Influence of Molecular Vibrational Energy Accommodation Modeling on Cone Surface Heat FLUX at Mach 10

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Abstract: In order to assess the influence of high vibrational temperatures typically found in shock-tunnel-generated flows on model surface heat flux, measurements are compared to simulations using the DSMC (direct simulation Monte Carlo) method. The two limiting cases of either full accommodation of molecular vibrational energy to the surface temperature or none at all are simulated for three shock tunnel conditions using Nitrogen (N_2) as a test gas. The conditions mainly differ by an order of magnitude in density, however, all three comparisons to the corresponding measurements suggest that vibrational surface relaxation happens only to a small extent. While model surface pressure is not affected, heat fluxes differ by up to 20%, depending on the modelling. Furthermore, lower flow densities generally lead to higher differences.

Key words: Shock tunnel, hypersonic, DSMC, heat flux measurement, thermal non-equilibrium.

1. Introduction

Hypersonic shock tunnels are useful and practical facilities to replicate flow conditions similar to those experienced by planetary entry vehicles in the upper atmosphere, hence providing the possibility to determine surface heating rates with an effort much lower than that of an atmospheric free-flight experiment. These tunnels usually operate in reflected-shock mode, where the hypersonic flow is created by a fast expansion of shock-heated and compressed gas through a Laval nozzle. Particularly for hypersonic low density flow conditions, this leads to nonequilibrium temperature effects during the flow nozzle expansion. For diatomic test gases, such as air or nitrogen, this so-called “vibrational freezing” results in lower nozzle exit velocities and also highly elevated vibrational temperatures in the freestream compared to

the translational and rotational temperature component, as also demonstrated by Nompelis et al. [1] and Ruffin [2]. The extra energy stored in the vibrational mode results in a flow condition different to an atmospheric flight test, and could lead to increased surface heat flux in case the molecules transfer vibrational energy during surface collisions. The issue has been addressed several times, however with vastly different assumptions and conclusions for the vibrational energy accommodation at the wall, ranging from nearly full accommodation [3] to hardly any, i.e. a vibrationally inert or non-catalytic surface [4].

While for air or Nitrogen, the relaxation rate in the nozzle, in the freestream and in the shock layer can be reliably calculated using the Landau-Teller model [5], the rate of energy transfer to the model surface depends on a large number of additional factors, such as surface material, surface temperature, surface roughness and also surface history, hence measured data for a particular gas-surface material pairing is scarce. Black et al. [6],

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for example, measured deactivation (or vibrational accommodation) coefficients (α_v) of N_2 excited to its first vibrational state ($v' = 1$) during collisions with various surface materials at approximately room temperature, all values for α_v ranging between 0.03 and 0.26%. Later on Parish and Janey [7] used more advanced CARS methods to determine N_2 deactivation also from higher vibrationally excited states up to five, showing that the probability increases with v' . While coefficients of all other tested materials remained below 1%, a particular chrome-nickel steel (SS 312) showed nearly complete deactivation from $v' = 4$. Assuming an equilibrium distribution of the vibrational states of N_2 , it is possible to calculate deactivation probabilities dependent on the vibrational temperature. This is done by multiplying the individual state population, calculated assuming a Boltzmann distribution, with the deactivation probability of the individual state, adopted from Parish and Janey [7]. The result for three selected materials is shown in Fig. 1. This calculation, of course, assumes fast repopulation of the fast-depleting higher vibrational states, an assumption which will probably not be satisfied in low-density, low-temperature hypersonic shock tunnel flows. Hence in reality, overall vibrational surface accommodation coefficients might be even lower, as the deactivation channels through highly excited states are blocked due to their slow repopulation. However, even assuming the scenario leading to highest α_v (i.e. SS 123 and an equilibrium distribution of v'), α_v remains below 3% for N_2 vibrational temperatures up to 3,000 K.

Nompelis et al. [1] showed that vibrational freezing in the nozzle flow leads to lower freestream velocities compared to equilibrium nozzle flows, which in turn leads to slightly lower heat fluxes and higher pitot pressures. Their comparison of Navier-Stokes-based CFD simulations with heat flux measurements on a biconcic model was in best agreement when assuming vibrationally adiabatic surface ($\alpha_v = 0$), although slip boundary conditions had to be used as a consequence of the low density flow condition.

Fig. 1 Vibrational deactivation rates for N_2 .

To also assess the influence of α_v on surface heat flux induced by a hypersonic shock tunnel flow around a double-cone, Moss and Bird [3] compared DSMC (direct simulation Monte Carlo) simulations with both full vibrational surface accommodation ($\alpha_v = 1$) as well as no accommodation at all ($\alpha_v = 0$), respectively, to heat transfer measurements taken at a low-density Mach 15.6 condition. They found that ($\alpha_v = 1$) leads to about 12% higher local heating rates compared to ($\alpha_v = 0$), however the differences to the measurements were of a similar magnitude.

The current work is in many aspects similar to their study, except that a simpler flow without separation is chosen, allowing to focus solely on the influence of vibrational surface accommodation. Also, three different density conditions allow to assess the influence of a change in Knudsen number by more than an order of magnitude.

2. Experiments

2.1 Shock Tunnel Conditions

The experiments were conducted in the ISL reflected shock tunnel, where high pressure hydrogen is used to rupture a membrane in order to create a shock wave heating and compressing the nitrogen (N_2) test gas. The nominal Mach 10 flow is created by a conically diverging nozzle with an opening half-angle of 14° .

The conditions in the shock tube before the nozzle

during the test were calculated with the equilibrium-chemistry code ESTC [8], using measured values of nozzle inlet (or reservoir) pressure, tube shock speed and shock tube initial fill conditions as input parameters. The equations for a normal shock wave are solved two times consecutively, as the shock wave reflects at the shock tube end wall. The measured nozzle inlet pressure is used to correct the calculated values by means of an isentropic expansion, which accounts for losses due to wall heat flux and flow drainage into the nozzle.

The freestream conditions were then calculated using the one-dimensional nozzle code STUBE [8]. The implemented Landau-Teller model [5] for vibrational-translational energy transfer uses relaxation rates from Vincenti and Kruger [9] and governs the non-equilibrium between vibrational and trans-rotational temperature components during flow nozzle expansion.

The calculated pitot pressure is fitted to a measured value by changing the effective nozzle angle in the code, accounting for the nozzle boundary layer displacement thickness. This strategy has been shown to predict measured freestream velocities to within 5% [10-12]. To further validate the freestream parameters, 2-d-axisymmetric CFD simulations using the commercially available Ansys Fluent code including a custom implementation of the Landau-Teller model were conducted additionally. One difficulty herein lies in the treatment of the re-laminarisation of the nozzle boundary layer, which cannot be simulated in a

realistic manner using standard turbulence models. Using them uncorrected generally leads to an overprediction of the nozzle boundary layer displacement thickness and hence pitot pressures higher than measured, as also pointed out by Nompelis [1]. To overcome this shortcoming, the turbulence model was switched off from a certain point in the downstream part of the nozzle. By adjusting the position of this point, the simulated pressure could again be matched to the measured one. Fig. 2 shows an up-to-scale schematic of the experimental setup, with simulated contours of the flow velocity.

The conditions of the current study are designed to resemble flight conditions at three different atmospheric altitudes and are listed in Table 1.

As the enthalpy of all three conditions lies below 5 MJ/kg, N_2 dissociation does not yet occur to a technically relevant extent. The total flow enthalpy can be expressed as a sum of bulk kinetic energy, trans-rotational energy, vibrational energy and the work of state formation:

$$h = \frac{\rho_\infty}{2} \cdot u_\infty^2 + \frac{5}{2} \cdot k_B \cdot T_{TR} + \frac{k_B \cdot \theta_V}{\exp(\theta_V / T_{VIB}) - 1} + k_B \cdot T_{TR} \quad (1)$$

Fig. 2 Setup and calculated velocity.

Table 1 Test flow conditions.

Equivalent altitude a.s.l.		km	50	60	70
Nozzle reservoir					
Reservoir pressure	p_{RES}	MPa	3.84	1.32	0.291
Reservoir temperature	T_{RES}	K	3,879	3,918	3,605
Freestream conditions					
Mach number	M_∞		10.5	10.5	10.6
Knudsen number (model dia)	Kn_D		0.0004	0.0011	0.0044
Reynolds number (model dia)	Re_D		36,700	12,800	3,200
Velocity	u_∞	m/s	2,845	2,827	2,684
Translational temperature	$T_{TR,\infty}$	K	177	173	155
Vibrational temperature	$T_{VIB,\infty}$	K	3,216	3,533	3,507
Density	ρ_∞	g/m ³	1.217	0.422	0.103

where, k_B is the Boltzmann constant and θ_V the specific vibrational Temperature (for N_2 , $\theta_V = 3,390$ K). Using the values of Table 1, it can be seen that while for all three conditions the flow kinetic energy is responsible for more than 80% of the total enthalpy, 10-15% are due to the elevated vibrational temperatures. That points out the importance of a realistic assumption for α_v when shock tunnel flow conditions are used in numerical simulations in order to calculate surface heat flux.

2.2 Model and Instrumentation

The steel model used is a blunted cone schematically shown in Fig. 3. It is instrumented with 11 fast response pressure transducers as well as 11 platinum thin film gauges for heat flux measurements distributed along the conical part of the model. The ratio of nozzle-exit-to-model diameter of three ensures that the model is well within the conically diverging core nozzle flow and not affected by the nozzle boundary layer.

2.3 DSMC-Modelling

The DSMC method simulates collisions between individual molecules and molecular surface collisions in a probabilistic manner. Collisions and particle motion are temporally decoupled and are simulated alternately, at numerical time steps smaller than the mean time between collisions. The DSMC code DS2V of Bird [13] was used with the VHS (variable hard sphere) model, which determines the effective collision cross section of the N_2 -molecules dependant on the molecular velocity. This allows obtaining a viscosity dependence on temperature in accordance with measured values. DS2V calculates the translational and the rotational molecular energy continuously (i.e. not quantized), while the vibrational energy level (v') of the molecule is implemented by discrete vibrational quantum states. The intermolecular vibrational energy exchange rates used in DS2V were derived from values of Vincenti and Kruger [9], also used for the nozzle

Fig. 3 Dimensions of the cone model in mm.

flow calculation described above. Due to the short test time in the order of a few milliseconds, the surface was modeled at a constant temperature of 300 K. The use of a conical nozzle results in a continuously diverging freestream, which was also considered in the simulations.

To obtain results which are independent of the number of molecules used in the simulation, their number was increased successively while monitoring the change in the heat flux result. Furthermore, it was taken care that the mean distance between modeled collisions was smaller than the molecular mean free path, as recommended by Bird [13]. Hence the numerical errors could be reduced to less than two percent.

3. Discussion

As opposed to Navier-Stokes based simulations, DSMC methods are also suitable for the modeling of rarefied flows—hence arbitrarily high altitudes can be simulated. As explained above, correlating literature data suggests nitrogen to behave nearly vibrationally inert at the surface. Still, this assumption is put to the test by comparing the shock tunnel heat flux measurements at each equivalent flight altitude to two types of simulations:

- FULL accommodation of vibrational energy when molecules hit the surface ($\alpha_v = 1$);
- NO accommodation, i.e. a vibrationally non-catalytic or inert surface ($\alpha_v = 0$).

The surface accommodation of rotational and translational energy was always modeled as complete. Also, the reflection at the surface was treated as fully diffuse. According to Bird [13], these assumptions should only be questioned for flight altitudes higher than 90 km. Three different tunnel runs were

conducted for each condition, the scatter between individual points at the same position indicating the magnitude of experimental uncertainty. Fig. 4 shows a comparison of both simulation variants with pressure measurements for the 50 km-condition. In accordance with the observation of Moss and Bird [3], the choice of α_v has no impact on pressure—both simulations agree well with the measurements. When comparing the simulations to measurements of heat flux at the same condition, however, differences show up, as shown in Fig. 5. There the heat flux is approximately 10% higher when vibrational energy accommodates at the surface. In general, the agreement with measured heat fluxes is better when the surface is treated as non-accommodating. At 60 and 70 km, shown in Figs. 6 and 7, the situation is similar—with, however, even larger differences between the two assumptions for α_v . While the effect of α_v on body drag, which is governed by surface pressure and skin friction, is below the accuracy of the DSMC simulation, it indicates significant differences on the total heating load on the model: for $\alpha_v = 1$, the heat fluxes are increased by 13, 15 and 19% for 50, 60 and 70 km, respectively.

The three conditions differ mainly in freestream density, but are also somewhat different as far as their velocities and vibrational temperatures are concerned. Hence correlating these values has to be done with caution. Still, due to multiple phenomena, there is a general trend towards smaller influence of α_v as freestream densities increase at lower altitudes.

In Fig. 8, the radial profiles of vibrational temperature at $X = 162$ mm from the nose tip are compared. It can be seen that for the vibrationally inert surface, T_{VIB} remains constant at 70 km but slightly decreases in proximity to the surface at 50 km. At the lower altitude, primarily the higher density and a longer gas residence time in the boundary layer leads to a small, however noticeable transfer of vibrational energy to translational/rotational modes, reducing the vibrational heat flux to the model surface, also for the $\alpha_v = 1$ case. A second reason is viscous heating in the

laminar boundary layer, the effect of which is more pronounced at low flight altitude, as the temperature profiles in Fig. 9 indicate.

Fig. 4 Surface pressure, 50 km equivalent altitude.

Fig. 5 Heat flux, 50 km equivalent flight altitude.

Fig. 6 Heat flux, 60 km equivalent flight altitude.

Fig. 7 Heat flux, 70 km equivalent flight altitude.

Fig. 8 Radial T_{VIB} profiles, 162 mm from nose tip.

Fig. 9 Radial T_{TR} profiles, 162 mm from nose tip.

Although not part of this study, small but nonzero values for α_v are also more significant at higher densities, as the long flow residence times that result from small boundary layer thicknesses with respect to

the model dimension promote multiple molecular surface collisions. Preliminary simulations not shown in this study indicate that the influence of α_v should become technically irrelevant for density conditions corresponding to atmospheric flight altitudes lower than 30 km.

4. Conclusions

An experimental test case of a non-reacting hypersonic shock tunnel flow around a blunted cone was compared against DSMC simulations in order to assess the influence of vibrationally highly excited nitrogen on surface heat flux. As literature data suggested, most surface materials should behave nearly noncatalytic for N_2 vibrational energy accommodation up to vibrational temperatures of 5,000 K. While simulations with corresponding modeling agreed to measured heat fluxes, the assumption of full accommodation, also applied in some previous work, lead to heat fluxes up to 19% high with respect to the measurements. Also, the influence of vibrational surface accommodation has been shown to be generally higher at lower freestream densities.

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