laminar continuum-flow regimes, providing a valuable overlap between the DSMC and N-S methodologies. The flow densities for the rarefied test cases bordered on the extreme for practical DSMC solutions. This proved to be a severe challenge and initially unsatisfactory results were obtained. However it stimulated significant improvements to be made to the core DSMC algorithms and in the numerical procedures used. The outcome was a series of computations from several sources that has demonstrated an ability to predict these complex flows which include shock/shock and shock/boundary layer interactions with remarkable precision[2]. The accuracy was comparable to that achieved using the Navier Stokes method for the denser flows. It should also be noted that these low density flows posed a significant challenge to the experimentalists and it is to their credit that they have been able to provide suitable data for the validation of the computed results.

All of these earlier studies were conducted with nitrogen as the test gas which avoided the complexities of chemical reactions within the flow. However, for the flows that occur during hypervelocity earth or other planetary re-entry, real gas and chemical reaction effects play a very significant role in the formation of the bow shock layer and in the regions of shock/shock interaction and separated flows associated with shock/boundary layer interaction. Since the last of these frequently leads to intense localized heating of the body, the prediction of the aerothermal loads on the vehicle is very dependent on modeling the real gas phenomena correctly.

Figure 1 shows fresh measurements that have been obtained for the sharp biconic body illustrating the effect of changing from nitrogen to air as the test gas. This test was conducted at the high enthalpy of 9 MJ/Kg. It can be seen that the differences in the flows, which are principally attributable to the chemical activity within the air, have resulted in a delay in the point of separation (indicated by the sharp fall in heat transfer on the forecone). The separation region is thus reduced in size but in the measured data similar profiles of heat transfer and pressure occur at and after reattachment on the aft cone. This is not echoed by the Navier Stokes predictions even though this was obtained using an advanced code and is indicative of significant unresolved problems in modeling the air thermo-chemistry.

To predict flows of this type using DSMC it is necessary to incorporate realistic yet computationally efficient models for the intermolecular and gas/surface interactions which replicate the reactions and internal energy exchange process that take place. Reaction probabilities are in most instances strongly coupled to the degree of vibrational excitation and thus the two phenomena are inexorably linked. To be usable in DSMC codes the collision models have to be, in some measure, approximated and thus the accuracy to which they perform in real flows has to be evaluated. The development of appropriate gas/surface collision models involving reactions and internal energy exchange has, to date, lagged behind what is available for gas phase interactions. So far there has been little opportunity to critically evaluate the performance of available models with carefully designed and executed experiments. For this reason the validation program described above is being extended to include chemical reaction and real gas effects.

EXPERIMENTAL PROGRAM

A new phase of the code validation study is being conducted in the CUBRC Aerothermal and Aero-Optics Evaluation Center Lens I and 48-inch shock tunnels. These experiments extend the range into the area where rarefied chemistry and real gas effects play significant roles. The study is being conducted using air and CO_2 for Mach numbers of 10 to 12 and with stagnation enthalpies ranging from 2 to 13 MJ/Kg. The tests are being undertaken in conjunction with computations in a code validation exercise and, as before, will provide data that spans the low-Kn rarefied and continuum regimes to provide an overlap between DSMC and N-S. New data have been obtained for the flow over the hollow cylinder/flare and double cone configurations used previously, but, in addition, studies of the region ahead of a sphere and a cylinder perpendicular to the flow, a flat-ended circular cylinder and a blunted 70° cone have been added. These latter bodies produce simpler flows without the shock interactions that occur on the first two configurations and are seen to be more suitable examples for the first phases of a collision model evaluation. Full data for these geometries will be published as part of CUBDAT specifically for DSMC code validation purposes.

A factor that is often glossed over in validation studies is that the precision of the experimental results can be no better than the accuracy to which the undisturbed test flow properties can be specified. For CFD a uniform approach flow is usually assumed but in wind tunnels some level of flow non-uniformity and uncertainty will exist. The complete characteristics of the test flow are rarely quoted, as there is always pressure to hide from public view any levels of imperfection. Characterizing the test flow precisely is an important issue that has been strenuously addressed in the present study. The test flow in wind tunnels operating in the high-enthalpy, high-Mach number range is produce by expanding it from a reservoir where high temperatures, in the present case, up to about 8,000K, exist. For air or CO_2 dissociation will take place and the internal energy states will be highly excited. For the former gas, significant mole fractions of NO are produced and the subsequent rapid expansion of the flow though the nozzle does not usually give sufficient time for the gas to regain equilibrium. Thus NO persists in the flow approaching the model which may influence the chemistry within its flow.

Deriving validation quality experimental data is always a difficult task; obtaining them on the hypervelocity low-density range is especially challenging. For high enthalpy flows, much reliance is placed on comparing computed data with measurements of surface static pressure and heat transfer. For blunt bodies and leading edges insight has also been gained by comparing computed bow shock profiles with those measured using Schlieren or shadowgraph photography, as these profiles are quite sensitive to the chemical activity in the flow. However all of these measurements give only very indirect evidence of the way that the reactions take place and for more fundamental comparisons it is desirable to have species concentration data from within the flow. As in integral part of our studies of real gas chemistry, we have sought to identify measuring techniques to determine the properties of non-equilibrium flows and the development of non-intrusive methods to do this has been seen as a high priority. We have ascertained that the most accurate method currently available, especially for short duration facilities, is to measure the concentrations of NO and O_2 using high-resolution tunable laser diode absorption spectrometry. This has become practical with the advent of continuous wave Quantum Cascade Laser (QCL) sources. Measurements have already been made in the CUBRC Lens I and 48-inch shock tube tunnel facilities to obtain concentrations of NO and O_2 for airflows with total enthalpies of 2, 3, 5 and 10 KJ/kg. The studies are reported more fully in reference[3].

The solid-state laser (Alpes Lasers) provides a continuous beam of 5.44 micron light that can be modulated very rapidly and precisely over about 10nm wavelength range by adjusting the applied current. The wavelength can also be varied from 5438nm to 5468nm by changing the instrument's temperature from -30 to 15°C. The distributed feedback QCL has an emission width which is one or two orders of magnitude narrower than the NO line widths and thus highly resolved absorption line profiles can be obtained by passing the light through selected parts of the flow. In the experiment the laser current was modulated using a 1 KHz ramp function and the transmitted light intensity detected by a 20 ns response-time LN_2-cooled InSb detector. Figure 2 shows a typical absorption spectrum for the $^{14}N^{16}O$ transition near 1835.56 cm^{-1} compared with a theoretical profile calculated using the HITRAN 2000[4] database with knowledge of the pressure of the test flow obtained from probe instrumentation. The temperature indicated by the fitted theoretical profile is 290K. Run 266 is a high enthalpy test case for which the reservoir temperature is about 6000K and the NO mole fraction in the free stream, predicted from the continuum full chemistry CFD, is about 5.8% whereas the measured value is 3.4% (see fig 3). Steady run conditions are established after about 12 msec. Evidently some degree of unexplained recombination has occurred in the nozzle.

Absorption by other NO isotopic transitions [Rl.5 ($^{14}N^{18}0$, 0.1993% isotopic abundance) and P2.5 ($^{15}N^{16}0$, 0.3654% isotopic abundance)] were observed. Because these transitions are based on a different lower state energy than our fundamental transition at 1835.56 cm^{-1}, the ratio of the integrated absorption feature compared to the integral of the fundamental absorption feature provided a reasonably sensitive measurement of the rotational temperature of the nitric oxide in the freestream. Calculations show that the rotational temperature of the gas for this run is about 190K whereas the expected value of the freestream temperature from the CFD using published reaction and internal energy relaxation rates (Park[5]) was 229K. The rotational temperature of the NO is likely to be in near equilibrium with the air in this test flow. Doppler measurements of flow velocity have also been obtained by using two inclined laser beams which pass obliquely through the free stream flow. From the shift in apparent wavelength between the two signals, see figure 4, a value for the flow velocity of 3634 m/s compared with the predicted value of 3551 m/s has been measured for run 266. This is only 2.36% higher than expected.

Although the use of the QCL spectroscopic technique has only recently begun, it is recognized that it is a valuable tool for acquiring more direct data for assessment of CFD computations for reacting flows. It permits fuller and more precise flow characterization to be made and in particular enables the levels of NO in the incident flow to be determined if the test gas is air. The technique will be applied to probing the composition of the flow within the shock layers of various bodies and the results will be published in the CUBRC database. The use of the method will be expanded to include the measurement of the nonequilibrium characteristics of CO_2 flows over a similar range of enthalpies. The direct measurement of species properties within these flows will provide direct and useful evidence for code validation. Historically shock profile and pressure and heat transfer surface flux data have been the principal sources of information for this purpose for hypervelocity flows. Well-tested techniques have been employed for many years to measure these fluxes; nevertheless care has to be excised if the flows are rarefied and chemically active. As the present experiments have concentrated on the high density end of the rarefied regime (Kn of the order of 0.002) correction for low density effects to the pressure readings has not been necessary except when surfaces are inclined at very small angle to the approaching flow as in the case of the hollow cylinder. Heat transfer measurements however are susceptible to error due to catalytic effects. In the present program a variety of gauges has been used to assess any differences due to changes in sensor composition. Coaxial chromel-constantan thermocouple gauges with chromium coatings thermocouples, exposed silver calorimeter gauges and platinum-on-Pyrex thin-film gauges with and without inert coating have been compared. The thin film gauges are the most precise whereas the coaxial gauges are the most robust. Consistency between the results from all gauges has been obtained for the cylinder, as can be observed from figure 5, and for the blunted 70° cone. All of the models tested were metallic and comparison of data with computations suggests that the surfaces act as fully catalytic and fully accommodated.

FLOW EXAMPLES

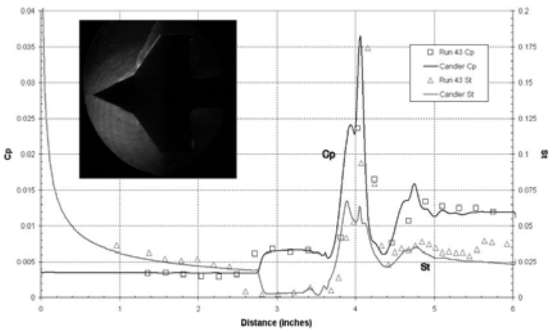
Studies in air were conducted at 5 MJ/kg and 10 MJ/kg with a cylindrical model with its axis normal to the flow. This is equipped with pressure and heat transfer instrumentation and high speed Schlieren was used to visualize the characteristics of the shock layer. Figure 6 shows the bow shock region ahead of a cylinder for total enthalpy levels of 10 MJ/kg; the contours indicate the results of a Navier Stokes computation. The Knudsen number based on cylinder diameter was 0.0011 but tests at lower densities are planned. In figures 5 we showed comparisons between N-S predictions and measurements of heating levels for a non- and fully-catalytic surface-reaction boundary condition and, in figure 7, the pressure around the cylinder is illustrated. It was evident from this test that while the pressure is accurately forecast for both enthalpy levels, at the higher level the heating rates to the model surface is not precisely predicted. This suggests that there remain problems within the N-S formulation in describing the flow and surface chemistry for high enthalpy airflows; it will be interesting to see if DSMC can resolve these difficulties.

Tests have also been conducted in carbon dioxide for all of the geometries. The results for the shock profile show very good agreement between the measured and predicted shock shapes at the low enthalpies (2 MJ/kg) where limited chemical activity takes place. However, at the higher enthalpy conditions (3, 5 and 10 MJ/kg), a discrepancy between measured and predicted shock shapes is seen. A major objective of the CO_2 studies is to obtain the levels of heating and assess the enhancement to this attributable to the catalytic activity at the wall. Tests on the blunted 70° cone have include an evaluation of the effect of using three different types of heat transfer instrumentation to investigate the relative effects of stainless steel, platinum and silver on catalytic heating of the gauges themselves.

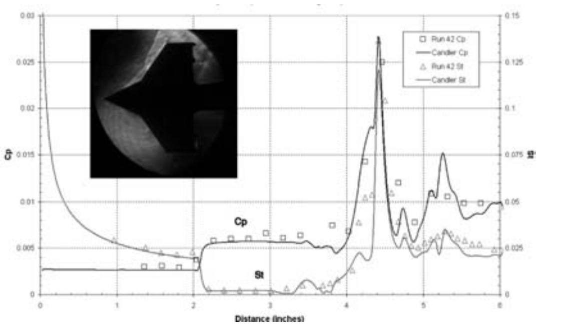
During the Lens 1 shock tunnel calibration for the studies of low-density flow, heat transfer measurements were made on two hemispherical nosetips over a range of freestream velocity and density conditions to obtain flowfields which spanned the continuum to the fully merged rarefied flow regime. Reynolds numbers down to 1000 were possible. We employed platinum thin-film gages, either uncoated or coated with a silicon dioxide, to provide catalytic and non-catalytic surfaces. Tests were also conducted to measure the heat transfer along the stagnation line of a small circular cylinder. The diameter of this was 4.3 mm and these provide information for Reynolds numbers (based on the cylinder diameter) down to a value of 100 (Kn = 0.019). Stagnation point heat transfer measurements for this body are shown in figure 8 and it be seen that these agreed closely with the simple Fay Riddell prediction technique for Reynolds numbers as low as 1000. However when this drops close to 100, there is a 20% decrease in the heating level relative to this prediction. The consistency between the measurements with the coated and uncoated instrumentation suggests that for these test conditions (i.e. < 3 MJ/Kg) surface catalysis does not have a significant influence on the stagnation heating value.

SUMMARY

A new series of tests specifically aimed at providing code validation data are being undertaken in the CUBRC Aerothermal and Aero-Optics Evaluation Center Lens I and 48-inch shock tunnels. These tests are aimed at extending the previous series which concentrated on the flows over a hollow cylinder/flare and biconic bodies to include simpler shapes to reduce the computational complexity. The range of test conditions has been chosen to include chemical reactions and enhanced real gas effects within the flow and will provide data for evaluation of collision models used within DSMC. A new non-intrusive solid-state laser spectroscopic technique has been developed which has been shown to give very good measurements of flow velocity, rotational temperature and NO concentration in the free stream. It will be used to investigate the flow in the shock layer around the blunt bodies. Data for these bodies will be published in CUBDAT but before the data is published it is proposed that another series of blind CFD tests be conducted in which only the body shapes and incident flow conditions will initially be made available.



(air)



(nitrogen)

FIGURE 1. Measurements of pressure and heat transfer on the biconic body showing the difference between air and nitrogen flow at 9 MJ/Kg.

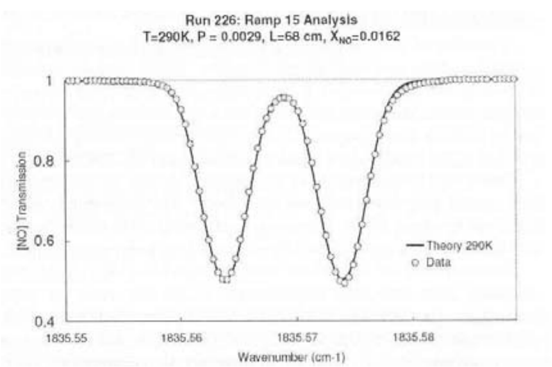


FIGURE 2. Measured and calculated (Voigt shape) NO absorption profile for run 266. This fit for the experimental data yields T =290K.

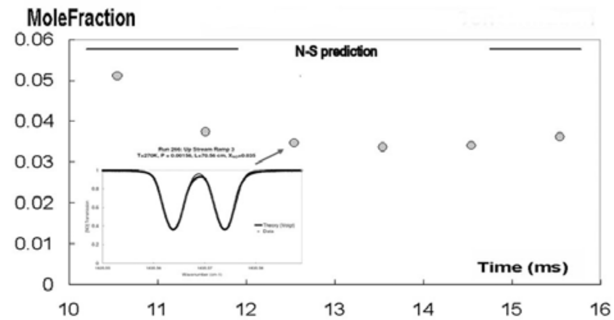


FIGURE 3. Mole fraction of NO in the free stream for run 266.

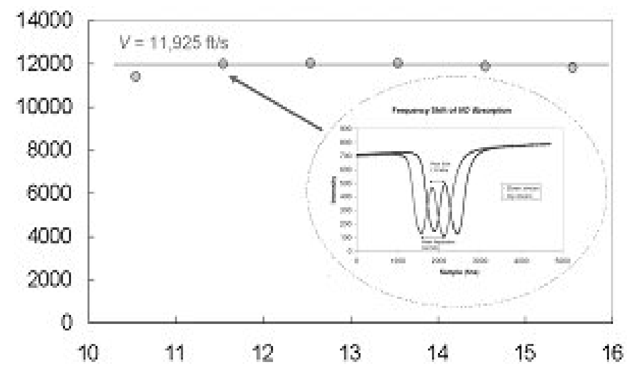


FIGURE 4. Doppler QCL measurements of the free stream velocity also for run 266. (Predicted value is 11650 f/s).

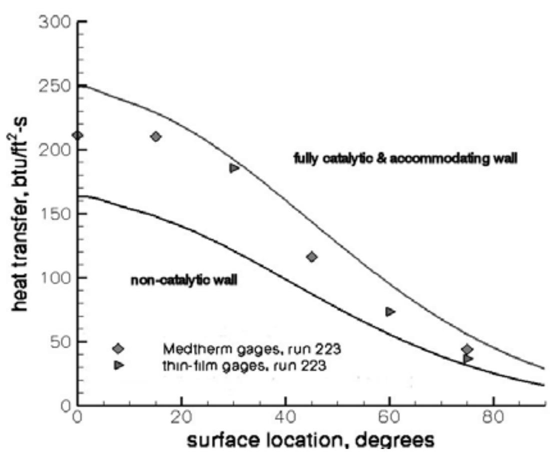


FIGURE 5. Heat transfer for a cylinder at 10 MJ/Kg. Diamonds: Medtherm thermocouple gauges; triangles: thin film platinum gauges. Kn(D)=0.0011.

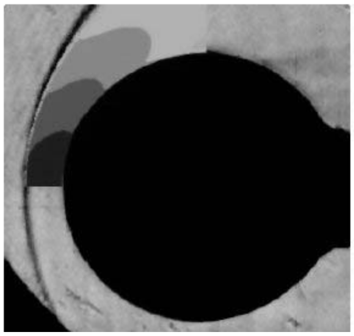


FIGURE 6. Comparison between measured and computed (N-S) shock stand-off distance for circular cylinder at 10 MJ/Kg.

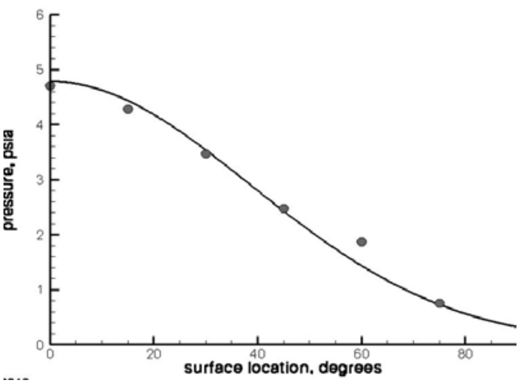


FIGURE 7. Pressure distribution on the cylinder at 10 MJ/Kg corresponding to figure 5.

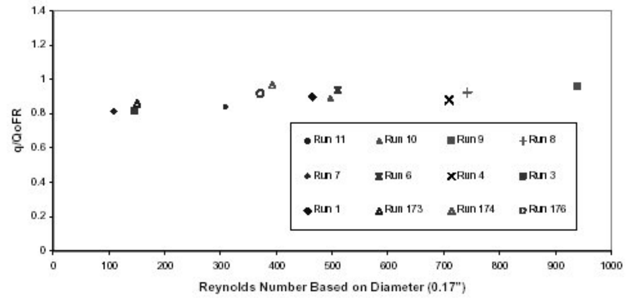


FIGURE 8. Stagnation point heat transfer on a circular cylinder compared with Fay and Riddel.

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