

MEASUREMENTS OF DIFFERENTIAL DIFFUSION IN TURBULENT NONPREMIXED FLAMES

B.B. DALLY and A.R. MASRI

Department of Mechanical and Mechatronic Engineering
The University of Sydney, NSW, AUSTRALIA

ABSTRACT

The differential diffusion parameter, $z = \xi_H - \xi_C$ is evaluated using recent single-point data collected in turbulent nonpremixed flames stabilised either by a pilot or on a bluff-body. Measurements are presented for flames of CH_3OH , H_2/CH_4 and H_2/CO fuel mixtures and over a range of jet Reynolds numbers. The effects observed in both bluff-body and pilot-stabilised flames are similar. Differential diffusion is generally found to decrease with increasing jet Reynolds number. The location of the reaction zone is found to be important in separating "hydrogen rich" regions on the lean side from "hydrogen deficient" on the rich side. This is true regardless of the parent fuel mixture. Profiles of mean z and its rms fluctuations are qualitatively similar in mixture fraction space, but in physical space, show a cross stream dependence. These findings are useful for modelling differential diffusion effects in turbulent combustion.

INTRODUCTION

Differential diffusion effects are usually assumed to be negligible in most conventional calculations of reacting and non-reacting turbulent flows. This, along with the unity Lewis number assumption, have been used conveniently by modellers, since they lead to a substantial simplification of the transport phenomena which is then represented by a single conserved scalar that is termed the mixture fraction. They also allow for the use of reduced chemistry to represent the reactive scalar field and substantially reduce the computational cost of turbulent reacting flows. Earlier investigations of differential diffusion in turbulent flames (Bilger and Dibble, 1982 and Drake *et al*, 1984) have concluded that these effects decrease with Reynolds number, and hence their neglect in highly turbulent flow calculations, seemed justified.

Recent advances in diagnostics and computational capabilities have rekindled interest in this issue. Experimental investigations such as those of Drake *et al* (1984) and Smith *et al* (1995) have confirmed

earlier expectations that differential diffusion effects decrease and become negligible at sufficiently high Reynolds number flows. Numerical efforts to model differential diffusion effects in reacting and non-reacting flows have recently been initiated (Kerstein, 1990, Kerstein *et al*, 1995, and Kronenburg and Bilger, 1997). The scaling of the mean and the dominant variance of the differential diffusion variable, defined as $z = \xi_A - \xi_B$, where A and B are conserved scalars, with the Reynolds number has been proposed along with simplified models (Kerstein *et al*, 1995 and Kronenburg and Bilger 1997). These scaling laws were suggested for isothermal flows and their applicability to reacting flows has been questioned (Smith *et al*, 1995).

Current understanding of differential diffusion remains very limited. Correlating it with the Reynolds number is empirical and does not account for the effects of chemical reaction and the nature of the parent fuel mixture. Advanced approaches to turbulent combustion modelling are in principle, capable of accounting for differential diffusion effects. This begs for reliable data for model validation.

In this paper, the differential diffusion parameters are evaluated from experimental measurements conducted in turbulent nonpremixed flames of different fuel mixtures and for a wide range of Reynolds numbers. Flames stabilised on both piloted and bluff-body burners are studied. The effects of parent fuel mixture, chemical reaction, localised extinction and burner geometry on differential diffusion are investigated.

MEASUREMENTS

The differential diffusion data presented here result from single-point Raman-Rayleigh-Laser Induced Fluorescence measurements in pilot and bluff-body stabilised flames. Temperature and the mass fractions of C-H(CH_4 or CH_3OH), CO, CO_2 , H_2 , H_2O , O_2 , N_2 , OH and NO have been measured and the results are reported elsewhere (Dally, 1997 and Masri *et al*, 1996). The full set of data is available on the World Wide Web (Data-base, Sydney University).

Information about the experimental setup may be found in Refs (Masri *et al*, 1996 and Dally *et al*, 1998). Twelve flames, covering a range of fuel mixtures and jet Reynolds numbers are selected here. Details about each of the flames are given in Table 1. Two of the fuel mixtures listed in Table 1

Fuel	Flame	U_J	U_C	Re_J	%BO	ξ_s
CH ₃ OH	PML1	62	15	37080	47	0.135
	PML3	117	"	69430	88	"
	PML3	127	"	74950	95	"
CH ₃ OH	BML1	80	40	23700	55	0.135
	BML3	121	"	35900	84	"
	BML3	134	"	39700	93	"
H ₂ /CO (2:1)	BHC1	134	40	17500	18	0.135
	BHC2	321	"	41990	43	"
	BHC3	536	"	70120	74	"
H ₂ /CH ₄ (1:1)	BHM1	118	40	15800	50	0.05
	BHM2	178	"	23900	75	"
	BHM3	214	"	28700	91	"

Table 1: Summary of the flames studied. U_J is the jet velocity in m/s, U_C is the coflow air velocity in m/s, Re_J is the jet Reynolds number, %BO is the percent of blow off calculated as the ratio of the bulk jet velocity over the velocity at blow off and ξ_s is the stoichiometric mixture fraction. Flames with names that start with (P) are stabilised on a piloted burner while those names that start with (B) are stabilised on a bluff-body burner.

have H₂ as part of the parent fuel. These are H₂/CO and H₂/CH₄. Methanol fuel produces H₂ as a major by-product since it dissociates to H₂ and CO, early in the rich side of the flame.

Accuracy of the Data

The differential diffusion parameter, z , is defined here as $z = \xi_H - \xi_C$, where ξ_H and ξ_C are mixture fractions determined from the hydrogen and carbon atomic balances, respectively. The accuracy of ξ_i and hence z depends on the error associated with each measured scalar. Measurement errors are classified into three types namely: random errors, which include shot and electronic noise and determine the precision of the single-point data; systematic errors, which include the drift of the calibration factors during experiment as well as errors associated with measuring the laser energy on a shot to shot basis; and interference errors, which may be due to a range of sources such as resonant fluorescence, incandescence, luminescence and Raman interference. A more detailed account of the various errors that are associated with the measurement technique used in this work can be found elsewhere (Dally, 1997, and Dally *et al*, 1998).

The error estimates reported below are based on the

random error only. The accumulated error associated with the calculation of the mixture fraction based on the hydrogen (ξ_H) and the carbon (ξ_C) atoms are presented in Figure 1 for two representative flames BML2 and BHC2. This figure shows that the

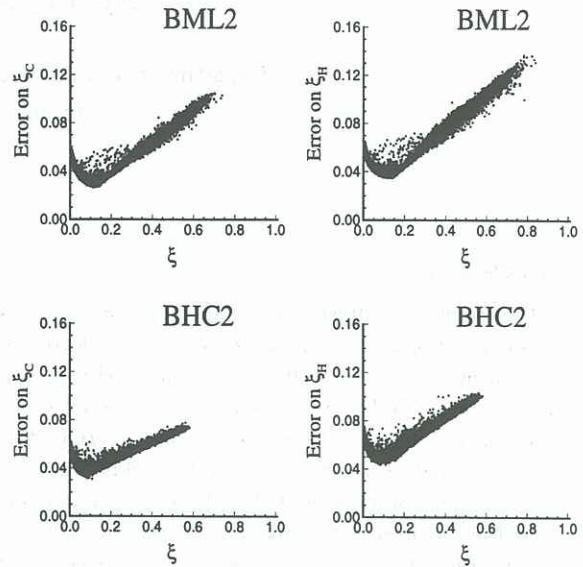


Figure 1: Accumulated error estimates for the ξ_H and ξ_C mixture fractions plotted versus the mixture fraction for flames BML2, and BHC2.

maximum accumulated error for the ξ_C is 15% for the BML2 flame and 10% for the BHC2 flame. The maximum error on the ξ_H is higher at 16% and 14% for the BML2 and BHC2 flames, respectively. These levels are acceptable considering that they compound the random error on all measured reactive scalars.

RESULTS AND DISCUSSION

Instantaneous Data

Figure 2 shows scatter plots of the measured differential diffusion variable ($z = \xi_H - \xi_C$), plotted against the general mixture fraction, ξ , for selected methanol flames that are listed in Table 1. These data are collected at similar axial locations in the various flames. The mixture fraction is calculated using Bilger's (Bilger, 1990) formula which conserves the stoichiometric value of the fuel mixture.

$$\xi = \frac{\frac{2(\xi_C - \xi_{C,O})}{W_C} + \frac{(\xi_H - \xi_{H,O})}{2W_H} - \frac{2(\xi_O - \xi_{O,O})}{W_O}}{\frac{2(\xi_{C,F} - \xi_{C,O})}{W_C} + \frac{(\xi_{H,F} - \xi_{H,O})}{2W_H} - \frac{2(\xi_{O,F} - \xi_{O,O})}{W_O}} \quad (1)$$

where ξ_i is a conserved scalar given by the total mass fraction of element i , and W_i is the atomic mass of element i . Subscripts (F) and (O) denote fuel and oxidant streams, respectively.

Experimental data for piloted and bluff-body stabilised flames with different jet Reynolds numbers

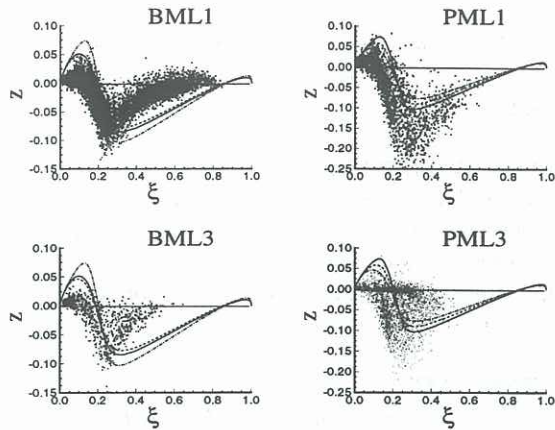


Figure 2: Scatter plots of the instantaneous measured z and the values calculated for laminar counterflow flames plotted versus the mixture fraction for the methanol flames. Black dots denote experimental data, dashed-dotted lines denote low stretch rate, 5 s^{-1} , solid lines denote intermediate stretch rate, 400 s^{-1} and the dashed lines denote high stretch rates, 800 s^{-1} .

are plotted. Also plotted on the same figure is the z value calculated from counterflow laminar diffusion flame simulations for three different stretch rates. These calculations define the extreme case of full differential diffusion in contrast to $z=0$ line which represents the equal molecular diffusion case. The calculated z profiles for the laminar flames of the same fuel mixture are weakly dependent on the stretch rate. Differences in the computed peak values of z at different stretch rates depend on the stoichiometric mixture fraction values and the chemistry of the fuel mixture.

Peak differential diffusion in both piloted and bluff-body flames is found at $\xi = 0.25$ which is the region where pyrolysis products, H_2 and CO , peak. A good agreement between the measured and computed values of z in these flames is seen for data in the range of $\xi \leq 0.5$. For $\xi > 0.5$, measurements show very little differential diffusion while the calculations show negative z values up to $\xi = 0.85$. In agreement with previous observation in similar flows the z value decreases with increasing of fuel jet Reynolds number. For flames BML3 and PML3, which are close to blow off, a significant number of data points lie on the $z = 0$ line. This is due to significant local extinction in these flames resulting in non-reactive mixtures of fuel and air. Such mixtures will naturally have $z = 0$ because there is only one component in the parent fuel.

It is clear from figure 2 that the geometry of the burner has minimal influence on the differential diffusion distribution in the mixture fraction space. On the other hand, other factors which can affect the differential diffusion, such as fuel pyrolysis and

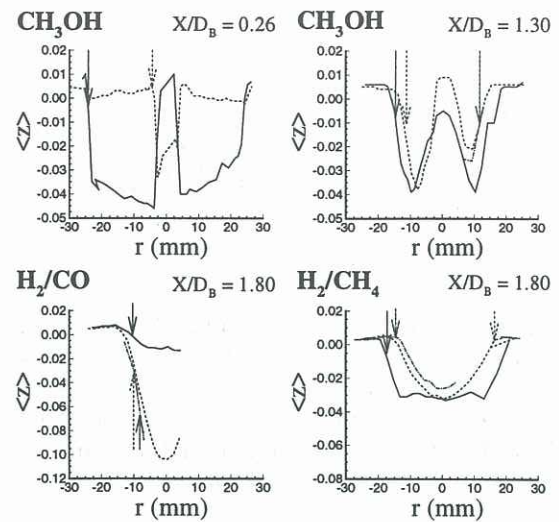


Figure 3: Mean differential diffusion variable plotted versus the radial distance for two axial locations in all bluff-body flames.

jet Reynolds numbers are found to be of great importance.

It is noteworthy that, for methanol fuel, similar results are obtained for the differential diffusion variable defined using the ξ_O conserved scalar ($z = \xi_H - \xi_O$).

Scatter plots for the H_2/CO and H_2/CH_4 flames are not shown here as these were reported earlier in Ref (Dally and Masri, 1997). Scatter plots of z for flames of H_2/CH_4 fuel mixture exhibit similar behaviour to those evaluated using the laminar flame calculations. On the other hand, the z values for the H_2/CO flames are substantially different from those of laminar flame calculations. This difference is not fully understood and more work is needed to resolve the discrepancy.

Averaged Data

Most of the previously proposed models for the differential diffusion effect, require the knowledge of the mean and the rms fluctuation of the differential diffusion variable. Four different quantities were considered in the past, namely: the ensemble mean, $\langle z \rangle$, its rms fluctuation, z' , and the conditional mean and its rms fluctuations, $\langle z|\xi \rangle$ and $\langle z'|\xi \rangle$.

Figure 3 shows radial profiles of mean differential diffusion variable, $\langle z \rangle$ plotted for selected axial locations in the H_2/CO , H_2/CH_4 and CH_3OH bluff-body flames. The axial location at $X/D_B=0.26$ is inside the recirculation zone, while the second profile is located outside the recirculation zone at $X/D_B=1.30$ for the methanol flames and at $X/D_B=1.80$ for the other flames. Flames BHC1, BHM1 and BML1 are plotted with solid lines, flames BHC2, BHM2 and BML2 are plotted with dashed lines while BHC3, BHM3 and BML3 flames are plotted with dashed-dotted lines. It is clear from this figure that the z variable distribu-

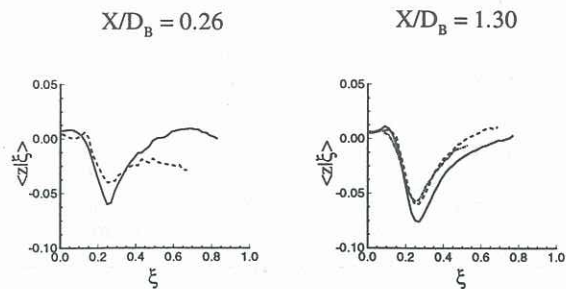


Figure 4: Conditional mean of the differential diffusion variable with respect to the mixture fraction plotted versus the mixture fraction for the methanol flames at two axial locations. Solid lines for BML1 flame, dashed lines for BML2 flame and dashed-dotted lines for BML3 flame ($X/D_B=1.3$).

tion has a high cross stream dependence which can be directly related to the mixing and reactive fields. Marked on this figure, with arrows, are the locations of the mean stoichiometric mixture fraction for the various flames. It is noticed that, in all flames, the $\langle z \rangle$ variable is mainly positive in the lean side of the reaction zone and tends towards negative values on the rich side of stoichiometric. This implies that the location of the reaction zone dictates the differential diffusion pattern regardless of the fuel mixture. Regions on the lean side of the flame are, mainly, "hydrogen rich" while those on the rich side are "hydrogen deficient". It should be noted that this behaviour is obtained for piloted as well as bluff-body stabilised flames.

Conditionally averaged mean and rms fluctuations of z with respect to the mixture fraction are needed for modelling the differential diffusion using the Conditional Moment Closure (CMC) approach. Figure 4 show profiles of $\langle z|\xi \rangle$ plotted against the mixture fraction at two axial locations for flames BML1, BML2 and BML3. It is clear from this figure that the profiles collapse irrespective of the jet Reynolds number or the location in the flame. Profiles of $\langle z|\xi \rangle$ and $\langle z'|\xi \rangle$ for other flames of the same fuel mixture investigated here (not shown) also collapse regardless of the Reynolds number and the position of the reaction zone. This is useful for modelling differential diffusion with the CMC approach.

CONCLUSIONS

Differential diffusion effects observed in turbulent piloted as well as bluff-body stabilised nonpremixed flames are consistent and, in the majority of cases, decrease with increasing Reynolds number. Transition in differential diffusion from "hydrogen rich" to "hydrogen deficient" regions along a given radial profile depend on the location of the reaction zone and appear to be independent of the parent fuel mixture. The mean and rms fluctuation of the differential diffusion have a cross stream dependency

but show similar profiles in mixture fraction space regardless of the axial location and jet Reynolds number.

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