HYPERSONIC BOUNDARY LAYER ANALYSIS COMPARISON OF VELOCITY MEASUREMENTS AND MONTE-CARLO CALCULATIONS

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1. Introduction

The study of gas-solid accommodation at low pressure is of paramount importance to several areas of scientific research and industrial development. In Chemical Vapor Deposition (CVD) processes for instance, ONERA has quantified the accommodation for several diatomic-solid pairs and shown that, near or below 100 Pa, the gas can be substantially colder than the surface being grown, at a distance less than one mean free path from that surface [1, 2]; this drastically lowers the rate of chemical reactions in the reactor volume with respect to the case where accommodation would be complete. In supersonic aerodynamics, a domain which is important for flight mechanics at high altitude, e.g. in the reentry of a space shuttle, boundary layers may slip, here causing vehicle performance to deviate from that which is computed using models that do not account for it. Work recently performed at Los Alamos indicates that momentum accommodation can be determined using a torsion balance [3]. Kinetics of molecules rebounding off a surface were carefully studied for many years [4, 5]. This expertise is key to the use of Monte Carlo simulations of flow slip next to the wall.

In accommodation studies, it is customary to define coefficients for the thermal accommodation related to the translational and internal energy and for the tangential momentum accommodation. Those are very delicate to measure, and it has often been impossible to obtain reliable values that could be used for numerical simulations. In aerodynamics, the momentum accommodation also matters. Depending on values of the accommodation coefficients one can find a corresponding violation of continuum at the surface becoming apparent in a velocity slip and a temperature jump, influencing the aerodynamic drag and heat transfer. This may be particularly important in wind tunnel tests where pressure is low and Mach number high. Measuring the coefficients in the flow is a result of confrontation between theory and experiment. The computational modeling of the experimental situation is the only way to extract accommodation coefficients in the transition regime and close to continuum.

The main objectives of this paper are threefold: 1) measurement of velocity profile in a supersonic flow over a flat plate, 2) comparison of experimental data and numerical results and 3) analysis of the effect of accommodation coefficients on the boundary layer. Section 1 is devoted to the experiment: the basic principle of the velocimetry technique is presented and the experiment described. In a second section, the gas/surface interaction model is described. Experimental results are reported and compared with calculations in section 3.
2. Experiment

2.1. The CARS velocimetry technique. CARS (Coherent anti-Stokes Raman Scattering) is a well-known four-wave mixing technique that is today commonly used for the optical diagnostic of reactive media. The CARS diagnostic is usually implemented in the frequency domain to get instantaneous and local measurements of the temperature and the concentration of major gas species. The technique has recently been applied to velocity measurements by using a single-shot approach in the time domain [6, 7]. Basically, the signal is now produced from the non-linear mixing of a short "Stokes" pulse with long-duration "pump" pulses (Fig. 1a). Then, the anti-Stokes response presents a fast increase during the two-photon excitation phase by pumps and Stokes pulses, followed by a slow decrease; the latter is caused by the pump beams scattering off the free oscillation of the Raman coherence, which persists after the Stokes is interrupted. The exciting beams are focused in the folded boxcars geometry [8] as shown in figure 1b). In a low-pressure supersonic flow, the response turns into a damped oscillation the frequency of which permits one to measure the local velocity.

The presence of a modulation in the anti-Stokes signal can be readily explained by use of a laser-grating picture. By using the phase-matching arrangement shown in figure 1b), the two intersecting pump beams create a fringe pattern in their region of overlap. The pump beam intensity is thus spatially modulated within the probe volume. Hence, the Raman coherence that results from the pumps and the Stokes excitation mimics the spatial distribution of the pump light. Therefore, one prints into the gas a coherence grating that is spatially in phase with the pump grating if the Stokes pulse duration is short enough that the molecules move by less than the fringe spacing during their excitation phase. When excitation stops, the coherence grating moves with the flow velocity. Thus, it comes periodically in and out of phase with the stationary pump grating acting now as a read-out grating. Consequently, the anti-Stokes response is modulated, maxima and minima being obtained when both coherence and pump gratings overlap or not. In reality, the molecular velocity is spread about the jet velocity due to the thermal motion of the molecules. This washes out the molecular coherence and leads to a damped beating that limits the persistence time of the signal and constrains the application to transonic and supersonic flows; molecular collisions also destroy the coherence, which restricts the range of application to low-pressures. Note that the CARS velocimetry is a seedless approach, which avoids the particle lag problem found in conventional laser anemometry, particularly in the low-pressure supersonic flows.

Fig. 1. a) time diagram in CARS velocimetry, the anti-Stokes response is shown for a static gas (solid line) and a supersonic flow (dashed line); b) : phase-matching diagram, the maxima of the pump gratings are schematically shown in the intersecting region.
To overcome the low velocity limitations, the frequencies of the two pump beams have been slightly shifted by means of a Bragg cell. Such a nearly degenerate approach allows us to extend the range of operation of the technique towards the subsonic regime [9]. With it, the pump grating now is moving and can be made to propagate in the sense opposite to that of flow, thus up-shifting the beat frequency. Low velocities then can be determined.

2.2. Description of the experiment. The experimental layout is depicted in figure 2a). The output of a Nd:YAG laser delivering 30 ns-long infrared Gaussian pulses at a 12.5 Hz repetition rate is divided into two parts. The first part goes through an acousto-optic shifter delivering two pump beams of equal intensity in the zero and first orders of diffraction. These two beams are produced with a 110 MHz frequency difference, which is imposed by the acoustic frequency driving the Bragg cell; after second harmonic generation, the pump pulse duration is 23 ns FWHM (full width at half maximum). The second part of the Nd:YAG laser beam is used to produce short pulses, typically 2 ns long, at the Stokes frequency. These short pulses are obtained using an original optical arrangement that consists of a dual-cavity optical parametric oscillator (OPO) [10] followed by an amplifier and a sum-frequency stage. Optical delays are adjusted so that the Stokes pulse is emitted at the maximum of the two pump pulses. At the output of the CARS bench, the output energy is 15 mJ for each pump beam and 1 mJ for the Stokes. In order to optimise both the persistence time and the intensity of the anti-Stokes signal, the OPO wavelength is adjusted for probing the most intense N\textsubscript{2} rotational lines, viz. S(6) and S(10) at 50 and 300 K, respectively. Hence the Stokes wavelength can be tuned between 534 nm and 540 nm whereas the pump wavelength is maintained at 532 nm.

![Fig. 2. a) CARS optical bench, X2: frequency doubler, AO: acousto-optic shifter, \(\omega_p\), \(\omega_s\), \(\omega_A\): pump, Stokes and acoustic frequencies); b) top view of the flat plate and laser beam mixing, \(\omega_{AS}\): anti-Stokes frequency, GT Glan Taylor polarizer, PC personal computer.](image-url)
Next, the Stokes beam is overlapped with the two pumps by means of an 800-mm focal-length lens; the half-crossing angle of the two pumps is 0.75° yielding a cylindrical probe volume that is 14 mm long and 0.2 mm in diameter. The axis of the probe volume is placed perpendicularly to the supersonic flow. To explore the boundary layer, the position of the probe volume is moved above the flat plate. Then, the anti-Stokes signal is filtered from the exciting lasers by means of a spectrometer and a Glan polarizer. Finally, the response is detected by a fast photomultiplier (Hamamatsu model R2566U) and displayed on a 1 GHz bandwidth storage oscilloscope (Tektronix, TDS684A), interfaced to a micro-computer.

The flat silicon carbide plate is 40 cm-long and 20 cm-wide with dimensions chosen to avoid edge effects. The plate was milled to obtain sub-micron surface flatness. Ideally, for clean slip flow studies, it should be flat to the atomic scale, which turned out impossible to achieve. The leading edge is a wedge cut at a 15° angle and features an estimated typical radius of curvature of 50 µm. The plate is aligned parallel to the flow axis and is translated about the flow centreline to vary the separation between the surface and the fixed laser beams.

The supersonic flow (0.2 m in diameter) is produced at the nozzle exit of a low-enthalpy wind tunnel operating with air or pure nitrogen. This facility maintains stable stagnation conditions with a good reproducibility in 60s-long runs. The jet velocity was previously measured by a Pitot tube [11] whereas the density and the temperature were obtained by using the dual-line CARS technique [12]. By comparison of velocity profiles and Navier Stokes calculations, it was deduced that the Mach number is 9.9 ± 0.07. Given the stagnation conditions that have been provided during this experiment (Pi = 2300±100 hPa and Ti = 1000±10 K), the expected flow conditions are Vjet =1382 m s\(^{-1}\) (air flow), static temperature = 48 K and static pressure = 5.5 Pa.

3. Numerical approach

The direct simulation Monte Carlo (DSMC) method is used in the present paper for numerical examination of the flow over a flat plate because it is one of the most promising approaches for the calculation of hypersonic rarefied flows. This method is the only one in computational rarefied gas dynamics that offers the capability of simulating flows across the range from continuum to free molecular; it is thus the most suitable for simulating flows where viscous and rarefaction effects are important [13-16].

The computations of the flow around the plate is performed by DSMC-software SMILE [17]. The following models were used in the computations:

- variable hard sphere [18] model for intermolecular collisions;
- Larsen-Borgnakke model [18] with temperature dependence;
- relaxation numbers for the energy exchange between translational and internal molecular modes of molecules;
- specular-diffuse gas/surface interaction model.

The flow above the flat plate at zero angle of attack was computed for the following conditions: stagnation pressure P\(_i\)=2270 hPa, stagnation temperature T\(_i\)=998 K, free-stream Mach number M\(_\infty\)=9.93. The wall temperature was a constant fixed to 278 K.

3.1. Gas/surface interaction model. The specular-diffuse model was introduced by Maxwell [19] and it is still widely used for computations. The model considers that a part of molecules (1-\(\alpha_\beta\)) are specularly reflected from the surface while a part of molecules \(\alpha_\beta\) are diffused following a Maxwellian law. The distribution function of reflected particles is [20]:

\[
f_r(t,x,v_r) = \left(1 - \sigma_r\right)f_i(t,x,v_i) + \sigma_r n_i \left(\frac{h}{\pi kT_i}\right)^{3/2} e^{-h v_r^2} \tag{1}
\]

where \(h = \frac{m}{2kT_i}\), \(f_i\) is the distribution function of incident molecules, \(m\) is the molecular mass, \(k\) is the Boltzmann constant. The function has three parameters \(\alpha_\beta\), \(n_i\), and \(T_i\); \(\alpha_\beta\) is the
accommodation coefficient of the tangential moment since it characterizes the part of tangential moment that is brought by incident molecules to the surface.

One introduces energy the accommodation coefficient [20]:

$$\alpha = \frac{E_i - E_r}{E_i - E_w}$$  \hspace{1cm} (2)

where \(E_i\) is the energy of incident molecules, \(E_r\) is the energy of reflected molecules, and \(E_w\) is the energy of reflected molecules taking \(T_r = T_w\) in Eq. 1. As a result, the distribution of reflected particles is defined given the accommodation coefficients and the wall temperature.

4. Results

Preliminary velocity measurements have been performed within the free stream in order to characterise the evolution of the jet velocity during a run. The wind tunnel operates with air. To improve the signal to noise ratio, each velocity measurement is obtained by averaging 30 laser shots. Under such conditions, the acquisition time of one measurement is 2.4 s, taking into account the data time transfer from the oscilloscope to the microcomputer. Thus, a set of 30 measurements is obtained along a run. At the beginning of the run, the CARS measurement gives 1380 ms\(^{-1}\), in good agreement with the expected value. This value decreases slightly to 1350 ms\(^{-1}\) at the end of the run. This small variation (2\%) can be attributed to a small decrease of the stagnation temperature. One estimates that the sensitivity of the technique to small velocity changes is comprised between 1.5 to 2\%. Obviously, the absolute uncertainty on the velocity measurement is higher, typically 6\% because of systematic errors, in the determination of the beam crossing angle [9].

In a second step, the boundary layer has been investigated 100 mm downstream the leading edge of the flat plate with a pure nitrogen flow instead of air. Velocity measurements have been collected between 5 and 25 mm above the plate. Experimental values as well as computed velocity profiles that have been performed for different accommodation coefficients (from unity to 0.5) are plotted in figure 3. The velocity profiles clearly show the reduction of the flow velocity through the boundary layer. Nonetheless, it was not possible to get velocity measurements within the 5 mm region apart from the surface since the signal to noise ratio was too poor at short distances. This is due to: i) the contamination of the anti-Stokes signal by stray light from the laser beams scattered off the surface, ii) the decrease of the anti-Stokes intensity resulting from the combined effects of reduced gas density, and increased temperature.

Fig. 3. Comparison between experimental and calculated velocity profile.
It can be seen from figure 3 that a decrease of the accommodation coefficient of tangential moment leads to a thinner boundary layer because fewer particles change their normal velocity component during a collision with the wall. A variation of energy accommodation coefficient has an opposite effect. Decreasing the coefficient increases the boundary layer thickness because diffusively reflected particles have larger energy. Note that all computed velocity profiles except one case ($\alpha_D = 0.5, \alpha_E = 1.0$) lie within the error bars of measured values so we cannot conclude on the effective $\alpha_D$ value.

In Figure 4, the intensity of the CARS signal has been plotted versus the position above the plate. Note that the variations of the signal intensity result from changes in the thermodynamic conditions (temperature and density) of the gas flow since the optical conditions (beam geometry and laser intensities) are not changed during the experiment. Hence, at long distances ($z > 25\,\text{mm}$), the CARS intensity depends on the thermodynamic conditions that are encountered within the free stream. Then, by decreasing the distance, one clearly observes a sharp increase of the CARS intensity, which is located about $z = 21.5\,\text{mm}$. Next, a plateau is recorded followed by a second decrease of the signal intensity. As explained below, the signal dependence can be explained by considering both the calculated evolutions of the gas density and the temperature through the boundary layer.

The calculated density and temperature profiles are shown in Figures 5 and 6, respectively. From Figure 5, it is seen that the density profile shows a fast increase at the position $z = 21.5\,\text{mm}$ which is attributed to the presence of an oblique shock generated by the leading edge of the plate. Next, the density decreases through the boundary layer. Also, we note that the influence of the accommodation coefficients on density profiles is small. For example, the difference between $\alpha_D = 1.0, \alpha_E = 1.0$ and $\alpha_D = 0.5, \alpha_E = 0.3$ cases is less than 5%. Conversely, the effect on temperature reaches up to factor of 2 close to the surface. At large distances (above 15 mm), it is seen that the temperature profile is roughly flat. From figures 5 and 6, one deduces that the anti-Stokes variation, which is observed at $z = 21.5\,\text{mm}$ is directly correlated to the density variation generated by the oblique shock since the temperature does not change in this region. In effect, the calculated density profile predicts an increase of a factor 2; such a variation leads to a factor 4 variation in the anti-Stokes signal since the CARS intensity varies as the square of the density. Figure 6 shows that computation for $\alpha_D = 1.0, \alpha_E = 1.0$ predicts a position which is in good agreement with experimental data. However, since the accommodation coefficients affect the flow in opposite ways, one can find combinations of accommodation coefficient values that produce the same shock position and our results do not permit us to conclude.

Fig. 4. CARS signal intensity through the boundary layer.
The analysis was pushed further by studying the surface quality of the SiC plate. An Atomic Force Microscope (AFM) was used, revealing a roughness scale in the range of 5-90 nm depending on the spatial frequency of the relief (Fig. 7 a). Clearly, slip is impossible on so rough a surface and the preceding results should not surprise us. A smoother surface of comparable size was then prepared from a silicon wafer used in the microelectronics industry. Figure 7 b presents an AFM surface analysis; the roughness is in the range 1-2 nm, and drops down to 1 nm after cleaning with an HF aqueous solution (Fig. 7 c).

For the same position downstream from the leading edge, and with an uncleaned plate, the same experimental velocity profile as with the SiC plate was found within experimental errors. No conclusive evidence of slip can be reported for those conditions where roughness, although smaller than with the SiC, remains rather coarse.

Fig. 5. Calculated density profiles. Fig. 6. Calculated temperature profiles.

Fig. 7. AFM micrographs of 15µmx15µm zones on the surface of the SiC plate (a) and of a silicon wafer before (b) and after (c) cleaning with an HF aqueous solution.
5. Conclusion

A DSMC study of a rarefied Mach 10 flow near a flat plate under zero angle of attack was conducted for different values of accommodation coefficients. Lowering tangential moment accommodation leads to thinner boundary layer and lowering energy accommodation thickens it. A novel velocity measurement technique was developed. Comparing experimental data with computed velocity profiles showed that all numerical results except one are within experimental error bars. Based on measured position of leading-edge shock wave, few sets of accommodation coefficients were found out which allow one to get the same position. However, flow velocity and temperature near the wall are rather different.

Surface quality remains too rough to reasonably expect slip, even if tangential moment accommodation was small. Future experiments should aim at 1) measuring flow velocity as close to the wall as possible or increasing flow rarefaction, 2) simultaneously measuring flow velocity and temperature and 3) using surfaces of SiC, Si or other materials with low accommodation with even better surface qualities. For the SiC, that will have to wait till large affordable single-crystal wafers become commercially available.

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