

**SPECIES MEASUREMENTS IN A HYPERSONIC,
HYDROGEN-AIR, COMBUSTION WAKE**

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(Running Title: Species in a Combustion Wake)

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ABSTRACT

A continuously sampling, time-of-flight mass spectrometer has been used to measure relative species concentrations in a two-dimensional, hydrogen-air combustion wake at mainstream Mach numbers exceeding 5. The experiments, which were conducted in a free piston shock tunnel, yielded distributions of hydrogen, oxygen, nitrogen, water and nitric oxide at stagnation enthalpies ranging from 5.6 MJ kg⁻¹ to 12.2 MJ kg⁻¹ and at a distance of approximately 100 times the thickness of the initial hydrogen jet. The amount of hydrogen that was mixed in stoichiometric proportions was approximately independent of the stagnation enthalpy, in spite of the fact that the proportion of hydrogen in the wake increased with stagnation enthalpy. Roughly 50% of the mixed hydrogen underwent combustion at the highest enthalpy. The proportion of hydrogen reacting to water could be approximately predicted using reaction rates based on mainstream temperatures.

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1. INTRODUCTION

The mixing and burning of a hydrogen wake or jet in air at hypersonic speeds is an essential process of very high speed scramjet propulsion^(1,2). It may occur in the combustion chamber of a scramjet, where rapid mixing and combustion is desirable, or it may occur in the inlet, in which case injection of the hydrogen with rapid mixing but delayed combustion is required. It has received limited attention up to the present^(3,4). Most studies of hydrogen-air wakes have been confined to air stagnation enthalpies below 2 MJ kg^{-1} ⁽⁵⁾. With precombustion temperatures of 800 K or more required for hydrogen, this implies that airstream Mach numbers have been limited to around 2.8.

Measurements of relative species concentrations in a two-dimensional wake at stream Mach numbers of 5.2 and above are reported here. The measurements were done in a shock tunnel, using a continuously sampling time-of-flight mass spectrometer, and involved a range of freestream temperatures sufficient to produce wake flows with and without combustion. Accompanying Pitot measurements in the wake were also made. The freestream Reynolds' number, based on the length of the wake, varied from 1.3×10^6 to 2.9×10^6 , indicating that the wake was well and truly turbulent.

2. EXPERIMENTAL ARRANGEMENT

The experiments were conducted in the free piston shock tunnel T4 at The University of Queensland⁽⁶⁾. This employed a 75 mm diameter shock tube with a free piston driver, and was operated in the shock reflection mode. A contoured nozzle, with a 25 mm diameter shock and a nominal area ratio of 110, was located at the downstream end of the shock tube, and produced a hypersonic free jet with a uniform core diameter of approximately 200 mm at the nozzle exit. Mixtures of argon and helium were used as driver gas.

The experimental arrangement is shown schematically in fig. 1. The hydrogen-air wake was formed inside a rectangular duct, located with its leading edge 120 mm from the nozzle exit. A fuel injection strut was mounted in the midplane of the duct, spanning the shorter dimension, and hydrogen was injected from its trailing edge. The mass spectrometer was mounted to traverse the wake in the centre of the duct at 500 mm from the injection strut trailing edge.

The duct and fuel injector are shown in more detail in fig. 2. The injector was 7.6 mm thick, and the hydrogen was injected at a Mach number of 3.2 through a two-dimensional nozzle which spanned the full 80 mm width of the duct. The leading edge of the duct was a wedge of 6.6° included angle and, as shown by the dotted lines in the figure, it was arranged that the flow disturbances from the wedge passed downstream of the measuring station without influencing the wake. The boundary layer on the strut was expected to be laminar, with a displacement thickness at the trailing edge of a fraction of a millimetre⁽⁷⁾, and this was not expected to have a significant effect on the development of the wake.

3. THE MASS SPECTROMETER

As shown in fig. 1, the flow was sampled continuously through a 2 mm diameter orifice in the first of three conical skimmers. The cavity between the second and third skimmer was connected to a pre-evacuated dump volume, and the cavity after the third skimmer, containing the gas analysis equipment, was connected to a separate pre-evacuated dump volume. Pressures were low enough to ensure that the test gas passed into the latter cavity in the form of a molecular beam. This beam was bombarded by an electron gun, and the ions produced were extracted from the beam and accelerated before passing into the drift tube, to be ultimately detected by the electron multiplier at the end of the drift tube. The electron gun

was pulsed on for 200 nanoseconds every 55 microseconds, and each pulse produced a packet of ions which, because their time of flight depended on the individual mass of the ions, could be detected and analysed for mass at the electron multiplier. Thus a complete mass spectrum, with a signal proportional to the numbers of ions of each mass arriving at the electron multiplier, was produced every 55 microseconds during the shock tunnel test time. This was recorded using a 50 MHz storage oscilloscope. More detail on the mass spectrometer is given in refs. 8 and 9.

To interpret the signal in terms of the number of particles of each species sampled by the mass spectrometer, published ionization cross-sections were used⁽⁹⁾. These were incorporated into calibrations which accounted for mass separation effects in forming the molecular beam, and in collecting the ions for passage through the drift tube, by using the mass spectrometer to sample known mixtures of helium-nitrogen, argon-nitrogen, and hydrogen-nitrogen in the tunnel freestream at varying stagnation enthalpies and Pitot pressures. The calibrations resulting from this process are considered to be accurate to within 20% in the measurement of hydrogen, 25% in water, 10% in oxygen, nitrogen, nitric oxide and argon, and 5% in helium.

Fig. 3 displays typical records of hydrogen and water mole fractions obtained in the wake, with a reading every 55 microseconds. The mainstream flow wake transit time was approximately 150 microseconds, so results were taken in the time interval from 0.5 milliseconds to 1 millisecond, in order that a steady flow state could be achieved. The error bars display the uncertainty in reading the records. It can be seen that, in this case, the mole fractions are not steady after 0.75 milliseconds, so readings were not taken after that time.

4. FLOW CONDITIONS

Experiments were conducted at the four flow conditions set out in table 1. The composition of the shock tunnel driver gas was varied with stagnation enthalpy to ensure that the pressure at the end of the shock tube remained steady (to within $\pm 5\%$) after shock reflection. The stagnation enthalpy was obtained by using the shock speed and the shock tube filling pressure to calculate the conditions after shock reflection, and expanding to the measured pressure where necessary. The Pitot pressure and static pressure were measured at the entrance to the test duct, and were used to guide the choice of area ratio for the shock tunnel nozzle expansion. Using this area ratio, the test conditions were calculated numerically⁽¹⁰⁾ for a one-dimensional steady expansion from the reservoir conditions at the end of the shock tube.

The hydrogen fuel was injected parallel to the mainstream flow, but was slightly over expanded and therefore the jet experienced some recompression to bring it to the mainstream pressure. The conditions in the jet after it was recompressed are displayed in table 1, and are based on calibrations of the injector with hydrogen flow⁽¹¹⁾. The fuel flow rates were chosen so that, at the lowest stagnation enthalpy, an equivalence ratio of one would be obtained if a section of the mainstream of 50 mm height was being fuelled. As will be seen below, this is slightly greater than the height of the wake at the measuring station, and therefore can be regarded as encompassing all of the mainstream involved in the mixing process. This "relative equivalence ratio" was increased with stagnation enthalpy, in accordance with what might be expected in a scramjet application.

Table 1. Test Conditions

<u>Mainstream</u>				
Stagnation enthalpy (MJ kg ⁻¹)	12.2	9.4	7.8	5.6
Driver gas composition (Ar/He)	12/88	17/83	23/77	25/75
Nozzle reservoir pressure (MPa)	40	40	40	40
Mach number	5.2	5.4	5.6	5.7
Temperature (K)	1750	1340	1050	760
Density (kg m ⁻³)	0.037	0.045	0.052	0.069
Velocity (M s ⁻¹)	4260	3840	3550	3120
Pitot pressure measured (kPa)	600	630	620	570
calculated (kPa)	625	615	605	618
Static pressure measured (kPa)	20	17	13	11
calculated (kPa)	19.4	17.6	15.8	15.1
<u>Hydrogen Fuel Jet</u>				
Mach number	2.8	2.8	2.9	2.8
Temperature (k)	117	114	113	114
Density (kg m ⁻³)	0.041	0.036	0.028	0.024
Velocity (m s ⁻¹)	2280	2300	2310	2300
Thickness (mm)	4.8	5.2	5.3	5.1
Relative equivalence ratio	2.2	1.9	1.4	1.0

It will be noted that the thickness of the jet after recompression was approximately 5 mm. The traverse measurements were done at a downstream distance which was 100 times greater than this, to enable a wake structure to be formed. This was confirmed by calculations of the air-hydrogen mixing layer at the top and the bottom of the jet^(12,13), which showed that the two

mixing layers closed to eliminate the inviscid core of hydrogen flow and form a wake at approximately 125 mm downstream.

5. RESULTS AND DISCUSSION

The number of particles of each species sampled by the mass spectrometer was converted into mole fractions by dividing by the total number of particles, and the results plotted in fig. 4 for each of the major species present, at each of the four stagnation enthalpies tested. Atomic species and the hydroxyl radical were not present in measurable quantities. The points plotted represent the mean of the values obtained from the sequence of mass spectra obtained in any one test, with the error bars representing the standard errors of those mean measurements.

The figure displays an increasing predominance of hydrogen in the wake as the enthalpy is raised, with an associated reduction in nitrogen. This is a reflection of the increased flow of hydrogen, as noted by the relative equivalence ratio of table 1. This also causes a reduction in the mole fraction of oxygen, but at the higher enthalpies this is due to combustion as well. This is shown by the increasing mole fraction of water formed. It will be noted that contamination of the test flow by the helium-argon driver gas increases with the stagnation enthalpy. However, this is not expected to significantly influence the results as the driver mixture is chemically inert, and a 20% mole fraction of the mixture would reduce the stagnation enthalpy by less than 10%.

As indicated by the vertical arrows, the measured levels of oxygen are some 50% in excess of expected values, in relation to nitrogen, at 15 mm at 9.4 MJ kg⁻¹ and 5 mm and 10 mm at 5.6 MJ kg⁻¹. This phenomenon has occurred occasionally in other tests with the mass spectrometer, and is not yet explained. Fortunately, the error incurred is not sufficient to

significantly affect the results below.

The results of Pitot surveys of the wake are shown at the top of fig. 5. The distribution of the average molecular mass, calculated from the results in fig. 4, is also presented and is seen to be similar to the Pitot pressure profile. Since the Pitot pressure may be closely approximated by ρu^2 , where ρ is the density and u the velocity, this similarity suggests that, through its influence on the density, the effect of hydrogen on the molecular mass is the main factor determining the variation of Pitot pressure across the wake.

Since the wake is well developed at the traverse station, it would be expected that the velocity and temperature throughout the wake would be reasonably close to the freestream values. This was confirmed by noting that the wake developed at constant pressure, and therefore it was possible to equate the momentum in the wake (as measured by the Pitot pressure profile) to the initial momentum of the hydrogen jet together with that of the mainstream fluid captured by the wake. Then, by assuming a linear variation of velocity with distance normal to the wake centreline, an estimate of the magnitude of the velocity could be obtained. The temperature was then related directly to the square of the velocity by making the further assumption that the distribution of Pitot pressure across the wake is identical with the distribution of average molecular mass, and the static pressure is constant. For the four test conditions considered, this process yielded a mean velocity in the wake which was within 95% of the mainstream velocity, and a mean temperature which was within 90% of the mainstream value.

Having established that the velocity variation across the wake is relatively small, it becomes possible to make an approximate check on the magnitude of the hydrogen concentrations

measured by the mass spectrometer. The mass of hydrogen flow in the wake can be written as

$$\begin{aligned}
 m_H &= 2 \int_0^\delta c_H \rho u \, dy \\
 &= 2 \rho_\infty u_\infty \left\{ \int_0^\delta c_H \left(\rho u^2 / \rho_\infty u_\infty^2 \right) dy + \int_0^\delta c_H \left(\rho u^2 / \rho_\infty u_\infty^2 \right) (u/u_\infty - 1) dy \right\}
 \end{aligned} \tag{1}$$

where c_H is the mass fraction of hydrogen (in any form) at any point, y is the distance normal to the wake centreline, with δ its value at the edge of the wake, and ρ_∞ and u_∞ are values of ρ and u at some reference condition; in this case the mainstream values given by table 1. Thus, putting $\rho u^2 / \rho_\infty u_\infty^2$ equal to the ratio of Pitot pressures, multiplying the total mole fraction of hydrogen (i.e. hydrogen + water) by the ratio of the molecular mass of hydrogen to the average molecular mass to obtain c_H , and integrating from the centre to the edge of the wake, the first term on the right hand side of eq. (1) is obtained. Noting that m_H is also given by the mass flow from the injector, which may be obtained from the density, velocity and thickness of the hydrogen jet in table 1, and that u has been assumed to be nearly equal to u_∞ , it is clear that the ratio of m_H obtained in this manner, to the first term on the right hand side of eq(1) should be a little greater than one. In fact, the results yield an average value of 1.15 for the ratio, with a variation of +13% and -8%, thereby approximately confirming the mass spectrometer measurements.

The total mole fraction of hydrogen is also plotted in fig. 5 for the four test conditions, along with the fraction of hydrogen which is mixed with air in proportions approximate to complete combustion. Where the mixture is lean in hydrogen, all the hydrogen is counted, and where the mixture is rich, only an amount of hydrogen sufficient for combustion with the oxygen and nitric oxide is counted. This is referred to on the figure as mixed hydrogen. At any point, the ratio of mixed hydrogen to total hydrogen can be taken as a local mixing efficiency, η_m .

Strictly, to obtain an overall mixing efficiency in the wake would require knowledge of the distribution of ρu in the wake, but if it is once again assumed that the velocity variation across the wake is relatively small, it is possible to follow the procedure leading to eq. (1), and to obtain the mixed hydrogen as

$$\begin{aligned} m_{H_m} &= 2 \int_0^{\delta} \eta_m c_H \rho u \, dy \\ &= 2 \rho_{\infty} u_{\infty} \left\{ \int_0^{\delta} \eta_m c_H \left(\rho u^2 / \rho_{\infty} u_{\infty}^2 \right) dy \right\} \{ 1 + O(u/u_{\infty} - 1) \} \end{aligned} \quad (2)$$

Performing the integration from the centre to the edge of the wake, and neglecting the term in $(u_{\infty}/u - 1)$, yields an approximation for the amount of hydrogen which is mixed. It is found that this amount is constant with $\pm 15\%$ for the results presented here, with no indication of a systematic variation over the test conditions.

An approximation for the overall mixing efficiency in the wake may be obtained from eqs. (1) and (2), again neglecting terms in $(u_{\infty}/u - 1)$, as

$$\eta_{mw} = \left\{ \int_0^{\delta} \eta_m c_H \left(\rho u^2 / \rho_{\infty} u_{\infty}^2 \right) dy \right\} / \left\{ \int_0^{\delta} c_H \left(\rho u^2 / \rho_{\infty} u_{\infty}^2 \right) dy \right\}$$

This yielded the values of η_{mw} presented in table 2. Because the amount of hydrogen injected was increased with stagnation enthalpy, but the amount of hydrogen mixed remained approximately constant, the wake mixing efficiency reduced with increasing enthalpy. It would seem that the increase in fuel flow serves no useful purpose, until it is noted that the hydrogen which is not "mixed", in the sense in which the term is used here, will still be effective in reducing post-combustion temperatures.

Table 2. Measurements of Overall Mixing Efficiency

Stagnation Enthalpy (MJ kg ⁻¹)	12.2	9.4	7.8	5.6
Mixing Efficiency η_{mw} (%)	30	42	63	60

The ratio of water concentration to that of mixed hydrogen indicates the proportion of mixed hydrogen that has reacted, and forms a local reaction efficiency. This is shown on the lower portion of fig. 5, where it is plotted as a series of bars indicating the expected uncertainty. It can be seen that more than half of the mixed hydrogen has reacted at the highest enthalpy, and very little indeed at the low enthalpies.

It is of interest to make a simple, first order estimate of the level of reaction. This can be done by assuming that the hydrogen-air mixture may be regarded as mixed for a period of time given by L/u_w , where L is the length of the wake, measured from the point of injection of hydrogen to the traverse station. During that time it first undergoes an ignition delay, given by ⁽¹⁴⁾

$$\tau_i = 8 \times 10^{-3} p^{-1} \exp(9600/T) . \quad (3)$$

Here the time τ_i is measured in microseconds, the pressure p in atmospheres, and the temperature T in K. In the remaining time it reacts, and the proportion of hydrogen which burns to form water can be expressed as

$$\alpha_H = (L/u_w - \tau_i) / \tau_R$$

where τ_R is the heat release time in microseconds, given by ⁽¹⁴⁾

$$\tau_R = 105 p^{-1.7} \exp(-1.12 T/1000) . \quad (4)$$

These expressions for τ_i and τ_R are subject to considerable theoretical uncertainty ⁽¹⁵⁾, but are taken as the best estimate of reaction rates for the present purpose. Assuming that T is equal to the mainstream static temperature then yields the levels for the ratio of water to mixed hydrogen which are shown by the broken lines in the lower part of fig.5 at 12.2 and 9.4 MJ kg⁻¹. It can be seen that they are reasonably consistent with the experimental values. The ignition delay predicted for 7.8 and 5.6 MJ kg⁻¹ is too long to permit the formation of water, and it is thought that the small amounts observed may be due to reactions involving nitric oxide ⁽¹⁵⁾, together with a very small residual amount, probably associated with outgassing.

6. CONCLUSION

Mass spectrometric traverses of a hypersonic combustion wake have yielded the distribution of hydrogen, oxygen, nitrogen, water and nitric oxide. Comparison with Pitot traverses indicated that the variation of Pitot pressure was largely due to the influence of hydrogen on the molecular weight, suggesting a wake structure dominated by hydrogen diffusion. The amount of hydrogen that was mixed in stoichiometric proportions was approximately independent of the stagnation enthalpy, in spite of considerable combustion taking place, and considerably more hydrogen being injected, at the highest enthalpy. When combustion took place, the degree of combustion could be approximately predicted using reaction rates based on mainstream conditions.

The prime purpose of the experiments was to assess the utility of the mass spectrometer in this shock tunnel application. However, it is worth making some remarks concerning possible implications of the results for scramjet operation. In a scramjet combustion chamber, pressures are expected to be almost an order of magnitude higher than in these tests and, as

shown by eqns(3) and (4), combustion will occur much more rapidly in relation to mixing. Thus, if fuel injection takes place in the combustion chamber, mixing limitations will be predominant. However, pressures in the inlet are likely to be an order of magnitude lower than in these tests, so that combustion will occur much more slowly. Noting that flow temperatures at the two lower enthalpy conditions tested are likely to be typical of inlet temperatures in flight, and that because of the lower pressures ignition delay and heat release times will be much greater than the minimum values of 0.5 milliseconds and 1 millisecond respectively which can be calculated from eqns(3) and (4) for the conditions of these tests, it is clear that wake lengths of several metres can be sustained without significant reaction. Therefore Reynolds' numbers equal to or greater than those obtained in the present tests can be achieved, leading to the same or a greater degree of mixing. Thus it appears that wake mixing efficiencies in the inlet exceeding 60% can be obtained without reaction, indicating that inlet injection ⁽¹⁶⁾ may offer an effective method of relieving mixing problems in the combustion chamber.

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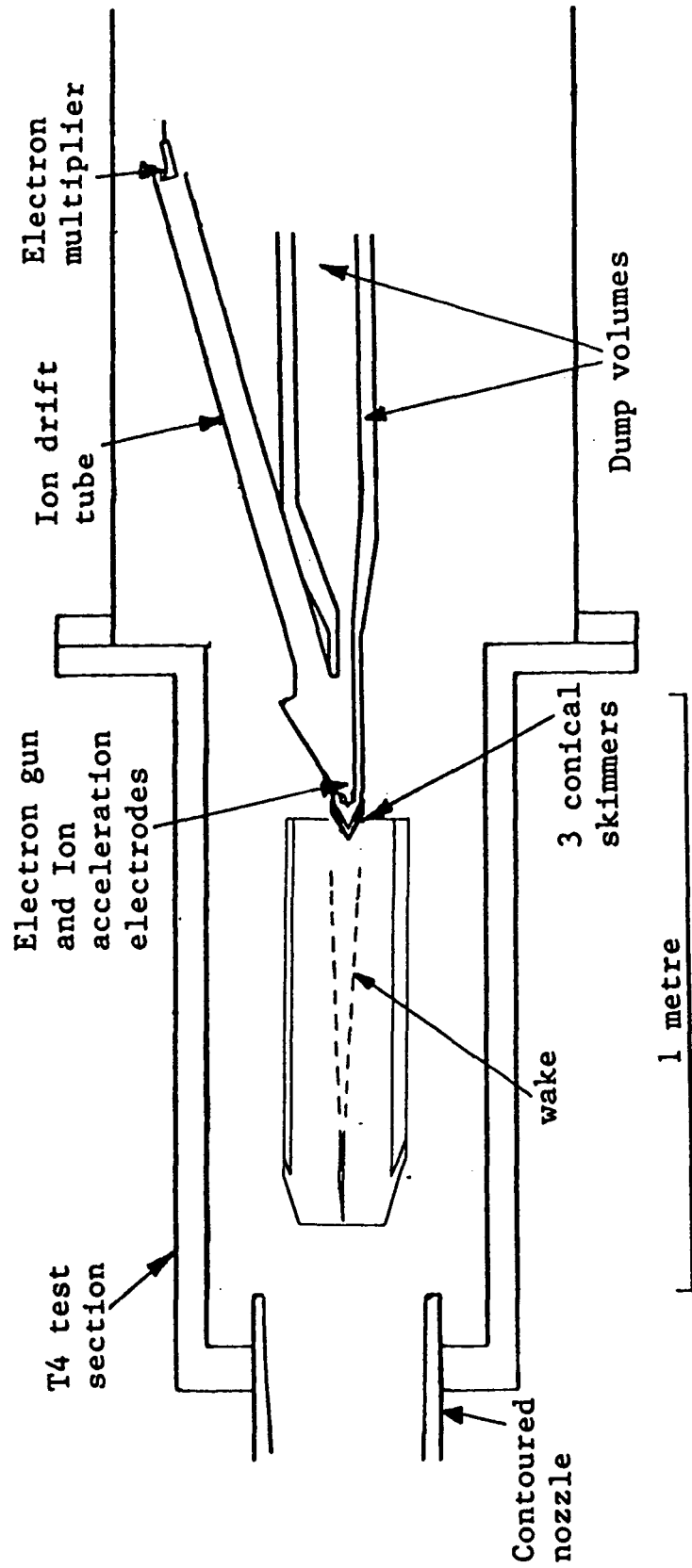


Fig. 1 Experimental arrangement.

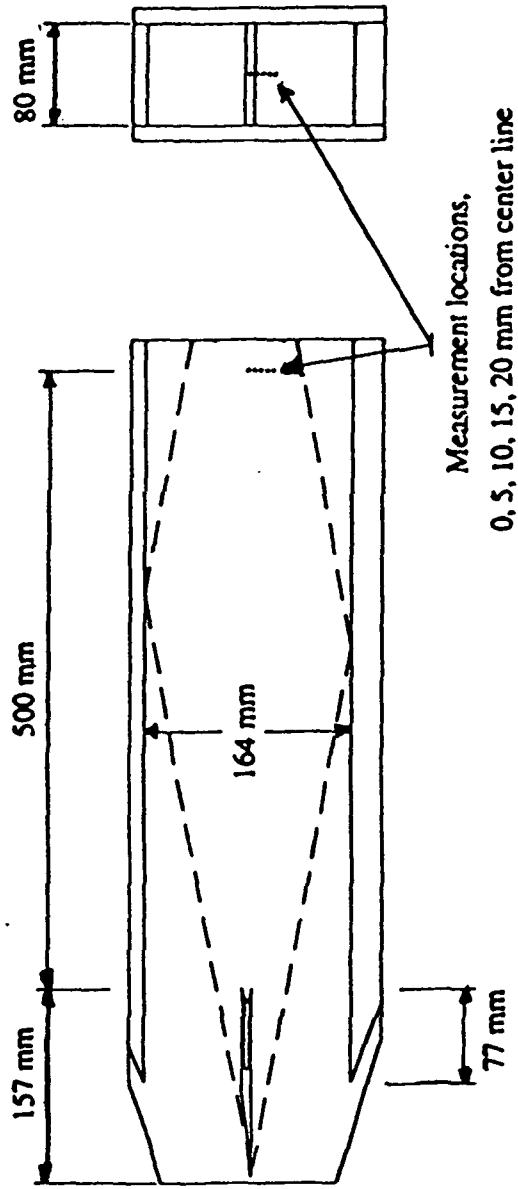


Fig. 2 Detail of experimental duct.

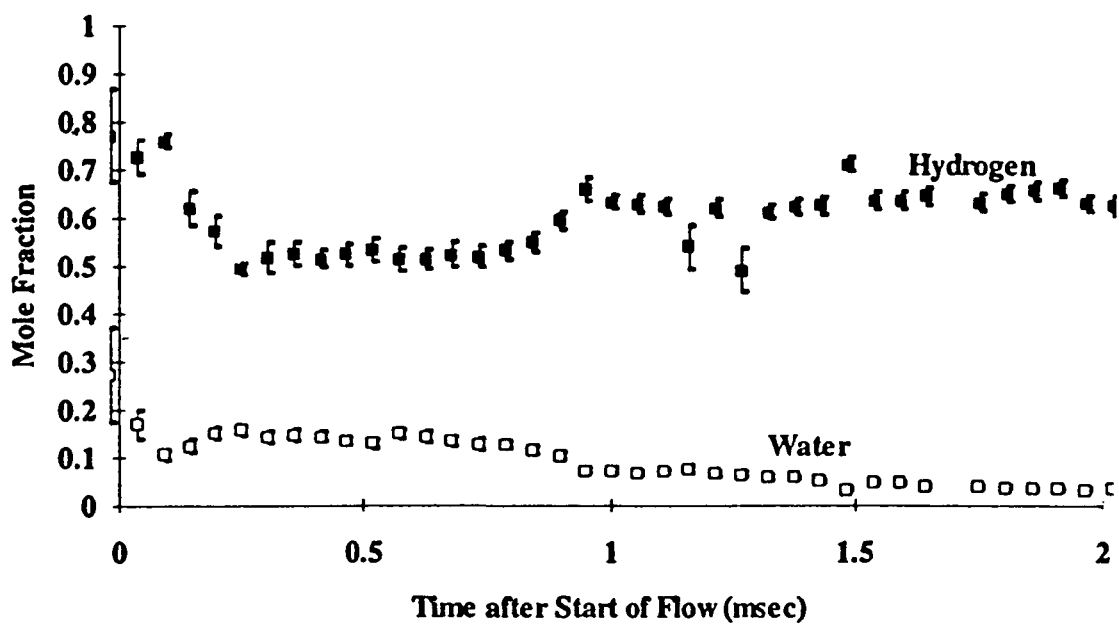


Fig. 3. Mass spectrometer records of hydrogen and water components (stagnation enthalpy = 12.2 MJ kg^{-1} , 10 mm from centre line)

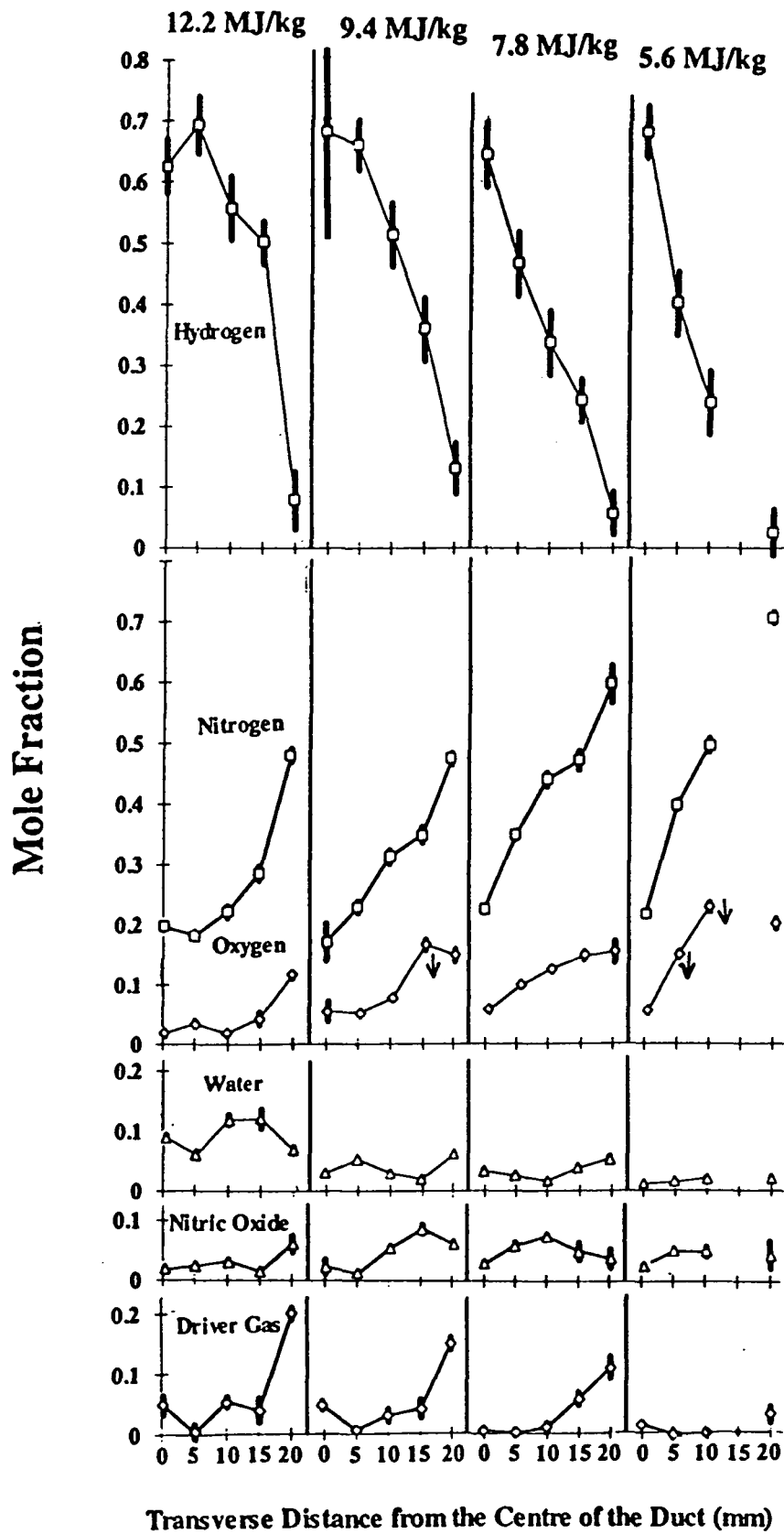


Fig. 4 Species distributions across wake.

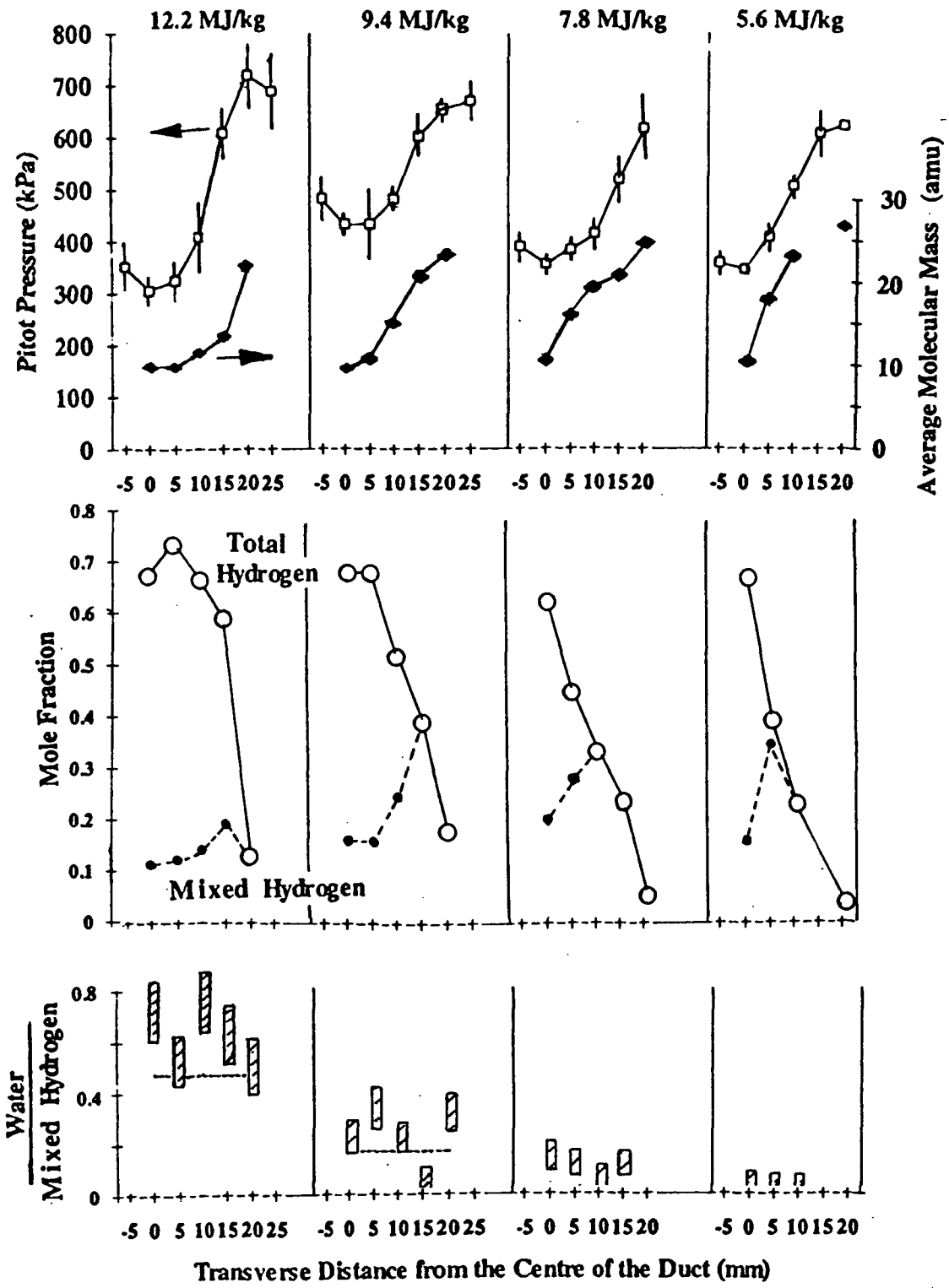


Fig.5 Diffusion of hydrogen and mixing and combustion in wake.
 (Reaction efficiency: \square expt, -----theory.)