Mixing and Reaction at Low Heat Release in the Non-Homogeneous Shear Layer

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Abstract

The effects of freestream density ratio on the mixing and combustion in a high Reynolds number, subsonic, gas-phase, non-buoyant, two-dimensional turbulent mixing layer, have been investigated. Measurements of temperature rise (heat release) have been made which enable us to examine the effect of freestream density ratio on several aspects of the mixed fluid state within the turbulent combustion region. In experiments with very high and very low stoichiometric mixture ratios ("flip" experiments), the heat release from an exothermic reaction serves as a quantitative label for the lean reactant freestream fluid that becomes molecularly mixed. Properly normalized, the sum of the mean temperature rise profiles of the two flip experiments represent the probability of fluid molecularly mixed at any composition. The mole fraction distribution and number density profile of the mixed fluid can also be inferred from such measurements. Although the density ratio in these experiments was varied by a factor of thirty, profiles of these quantities show little variation, with integrals varying by less than 10%. This insensitivity differs from that of the composition of molecularly mixed fluid, which is very sensitive to the density ratio. While the profiles of composition exhibit some similarity of shape, the average composition of mixed fluid in the layer varies from nearly 1:2 to over 2:1 as the density ratio is increased. A comparison of data and available theory for this offset or average composition is discussed.

Introduction

The two-dimensional turbulent shear layer has been the subject of investigation for many years, particularly the gas phase layer with uniform freestream densities. This flow represents one of the simplest in which turbulent mixing occurs between two separate streams. Relatively simple boundary conditions and strong similarity properties combine to make this one of the more attractive flows to experimentalists, theorists and modelers.

Although it has been the subject of study in the past, there are several reasons why the present work focuses on the effects of freestream density ratio on the shear layer. As noted by Brown & Rossho (1974), this knowledge is a necessary precursor to the study of compressibility effects. The renewed interest in supersonic mixing and combustion, combined with the experimental difficulties of producing density matched supersonic shear flows has given a new impetus to the search for an understanding of the effects of the density ratio in these flows. However, this is not to imply that the only interest rests in the connection to compressible flows. In many important engineering applications the shear layer geometry is used to mix reactants or to ignite premixed streams which release large amounts of heat. Optimization of combustion systems used in propulsion and energy "production" roles requires knowledge of the physical mechanisms involved. Again, a study of turbulent combustion with large heat release and therefore large density differences, is aided by an understanding of density ratio effects.

Several investigations in the past have dealt directly with this issue. Brown & Rossho (1971, 1974) performed a series of experiments in subsonic non-homogeneous layers and concluded, contrary to proposals entertained at the time, that the large reductions in spreading rate found in compressible layers could not be attributed to density ratio effects. Based on directly measured concentration fields in shear layers at two freestream density ratios, Konrad (1976) concluded that the composition of the mixed fluid was strongly affected by the density ratio of the freestreams but that for each case it did not vary within the mixing region as expected based on conventional gradient transport modeling. Wallace (1981) investigated the product formed due to mixing and reaction for both density ratios studied by Konrad. By measuring the temperature rise for several values of the freestream reactant concentration, he found the mean composition of the mixed fluid to be in good agreement with Konrad for the uniform density case, but was unable to use the technique for the non-uniform density case.

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Although it did not deal specifically with non-homogeneous flows, there is another study which helped lay the ground work for the present investigation. Koochesfahani & Dimotakis (1986) measured the amount of reaction product in a liquid shear layer at flow conditions comparable to the uniform density case of Konrad. They concluded that the amount of mixed fluid was much less than that found in gas phase shear layers and argued that this difference indicated the importance of the Schmidt number as a parameter. This dependence countered fundamental assumptions in classical analyses of high Reynolds number flow, where the molecular transport coefficients are several orders of magnitude smaller than the effective turbulent transport coefficients.

Of particular interest to this work, they also demonstrated how several quantities could be determined from reacting flow measurements as if directly measured with the requisite resolution. This is one of the motivations for the present work. Breidenthal (1981) noted that in all techniques which attempt to directly measure the composition field, any failure to resolve fully all the features of the flow field leads to an over-estimate for the amount of mixed fluid. As demonstrated by Koochesfahani & Dimotakis, by using the molecular nature of chemical reactions and measuring only the mean value of the product concentration, an estimate can be derived which is conservative.

In 1982 a new facility was completed which permits the investigation of reacting, gas-phase shear flows. This study follows in the wake of the low heat release study (Mungal & Dimotakis 1984), the study of heat release effects (Hermanson 1985, Hermanson et al. 1987), the study of Reynolds number effects (Mungal et al. 1985) and the investigation of Damkohler number effects (Mungal & Frieler 1988). Using the same facility, the present study has extended the range of topics to include the effects of freestream density ratio.

Experiments

The facility consists of a blowdown tunnel described in detail in Mungal & Dimotakis (1984) and Hermanson (1985). Gases are loaded by a partial pressure technique into high pressure reactant tanks. Driven by a large (nearly) constant pressure source, these gases flow during a run through sonic metering valves and into the apparatus test section. In the present experiments, the high-speed flow issues from a 6:1 contraction through a 5x20 cm² exit at a velocity of $U_1 = 22$ m/s. The low-speed flow emerges from a 7.5x20 cm² exit after a 4:1 contraction at a velocity of $U_2 = 8.5$ m/s. These streams enter the test section as shown in Fig. 1.

Experiments involving chemical reaction between mixtures of hydrogen and inert gases in the high-speed stream and fluorine and inert gases in the low-speed stream have been performed. Table 1 contains the detailed composition of each stream for all experiments for which results are presented here. The apparatus allows the use of precise mixtures of gases which have significant density differences, keeping most other relevant quantities constant. The choices of diluent gases allowed experiments to be carried out for the range of freestream density ratios $1/8 < p_2/p_1 < 8$, with the heat capacity of the mixtures carefully matched. Unfortunately, results for $p_2/p_1 > 4$, which could be directly compared to the $p_2/p_1 = 7$ case of Konrad, are not included. We suspect that a new mode of instability, details of which were discussed in Koochesfahani & Frieler (1987), becomes important for large values of the density ratio. Although results for $p_2/p_1 = 4$ show only a hint of the effects, results for higher density ratios were sufficiently different that comparison with "normal" shear layers would be outside the scope of present work. The data presented here cover the range of density ratios $0.136 < p_2/p_1 < 4$, which corresponds to a factor of 30 for that parameter.

![Figure 1. Turbulent Shear Layer Geometry](image-url)

Table 1. Composition details for each experiment.
Based on an estimation technique described in Mungal & Frieler (1988) and refined in Dimotakis & Hall (1987), kinetic rates for these experiments were established to be more than a factor of two higher than the rates at which product formation may be assumed to be mixing-limited. The HF chemical system may be regarded as a fast and hypergolic reaction system, even at low concentrations of reactants and at extreme stoichiometric ratios. This allowed experiments to be performed with the heat release maintained below the threshold suggested by Wallace (1981) and confirmed by Hermanson (1985) and Hermanson et al. (1987), beyond which density changes resulting from heat release begin to affect the fluid mechanics of the turbulent shear layer. At the downstream location where our measurements were made (x = 46 cm) the Reynolds number for these experiments, based on properties of the nitrogen diluent and the velocity difference between the two freestreams, was \( Re = \frac{AU}{v} = 6.7 \times 10^6 \). Here the length \( \delta \) is the reference length scale used throughout the present work and is defined as the distance between the 1% points of the mixed fluid probability profiles, \( p_m(y) \) in Fig. 4. This width has been found to correspond closely to the visual thickness of the mixing region. Measurements of temperature rise were made using a rake of eight resistance wire (2.5 \( \mu \m) thermometers, as described in Mungal & Dimotakis (1984). Run times were 6 seconds with 1.5 second start-up and 4 seconds of data acquisition. Probes were sampled at an aggregate rate of 240 kHz for a total of \( 10^6 \) data points for each run.

In the limit of low heat release, temperature rise measures the number density of product molecules. As a result of the finite heat release in these experiments, however, the number density of molecules is not constant. Because of the careful matching of specific heats, we can still relate the measurements to the amount of product formed in the present experiments. In particular, 
\[
\frac{\Delta T}{n} = \Delta \eta
\]
where \( \Delta T \), \( \eta \) and \( n \) are respectively the temperature rise above ambient, the number density of product molecules and the total number density. Assuming isobaric conditions, the quantities \( \eta \) and \( n \) can be inferred separately from the temperature rise and the perfect gas law, i.e.
\[
\frac{\Delta \rho}{\eta_0} = \frac{\Delta T}{T_0 + \Delta T}, \quad \text{and} \quad \frac{n}{\eta_0} = \frac{T_0}{T_0 + \Delta T},
\]
where \( T_0 \) is the ambient temperature (~300 K) and \( \eta_0 \) is the number density of molecules in the freestreams at \( T_0 \). Fortunately, as argued by Mungal & Dimotakis (1984), the probes used in these experiments produce very accurate measurements of the mean temperatures. Therefore the mean of the ratio \( \frac{\Delta \rho}{\eta_0} \) can be reliably determined, although averages of \( \frac{\Delta \rho}{\eta_0} \) and \( \frac{n}{\eta_0} \) separately will suffer to some degree from inadequate probe resolution.

A sample of the results of a single experiment is shown in Fig. 2. Measured mean temperatures at each of the eight probe locations are indicated by the circles (\( \Delta T_{ave} \)). Fitted profiles are also shown for the mean temperature, mean number density of product \( (\eta_0/n) \) and mean number density \( (n/\eta_0) \).

These curves are of the form
\[
\Delta T(n) = n - (c_0 + c_1 \eta + c_2 \eta^2 + c_3 \eta^3 + c_4 \eta^4)
\]
where \( \eta = y/(x-x_0) \).

**Analysis**

The major concepts involved in the analysis of the data were derived for the laser induced fluorescence (LIF) technique in liquids by Koochesfahani & Dimotakis (1986). Some differences exist, however, which will be described here.

Starting with two distinguishable fluids, we will label the pure fluid from the low speed side as \( \xi = 0 \), and pure fluid from the high speed side as \( \xi = 1 \). We define \( \xi \) as the (conserved scalar) composition, with intermediate values, \( 0 < \xi < 1 \), corresponding to the fraction of high speed fluid in the mixture. If we were able to make measurements with perfect resolution in both time and space, a properly normalized histogram of composition sampled at discrete times would approximate the probability density function (PDF) of composition, \( \Phi(\xi) \). Although laboratory measurements of sufficient resolution can not currently be made in high Reynolds number flows, for the present discussion it is only necessary to accept the existence of the PDF. A conceptual model of the PDF of composition appears in Fig. 3.

Next we apply the change of variables from composition to temperature shown in Fig. 4. This temperature dependence, \( \Delta T(\xi) \), represents the temperature rise above ambient which results from a fast, irreversible exothermic reaction occurring between two fluids containing reactants mixed at a composition \( \xi \) (cf. Bilger 1980). For the chemical system used here, the stoichiometric mixture ratio is equal to the ratio of the freestream reactant concentrations, \( \Phi = c_2/c_1 \).
we then relate the mean temperature, at a specific value of $\phi$, to $P$ we obtain

$$\frac{\Delta T}{\Delta T_f} = \frac{\Delta T}{\Delta T_f} \int_0^\infty \frac{\Delta T}{\Delta T_f} P_\phi(\Delta T) \, d(\Delta T)$$

The second form results from a change of variables from $\Delta T$ back to $\xi$.

There are two interesting limits immediately apparent from this expression. These are the "flip" experiments described in Koochesfahani, Dimotakis & Broadwell (1985). If we let the stoichiometric composition $\xi_0 \rightarrow 1$, then the second integral vanishes and we are left with

$$\frac{\Delta T}{\Delta T_f} \rightarrow \int_0^1 \xi P(\xi) \, d\xi = \bar{\xi}.$$ 

Here $\bar{\xi}$ is the mean composition and also represents the mean high speed fluid mixture fraction. If we let $\xi_0 \rightarrow 0$, the first integral vanishes and we are left with

$$\frac{\Delta T}{\Delta T_f} \rightarrow \int_0^1 (1-\xi) P(\xi) \, d\xi = 1 - \bar{\xi}.$$ 

Here the roles of $\xi = 0$ and $\xi = 1$ have been reversed (i.e. $0 \rightarrow 1/\phi$) and therefore $\bar{\xi} \rightarrow 1 - \bar{\xi}$, which represents the low speed fluid mixture fraction.

It is necessary to consider an aspect of the data which affects this analysis. Previous experimental work (Konrad 1976, Koochesfahani & Dimotakis 1984) demonstrated that there is a finite probability of observing pure fluid from each of the freestreams in the interior of the layer. Consequently, we must admit integrable singularities (delta functions) in $P(\xi)$ at the values $\xi = 0$ and $\xi = 1$. The process of taking the limit in each case above relied on the integrand being finite at these points, though delta functions at any other value of $\xi$ would not pose a problem. Note that measurements of temperature cannot distinguish between pure high-speed or pure low-speed fluid since $\Delta T(0) = \Delta T(1) = 0$. Because the transform introduces an ambiguity at points where the PDF is singular, the connection between mean temperature and mean composition cannot be made. However, since this ambiguity arises from the probability of seeing pure fluid from the lean reactant freestream, it can be avoided if we restrict our attention to the molecularly mixed fluid (compositions $\xi \neq 0, 1$).

We have examined how the mean temperature rise is related to the mean composition. Another useful, though perhaps less precise, interpretation is that in these limits $\Delta T/\Delta T_f$ measures the amount of fluid originating in the lean reactant freestream.
Building on this idea, we can define two reduced
temperature profiles as

\[
\theta_1(y) = \frac{\xi_0}{\Delta T_f} \frac{\Delta T_f(y)}{\xi_0} \leq \int_0^{1-\epsilon} \xi P(\xi, y) d\xi,
\]

and

\[
\theta_2(y) = \frac{1-\xi_0}{\Delta T_f} \frac{\Delta T_f(y)}{1-\xi_0} \leq \int_\xi^{1} (1-\xi) P(\xi, y) d\xi.
\]

An arbitrary small number, \(\epsilon\), has been introduced in the limits of integration solely to indicate that contributions from the pure fluid originating from either stream have been excluded. Note the dependence on the spatial coordinate, \(y\), which appears in these expressions. This dependence was left implicit to the present but will be explicitly included for the remainder of this discussion.

The limits discussed above may now be reexamined. As \(\xi_0\) approaches 1, the equality in the first expression is realized and \(\theta_1\) becomes equal to the amount of high speed fluid which is molecularly mixed. Similarly, in the limit of \(\xi_0\rightarrow 0\), \(\theta_2\) measures the amount of low speed fluid which is molecularly mixed. As shown in Fig. 4, the normalization has been chosen such that for any other stoichiometric composition, \(\theta_1(y)\) and \(\theta_2(y)\) provide conservative estimates for the profile of mixed fluid which originated from the respective freestream.

We can now estimate the probability of mixed fluid at any composition, \(p_m(y)\). In particular, if we add the reduced temperatures we obtain

\[
\theta_1(y) + \theta_2(y) \leq \int_\xi^{1} \frac{\xi P(\xi, y) d\xi}{\xi} + \int_\xi^{1} \frac{(1-\xi) P(\xi, y) d\xi}{\xi} = \int_\xi^{1} P(\xi, y) d\xi = p_m(y)
\]

where this is again a conservative estimate for this quantity. This particular result was introduced in a previous discussion (Dimotakis 1987) in a somewhat more direct fashion. There, the mixed fluid function, \(\theta_m(\xi)\), was defined to be the normalized sum of the temperature rises for the "flip" experiments, i.e.

\[
\theta_m(\xi) = (1-\xi) \left( \frac{\Delta T_f(\xi, \xi_0)}{\Delta T_f(\xi_0)} + \frac{\Delta T_f(1-\xi, \xi_0)}{\Delta T_f(1-\xi_0)} \right).
\]

This transform provides an estimate for the amount of mixed fluid through the relation

\[
p_m(y) \geq \int_0^{1} \theta_m(\xi) P(\xi, y) d\xi.
\]

As shown in Fig. 5, this estimate will be quite good for small values of \(\xi_0\). Note that the figure corresponds to the stoichiometry \(\xi_0 = \xi_0\) at which these experiments were performed. These two approaches are clearly equivalent.
The small systematic differences displayed by these distributions are interesting. They could be a manifestation of the weak effects of finite heat release in these experiments. Note that the density decrease owing to heat release is different for each experiment of the 'flip'. This could rearrange the distribution of the mixed fluid probability slightly for each case and thereby cause the sum of the reduced temperatures to be skewed toward one side. Since this heat release effect is partitioned within each of the flip pairs in a fashion which depends on the density ratio, this could result in the observed systematic trend. It is important to note that although this would reflect on the accuracy of the local distributions, it would not affect their integral values, e.g. \( P_m \). Whether this trend in the profiles is a result of density ratio or the effect of the slight heat release will have to be determined by subsequent experiments.

![Figure 6. Mixed Fluid Probability Distributions.](image)

The mean number density of product and mean molecular number density were also determined for each experiment. The results of adding the number density of product for the flip experiments are the bell shaped profiles shown in Fig. 7. These distributions represent the mean number density of mixed fluid, \( n_m(y) \), within the shear layer. Note the similarity of these distributions despite a variation in the density ratio of a factor of thirty. Their integrals (\( \delta_m \)) shown in the far right column, represent the total amount of mixed fluid expressed as a thickness. The lack of variation with density ratio shown by this quantity is particularly noteworthy, with the mixed fluid fraction, \( \delta_m/\delta \), changing by less than 5%. Also shown in Fig. 7 are the profiles of mean number density for each case. The integrals of molecular number density, \( \delta' \), can be used to estimate the dilatation resulting from heat release. In each case, \( 1 - \delta'/\delta \) is below 0.1, indicating that the average number density in the layer has been reduced by less than 10%. Using the same approximations, the mean number density of mixed fluid can be divided by the mean number density to estimate the profiles of mixed fluid mole fraction. These profiles are shown in Fig. 8. In the far right column is the integral mole fraction of mixed fluid (\( \delta_m \)) determined using this approach.

![Figure 7. Mixed Fluid Number Density and Total Number Density Profiles.](image)

Note the close similarity in the data in Figs. 6 and 8. The mole fraction profile, \( n_m(y)/n(y) \), differs from the mixed fluid probability profile, \( P_m(y) \), only because we have taken the quotient of time averages, rather than the time average of a quotient. The relative insensitivity of these profiles to this averaging process indicates that the statistics are not too pathological. This suggests that possible resolution inadequacies in this work are not serious in this context, and provides support for the approximations used to produce Figs. 6 and 8. Remember that, in the heat release Figs. 6, 7 and 8 would be identical. All four of the integral quantities, \( P_m \), \( \delta_m \), \( \delta_m/\delta \) and \( \delta'/\delta \) are plotted in Fig. 9 versus the freestream density ratio. Note the insensitivity of these quantities to the factor of thirty change in density ratio.

Using the approximations detailed in the analysis section, the mean composition profiles of the mixed fluid, \( \delta_m(y) \), were also estimated. Shown in Fig. 10 are the composition profiles for each of the density ratios investigated. With the exception of an offset or average composition which
the evolution of a "typical" vortex as viewed in its rest frame, Dimotakis envisions $E_v$ as being the volume flux ratio of fluid entering the large scale structure from the freestreams. This ratio is related to both the flux ratio and the composition ratio, and as such, cannot be related rigorously to a function of the field quantities. However, since some models (e.g. Broadwell Breidenthal 1982, Dimotakis 1987) treat the mixing process as being independent of the transverse coordinate and it is precisely in this case that the distinction between flux and composition ratios vanish, a comparison is in order. If we proceed under this assumption and further assume that the fluids mix at the ratio they are entrained, we arrive at a prediction for the average mixed fluid composition, for the present velocity ratio, of

$$E_v = \frac{E_v(r,s)}{1 + E_v(r,s)} = \frac{1.3 \xi^{1/2}}{1 + 1.3 \xi^{1/2}}$$

Shown in the far right column of Fig. 10 are the average mixed fluid composition for each density ratio. A comparison between our inferred experimental values and the theoretical estimate for the average composition versus density ratio, is shown in Fig. 11. It is important to note that, analogous to the integrals of mixed fluid probability, these values are not affected by the heat release as are the distributions. However, the small systematic variation between data and theory could stem from several sources. Most obviously, one could question the basic premise which led to the comparison, that the distinction between flux and composition ratios is negligible. Secondly, there is some evidence based on flow visualization that the fluids may not mix at the same ratio as they exist within the mean boundary of the turbulent region. Still Schlieren photographs indicate that regions within the mixing layer of unmixed fluid increase in size on the light fluid side as density differences increase. Finally, the determination of mixing by chemical reaction implicitly assumes that diffusivities of all the species involved are equal. This is clearly not the case when $H_2$ is one of the reactants. The extent to which these considerations may affect the inferences drawn from these measurements is being investigated.

### Conclusions

Based on the similarity of the profiles in Figs. 6, 7 and 8 we conclude that the distribution of mixed fluid within the two-dimensional shear layer is relatively insensitive to freestream density differences. This is reinforced by the invariance of the integral amounts (Fig. 9) which differ by only 10% for all density ratios investigated. This is not the case for the composition of mixed fluid, which is quite sensitive to the density ratio. The average composition of mixed fluid in the layer varies from nearly 1:2 to over 2:1 as density ratio increases. Small differences notwithstanding, the agreement between theory based on the large structure dynamics and experimental results is compelling evidence for the central role of the large structures in the mixing process.
Our results indicate that simple models can represent several aspects of mixing in a turbulent non-homogeneous shear layer. When normalized by the local width of the mixing region, the distribution of mixed fluid could be modeled as a function of the position in the layer only. Also the composition of the mixed fluid could be represented by an average composition which is qualitatively predicted by theory, multiplied by a function of position only.

References


