SHORT COMMUNICATION

Stretch Effects in High Speed Reacting Mixing Layers

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Abstract—The weak thermal development of a reacting high speed high enthalpy hydrogen-air mixing layer which seems to depart from equilibrium only slightly in terms of reaction rates is analysed through the examination of stretch, and details of chemistry from the direct numerical simulations of the reacting mixing layer with full chemistry. The analysis of these parameters clearly indicates that the peak temperatures and the local composition depart from equilibrium significantly consistent with the high stretch even though the departures of the reaction rates from equilibrium apparently are not large. A serious consideration of chemical non-equilibrium effects in high speed mixing layers is called for.

NOMENCLATURE

Y_i : Mass fraction of species i
p : Pressure
T : Temperature
t : Time
u : Streamwise velocity
v : Transverse velocity
$\dot{w}'''$: Volumetric reaction rate
x : Streamwise coordinate
ρ : Density

INTRODUCTION

Studies on reacting supersonic mixing layers have been encouraged by the recent interest in the development of scramjet combustors. Basic studies, both experimental and computational have been conducted by several investigators (Beech et al, 1972; Jarrèt et al, 1988; Cheng et al, 1991; Drummond and Mukunda, 1988; Sekar and Mukunda, 1990). The experimental studies have concentrated on mixing layers and coflowing jet streams without or with combustion. Though early experimental combustion studies have been conducted at conditions far removed from the realistic high Mach number and high stagnation enthalpy conditions, experiments with higher enthalpies and temperatures have been conducted in recent times. For instance, the fuel temperatures are between 500-800 K and the vitiated air temperatures are around 1200 K (Cheng et al, 1991).

Few computational studies on reacting high speed mixing layers have been conducted. The previous studies with single step chemistry show that exothermic chemistry does not affect the growth of the mixing layer at high speeds (Sekar and Mukunda, 1990). This result is substantially different from that at low speeds where the growth rate of a mixing layer has been shown experimentally to decrease with the extent of heat release by combustion (Hermanson and Dimotakis, 1989). This result has been analysed and it is argued to be related to the reduction of density due to heat release by combustion. Sekar and Mukunda (1990) have showed consistency of these results with those at high speeds by showing that the changes in density due to gas dynamics are more dominant than due
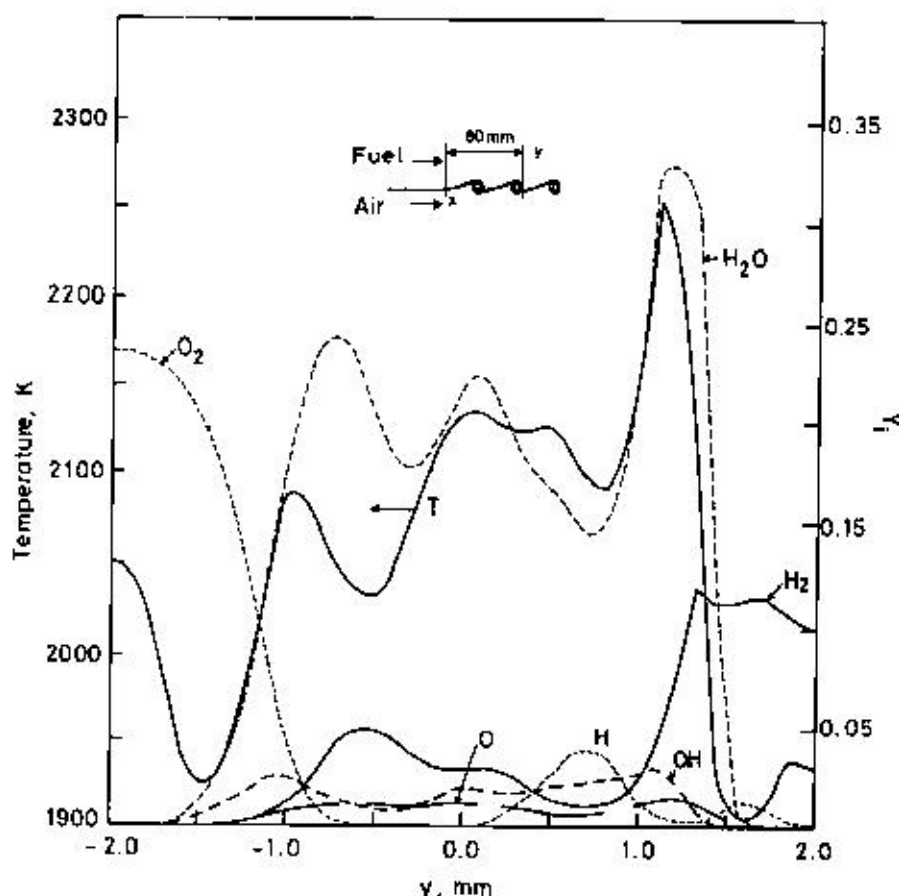
Figure 1 Variation of temperature and specie mass fractions across a reacting mixing layer, $x = 80$ mm downstream of the splitter plate. Inplane temperature is 2000 K at $z = 0$. The region $y > 0$ is fuel stream and $y < 0$ is the oxidant stream.

to heat release by combustion because (a) the compressibility effects make the changes in density significant and (b) the heat release is limited by dissociation processes at high temperatures generally prevalent at high speeds. In this study (Sekar and Mukunda, 1990), the parameters of the single step chemistry were chosen from subsonic premixed flame propagation data. It was shown from full chemistry calculations made later (Sekar et al, 1990) that the development of the temperature profile along the mixing layer is much weaker than expected from single step chemistry. While the causes for the single step chemistry giving a much higher temperature rise form a separate subject of examination the fact that full chemistry results show slow thermal development was considered worthy of study. A possible explanation was that the flame which is generated in the vortical regions is subject to intense and large strain rate. This strain rate can cause significant departures from equilibrium. An opposing consideration was that at these temperatures ($\sim$1500-2000 K) one would expect the reaction rates to be so large that chemical equilibrium must be established early and hence it may not be proper to expect large departures from equilibrium. A literature study showed that these issues
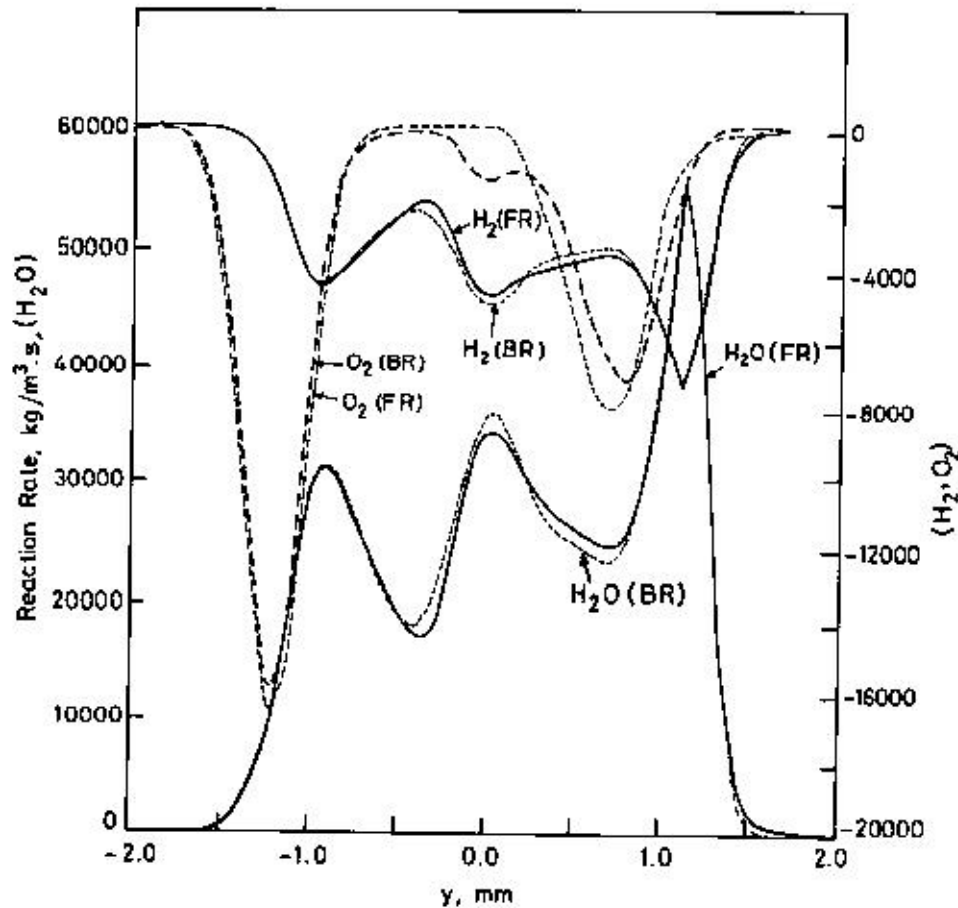
Figure 2 The reaction rates of water vapour, hydrogen and oxygen across the mixing layer.

had not been addressed earlier and therefore, it was thought appropriate to attempt to clarify the issues through an analysis of the results of the mixing layer.

RESULTS FROM MIXING LAYER SIMULATION

The studies reported in Sekar and Mukunda (1990) and Sekar et al (1990) are on mixing layers formed out of streams of fuel (H_2 and N_2 mixture) and air at 2000 K coming off a splitter plate at substantially different velocities the parameters for which are shown in Table 1. The case 1 has equal Mach numbers, but different velocities, but the second case has different Mach numbers and velocities.

The model-free two-dimensional Navier Stokes calculations with hyperbolic tangent initial profiles were carried out with very fine grid resolution to capture the early stages of the growth of the layer. These calculations were made with single step and full chemistry. Full chemistry implies seven species and eighteen reversible steps. The details of the chemistry are available in Drummond and Mukunda (1988). The calculations were carried out in a time accurate mode with disturbances of a small amplitude at the initial plane. Time data of the various quantities were stored after statistical steady state was obtained and the
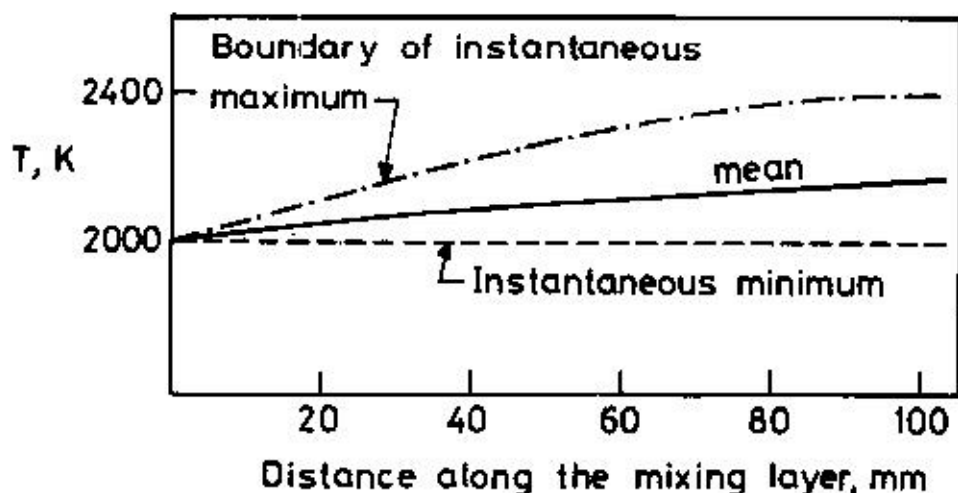
Figure 3   Averaged peak and boundaries of the peak and the minimum instantaneous temperatures along the mixing layer.

TABLE 1.
INFLOW PARAMETERS

composition	quantity	case 1	case 2
	u, m/s	2670.0	same
Fuel	M	2.0	same
$0.1H_2 + 0.9N_2$	γ	1.3133	same
	u, m/s	1814.0	4330.0
Oxidant	M	2.0	5.25
$0.232O_2 + 0.768N_2$	γ	1.296	same
	M_c	0.385	0.76

T = 2000 K, p = 0.101325 MPa

data were analysed for their statistics. The appropriate results from these calculations are presented in Figures 1 and 2. Figure 1 shows the instantaneous plots of temperature and mass fractions of most species across the mixing layer about 80 mm downstream of the splitter plate (this corresponds to about 60 momentum thicknesses). The several humps and valleys in these plots are due to the vortical structure which engulfs the fluids from both the streams. One can have alternate regions of fuel and oxidiser richness and this leads to temperature and concentration profiles which have humps as seen in the figures. A more remarkable feature of the results can be seen in Figure 2 where the reaction rates of H_2O, H_2 and O_2 are plotted. It is seen that the forward and reverse rates are nearly equal and one would infer that the departure from equilibrium is small. The plots of the rates of H, O, and OH (not shown here) also exhibit similar trends. A good estimate of the reaction time is obtained from the inverse of the ratio of reaction rate and density, $[\dot{w}'''/\rho]^{-1}$ as about 3-5 μs and the flow time through the field as (0.1 m / 2200 m/s) = 45 μs. Thus the reaction time is at least ten times as small as the flow time and therefore one would expect chemical equilibrium to prevail. Further, calculations of ignition delay of premixed H_2 - air mixtures by Rogers and Schexnayder (1981) show that the ignition delay for stoichiometric composition of H_2 - air is about 1 μs at 2000

conditions. It may be tempting to conclude that because high temperatures are involved the non-equilibrium effects are insignificant. The present work indicates clearly that such is not the case.

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Table 2
The local mass fractions, temperature and equilibrium temperature

Point	H_2	O_2	H_2O	OH	H	O	N_2	T, K	T_{ad}, K
a	0.0262	0.0291	0.2909	0.0409	0.0115	0.0233	0.5781	2317	3069
b	0.0037	0.0674	0.1320	0.0299	0.0035	0.0256	0.7379	2321	2939
c	0.0301	0.0103	0.3109	0.0349	0.0115	0.0112	0.5911	2546	3047

K. This would imply that if there are no effects other than mixing, then the build up of the temperature profile through the mixing layer should have been much stronger than observed. However, the variation of the mean temperature shown in Figure 3 indicates that the increase in 100 mm of the axial distance does not exceed 100 K. Also the plot of the boundary of the peaks in the instantaneous temperature field shown by dotted lines in Figure 3 indicate peaks no more than 2350 K-350 K from the ambient. The minimum temperature has gone below the ambient essentially due to the expansion waves in the flow. These results imply that the departure of the temperature from equilibrium must be significant or the departure from ambient temperature small.

In order to understand the behaviour, the mass fractions and temperature were sampled at a few points and the adiabatic temperature was calculated. These results are set out in Table 2 for case 1. Points a, b and c in the table correspond to the locations 0.812, 2.132 and -7.303 mm from the centre line of the shear layer.

An examination of the above table shows that the adiabatic temperature is much higher than the local temperature. This means that the composition is still far from equilibrium. The fact that the net reaction rates are relatively small is argued to be a property of high stream temperatures leading to very high reaction rates, whether near or far from equilibrium. The nonequilibrium must have been caused by the large stretch in the flow. The stretch experienced by the flow is estimated from the relation

$$\text{stretch rate} = \frac{\partial u}{\partial s} + \frac{1}{r_f}\frac{dr_f}{dt} \tag{1}$$

where u and s are the velocity and the coordinate along the flame surface. The local radius of curvature of the flame surface (r_f) is defined with respect to the local centre of curvature. In order to determine them, contour plots of temperature are obtained and an isotherm slightly below the peak temperature was chosen as the flame surface and the stretch rate is evaluated from the above expression. Typical value of the $(\text{stretch})^{-1}$ varied from 15-25 μs the lower range of values being found more often in the high Mach number case (case 2). The inverse of the characteristic stretch rate of the flow can be obtained from the ratio of the difference in the velocities of the streams to the mixing layer thickness. This works out to 2.5 μs. The Damkohler number defined by the ratio of the inverse stretch rate to reaction time is about 5-8. This value is so small that nonequilibrium effects can be expected to be very important. The fact that the reaction rates show small differences between the forward and reverse rate though the composition and temperature are significantly different from equilibrium is inferred to be due to the fact that at high temperatures the reaction rates, forward or reverse will be very high and the small differences between them hides the departure from equilibrium. The more obvious difference between equilibrium and the actual state is shown up in the composition and temperatures.

Thus the present work which has considered reacting high speed mixing layers shows explicitly that the weak departures of the reaction rates from equilibrium are due to the very high reaction rates at high temperatures, this result being consistent with the other result that the local composition and temperature are very far from adiabatic equilibrium