Advanced laser diagnostics in combustion for prototype and modelling development

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ABSTRACT

This paper addresses the questions of how advanced laser diagnostics for the measurement and imaging of scalar quantities are helping in the development of new high-performance combustors and engines. Such diagnostics have greatly improved our understanding of combustion processes but their early promise for aiding more directly the development process are perhaps unfulfilled as yet. Some examples of the direct use of these diagnostics in the development of prototype engines and combustors are reviewed. It is concluded that most applications are still in the realm of the research laboratory, but that there may be an opportunity for commercially-hardened systems for use in routine development in the automotive industry. The alternative approach of using the diagnostics to improve the modelling of combustion used in computational fluid dynamics (CFD) codes is also discussed. Such codes are already widely used in prototype development for prediction of flow and mixing processes in engines and combustors. At present they are not capable of quantitatively predicting for practical combustors the effects of coupling between the flow and combustion such as those involved in pollutant formation and in flame-stabilisation, extinction and ignition processes. Joint Rayleigh/Raman/LIF measurements in turbulent jet diffusion flames and bluff-body flames of gaseous fuels are, however, providing accurate and challenging data bases for validation of advanced combustion models. Interaction between the diagnostic measurements and the modelling is the subject of an important series of international workshops. Models such as Monte-Carlo simulation of the PDF transport equation and Conditional Moment Closure are proving to have considerable success in predicting these data and the application to practical systems is likely in the near future. Advanced laser diagnostics are now capable of addressing questions of flame structure in turbulent premixed flames. It is necessary for combustion models to be based on valid concepts of flame structure. Recent measurements with joint planar Rayleigh scattering and PLIF for OH and of joint PIV and PLIF for OH indicate that considerable revision of the concepts and bounds for regimes of flame structure may be necessary.

1. INTRODUCTION

Laser-based methods of measurement in flows have been developed intensively over the last 30 years. They have had a particularly significant impact in combustion. This is because intrusive probe methods have been of very limited usefulness due to the extreme hostility of their environment. Our understanding of flame structure and combustion processes has advanced quite wonderfully over this time and this hugely complex subject has developed from being a "black art" into an emerging engineering science. This conference series has always had a substantial contribution from the combustion community and I am very grateful to the organisers to have the opportunity to give this invited plenary lecture.

It is not my purpose here to give a broad overview of laser diagnostics in combustion. Indeed, I am not competent to do so. Furthermore, Wolfrum (1998) has recently done a superb job in this regard, covering the whole field from the basic science and spectroscopy of the many diagnostic methods through to applications to elementary reaction mechanisms, laminar and turbulent flames, engine combustion and combustor control. I will confine my scope to the application of laser-diagnostic methods to prototype combustor development and to the development of combustion models for use in Computational Fluid Dynamic (CFD) predictions of combustion systems. I address the question: "how is laser diagnostics helping in the development of better combustion systems?" I leave aside velocimetry, except where its joint use with scalar measurements has been useful. I will also leave aside the application of lasers to combustion control: Wolfrum (1998) gives a good entry to this area.

As the terminology "laser diagnostics" implies, the original concept was that these laser methods would not be just for laboratory science but would be applied directly to engineering measurements in prototype combustors. A long held principle of engineering has been that objective measurement will speed development even if the process itself is not well understood. Such was the goal held out to counter early criticism that the techniques were expensive and largely confined to small laboratory burners. As the difficulties of making worthwhile measurements in prototype engines became better understood, some of us held out the alternative goal of using measurements in somewhat larger laboratory burners to help the formulation and validation of improved combustion models for use in CFD codes. Where are we along that route? Has that route been outflanked by a resurgence in direct measurement in prototype engines and combustors? I address this last question first and then review recent work on model validation using laser measurements and on improving our understanding of flame structure.

2. MEASUREMENT IN PROTOTYPE ENGINES AND COMBUSTORS

Zhao and Ladommatos (1998a) give a recent review of the use of laser diagnostics for measurements of in-cylinder mixture formation in IC engines. Rayleigh scattering, spontaneous Raman scattering, laser induced fluorescence have all been widely used for measurement of fuel vapour concentration while laser induced exiplex fluorescence has been used to simultaneously image both liquid droplets and vapour concentration (see also Bruneaux *et al*, 1999).

Gold, *et al* (2000) report results of collaborative work between Imperial College and Rover on measurements in an optical engine, based on the Rover K16 design, using planar laser-induced fluorescence (PLIF) to measure fuel vapour concentration. Measurements of air flow were made with laser Doppler velocimetry (LDV) and the velocity and size distribution of the fuel droplets with phase Doppler anemometry (PDA). Mie scattering from the fuel droplets was used to visualise their location. The effect of various port injection strategies and other design variables on the mixture formation were studied. Figure 1 shows the sort of results reported. The measurements also gave insight into sources of cycle-by-cycle variability. Greenhalgh and his colleagues at Cranfield University have used four-dimensional (several laser sheets at successive times) PLIF imaging to study mixture formation in the Honda VTECT-E stratified charge engine (Greenhalgh, 1996; Berckmuller *et al*, 1996, 1997). PLIF of nitric oxide, NO, was used to measure recycled end gas concentrations. Spontaneous Raman scattering also continues to be used to study these questions (Hinze and Miles, 1999)

The rapid development of a whole range of exciting new reciprocating engines such as gasoline direct injection spark ignition (GDI or DISI) engines (Takagi, 1998, Zhao *et al*, 1999) and homogeneous charge compression ignition (HCCI) engines has relied heavily on the use of such advanced laser diagnostics to study and gain understanding of the mixture formation process within the cylinder (Drake *et al*, 1996; Richter *et al*,1999).

Measurement of pollutant formation in prototype engines is also feasible although most work has been done so far in laboratory (rather than prototype) engines. PLIF has been used to measure crevice hydrocarbons in a four-stroke SI engine (Marran *et al*, 1998). Measurement of soot concentration and particle size in diesel engines by light scattering and extinction and in imaging using laser scattering and laser induced incandescence (LII) has been recently reviewed by Zhao and Ladommatos (1998b). Dec (1997) has used such measurements to develop a new conceptual model for the ignition and combustion of the fuel spray in direct injection diesel engines. PLIF measurements of NO formation have been carried out in SI engines (Hildenbrand *et al*, 1999) and compared with various numerical models (Josefsson *et al*, 1998; Schultz *et al*, 1998).

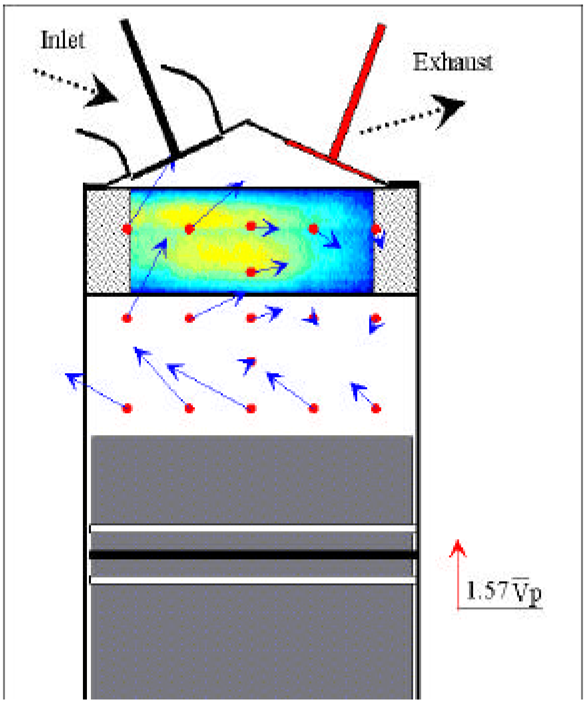

Figure 1. Fuel vapour concentration measured by PLIF and velocities measured by LDV in an optical engine at 270°CA with closed valve port injection of the fuel (Gold *et al*, 2000).

For gas turbines Greenhalgh *et al* (1996) have used PLIF imaging of fuel to study pre-mixing of the fuel and air in a laboratory lean premixed prevapourized combustor and of the spray in a liquid-fueled combustor. Correa (1998) holds that direct use of lasers in prototype development have not made a significant impact as far as the gas turbine is concerned. He asserts that the major contribution from laser diagnostics has been in advancing concepts of flame flow interactions in a qualitative way.

Smith *et al* (1998) and Parham *et al* (2000) have used PLIF of dyes to characterise the mixing process in water flow models of a novel coal-fired precessing jet burner that gives low NO_x emissions when used in cement kilns and other furnaces. PLIF of OH has also been used in a mechanically precessed version of the burner fired with natural gas (Reppel *et al*, 1999). Results at three different phase angles are shown in Fig. 2. St is the Strouhal number formed from the rotation frequency, the jet diameter and the jet exit velocity.

These few examples of the use of advanced laser diagnostics in engine and combustor development do not constitute a comprehensive survey. They are enough, however, to give the flavour of what advanced laser diagnostics are being used for in this area. It is evident that the techniques are still in the realm of the research laboratory and not yet in use as an engineering development tool in the prototype development department. They are being used to develop an understanding of the mixing and combustion processes, rather than as a routine aid to development. The systems are custom built and need PhD level graduates to install, tune and operate them and to interpret the results. Interest from the automotive industry appears to be strong and there may be an opportunity for a commercially-hardened system to be marketed for routine development use. Others will be better able to judge whether this prospect is realistic and what the specification of such a system might be. It seems unlikely, at present, that such commercial systems will become available soon for gas turbine and furnace combustors.

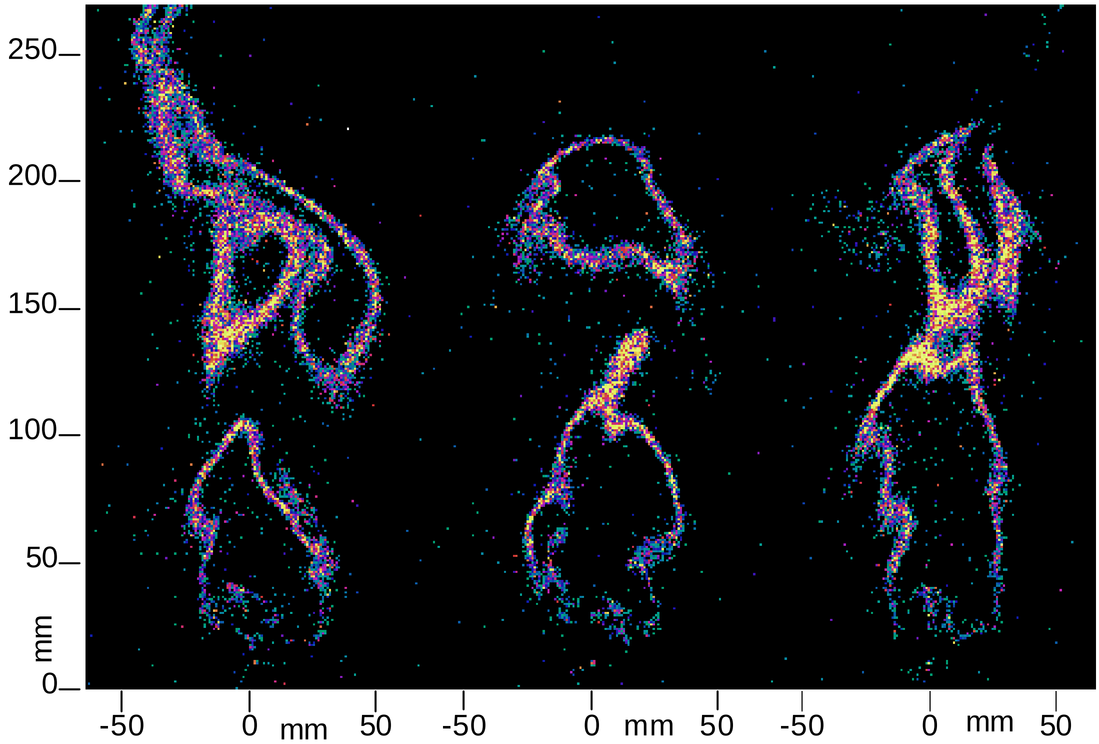

Figure 2. OH distributions measured by PLIF in the flame from a mechanically precessed natural gas jet (Re ~ 2500, St = 0.016) rotating at 80 Hz (Reppel *et al*, 1999)

3. MEASUREMENTS FOR VALIDATION OF COMBUSTION MODELLING

I will be concerned here primarily with measurements made for the improvement of modelling for finite rate kinetic effects using combustion models incorporated in Computational Fluid Dynamic (CFD) codes. Such models are needed for the prediction of autoignition in diesel engines and lean premixed prevaporised gas turbines, for prediction of flame stabilization and extinction and for prediction of pollutant formation and emissions.

Modelling methods for premixed systems have been recently reviewed by Brewster *et al* (1999). Bray (1996) and Libby and Williams (1994) review turbulent combustion modelling in general. The major problem of interest is to account for turbulence-combustion interactions. The major approaches of current interest are laminar flamelet methods, Monte-Carlo simulation of the joint probability density function equations (MC-PDF) and conditional moment closure (CMC). In laminar flamelet methods (Peters, 1986) the combustion is assumed to equivalent to an ensemble of stretched laminar flamelets. In MC-PDF methods (Pope, 1985) the fluid processes are simulated by an ensemble of stochastic particles that are convected with the flow and undergo reaction and molecular scale mixing. In CMC (Klimenko and Bilger, 1999), equations are solved for conditional averages and higher moments of species mass fractions and enthalpy, the conditioning variable being the mixture fraction in non-premixed systems. In systems with little fluctuation about the conditional average due to local extinction and ignition, the closure for the conditional average reaction rate terms can usually made at the first moment level. These methods potentially can handle the large detailed kinetic schemes that are needed to adequately model CO, NO_x and soot.

CFD calculations for finite-rate kinetic effects in turbulent combustion include many other sub-models for the other processes involved such as for turbulent momentum exchange, mixing and radiant heat transfer. In order to properly validate the modelling it is necessary to have comprehensive data sets of high quality that measure as many of the velocity and scalar variables as possible at many spatial positions, including the boundary conditions. Only in this way is it possible to properly validate the combustion modelling: one needs to get the right answers for the right reasons - not because a deficiency in one sub-model is compensated for by a balancing deficiency in another sub-model. To this end it is helpful to have experiments which are not too complex from the flow point of view, that is, the flow structure is one that can be expected to be well modelled for the velocity and mixing field by well-established turbulence models.

For non-premixed combustion, the jet diffusion flame and piloted jet diffusion flame have become established as model problems for addressing issues of modelling finite-rate kinetics effects. Turbulence modelling for such flows is well established. Single-shot point measurements using joint Rayleigh and spontaneous Raman scattering provide accurate results for major species mass fractions and temperature together with simultaneous LIF measurements for OH and NO. Masri *et al* (1996) review the earlier work in this area. Recent improvements in laser systems have led to further improvements in the quality of the data, including measurements of the velocity field and radiation losses. These data bases have become the focus of a series of international workshops on turbulent non-premixed flames (web site: http://www.ca.sandia.gov/tdf/Workshop.html).

Early workshops were concerned with nitric oxide formation in turbulent jet diffusion flames of hydrogen and hydrogen diluted with helium for which comprehensive data is available for the scalars (Barlow and Carter, 1994, 1996) and for the velocity field and radiation loss (Flury and Schlatter, 1997). Detailed comparisons of predictions of these flames by MC-PDF and CMC modelling have been made (Smith *et al*, 1995; Barlow *et al*, 1999) with generally satisfactory results being achieved. Radiation effects are significant for the undiluted flames but are well predicted using an optically thin assumption. Chen, *et al* (1995) present further MC-PDF results for these flames. Kronenburg *et al* (1998) show that second order effects on the CMC closure of the reaction rate for NO are not large but do improve the predictions. Kronenburg and Bilger (2000) make CMC predictions for differential diffusion

Figure 3. Piloted diffusion flame burner (Barlow and Frank, 1998a).

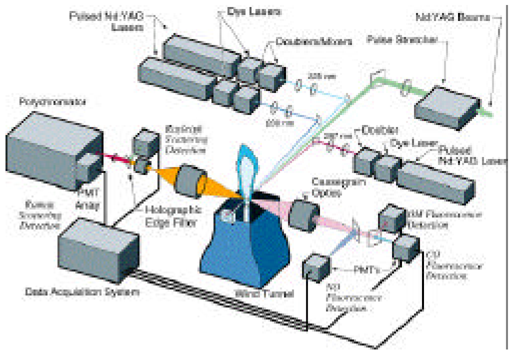

Figure 4. Optical diagnostics for Raman/Rayleigh/LIF measurements (Barlow and Frank, 1998a)

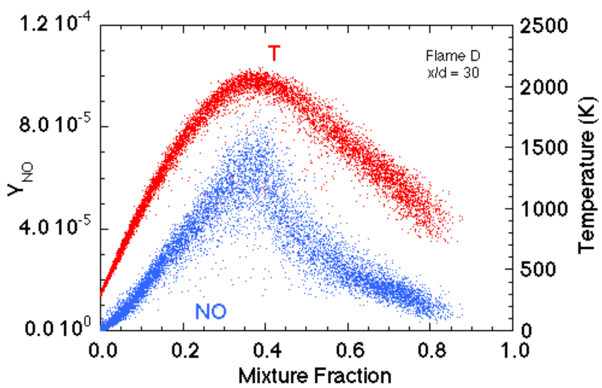

Figure 5. Scatter plot of temperature and NO mass fraction versus mixture fraction in Flame D (Barlow and Frank, 1998a).

effects on NO formation. Data on turbulent jet diffusion flames of H_2-N_2 mixtures is also available through the workshop web site quoted above. Data on $CO/H_2/N_2$ flames (Barlow *et al*, 2000) and on $CH_4/H_2/N_2$ flames are also available through the workshop web address.

Current interest is focussed on the prediction of CO, NO and local extinction in piloted jet flames of partially premixed methane-air mixtures (Barlow and Frank, 1998a). Figure 3 shows the burner used and Fig. 4 the diagnostics set up. Typical results obtained are shown in Fig. 5 for temperature and NO mass fraction plotted as a function of mixture fraction. Data are available for six flames A-F ranging from a laminar flame, A, to a turbulent fame, F, that shows considerable effects of local extinction. Flame D, results for which are shown in Fig. 5, is fully turbulent and plotting of the results versus mixture fraction shows that most of the fluctuation in temperature and species mass fractions are associated with fluctuations in the mixture fraction. A curve drawn through the middle of these plots would correspond closely to the conditional average of temperature and NO mass fraction conditional on the mixture fraction. It is seen that there is relatively small scatter about these conditional average curves. For Flame A, the scatter is somewhat less and corresponds to the uncertainty in the measurements. In Fig.5 the increased scatter is due to turbulence chemistry interactions. In Flame F the scatter is much larger and is indicative of local extinctions. Data for all flames in the form of conditional averages as a function of mixture fraction and conditional rms fluctuation from the conditional average is available at the web address quoted above. Unconditionally averaged data is also available. Prediction of the conditional averaged data is a more useful test of the modelling validity since it is less sensitive to errors in prediction of the mixing field than are predictions of the unconditional averages.

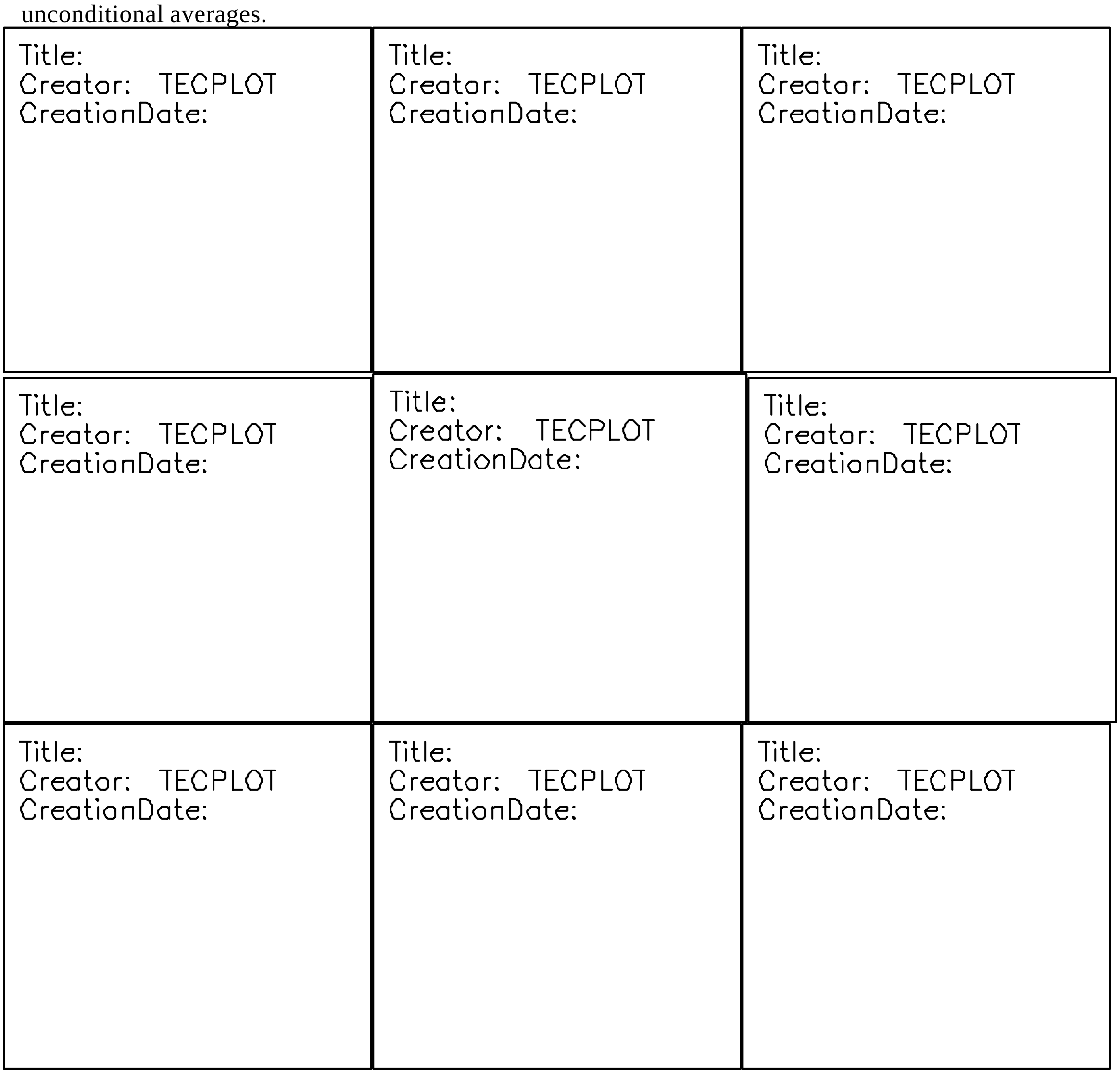

Figure 6. CMC predictions (full curves) of Roomina (1998) versus conditional averages (points) measured by Barlow and Frank (1998a) for Flame D at 30 diameters from the jet exit.

Figure 6 shows CMC predictions for Flame D obtained by Roomina (1998) using first-order closure for the conditional chemical reaction rate terms. The results shown are for a large kinetic mechanism using 49 species and 279 reactions and a radiation model that assumes that the flame is optically thin. It is seen that the predictions are quite good except that NO is somewhat over predicted. There is also some over prediction of fuel conversion to CO and H_2 on the rich side of the reaction zone. The predicted radiation loss from the flame is much higher than that measured and indications are that the 4.3 micron band for CO_2 is not optically thin. More recent calculations by the MC-PDF method (Tang *et al*, 2000) using a 19 species, 15 reaction augmented reduced mechanism show even better agreement for CO and NO and also give good results for Flames E and F where local extinction is extensive.

A further model problem of interest in the turbulent non-premixed flame workshop series is the bluff-body stabilised non-premixed flame as comprehensively measured for various fuels by Dally *et al* (1998). Although the flow field here is much more complex than in the jet flames and is not well predicted by conventional turbulence models, this problem allows the question to be addressed of whether the combustion models can perform satisfactorily in more complex recirculating flow fields. Kim *et al* (2000) report CMC predictions for the case with methanol fuel that show generally satisfactory agreement for the major species and temperature. The computation is carried out for a grid of 72×52 in physical space and 40 nodes in mixture fraction space. Computer memory and CPU time requirements are not overly large and indicate that fully 3D predictions will be feasible soon.

CMC predictions of soot formation in turbulent jet diffusion flames have been made by Kronenburg *et al* (2000) including the effects of differential diffusion which are quite significant. Good agreement was found with extinction measurements made in methane jet flames (Brookes and Moss, 1999) at one and three atmospheres pressure. Measurements with laser induced incandescence (LII) together with Rayleigh/Mie scattering as has been done in ethylene flames (Tait and Greenhalgh, 1993) in such flames would be valuable. Unfortunately, the "mixture fraction probe" of spontaneous Raman scattering, that has been of such great benefit in the study of non-sooting flames, is not available here. New techniques for point measurement and imaging of mixture fraction in sooting flames would be very beneficial.

Detailed measurements in premixed turbulent flames are beginning to appear, e.g. Barlow and Frank (1998b). These measurements will be of great value when the capability of modelling turbulent premixed combustion has been advanced sufficiently for prediction of pollutant species such as CO and NO_x to be possible. CMC modelling for premixed turbulent flames has been outlined (Klimenko and Bilger, 1999).

Advanced laser diagnostics can also be of help in advancing turbulence models for prediction of flow fields and mixing. Conventional Reynolds stress and k-e models do not do an adequate job in flows with swirl and recirculation. Measurements such as those of Gold *et al* (2000) and Dally *et al* (1998) will be of value in validating advanced turbulence modelling techniques. PDF methods appear to be showing advancement in such modelling (Van Slooten and Pope, 1999; Masri *et al*, 2000) for swirling flows. Direct measurement of turbulence quantities such as scalar fluxes (Kalt *et al*, 1998) using joint particle imaging velocimetry (PIV) and LIF for OH can be of help in developing new modelling approaches (Kalt and Bilger, 2000).

4. MEASUREMENT OF FLAME STRUCTURE

Assumptions about flame structure are inherent in any combustion model for turbulent combustion. Many of these models assume that the flame is that of a stretched laminar flamelet (Bray, 1996). For this modelling to be valid it is necessary that the flame be thin compared with the Kolmogoroff scale of the turbulence, $h \equiv (n^3/e)^{1/4}$, where n is the kinematic viscosity of the fluid and e is the rate of dissipation of the turbulence kinetic energy. For non-premixed flames the mixture fraction gives a good measure of the mixing scales and the theoretical basis for the existence of flamelets is on firm ground (Bilger, 2000). For premixed flames there is considerable uncertainty in the definition of the length scale to be used for the flame thickness and experimental evidence from advanced laser diagnostics (Mansour, 1999; Chen and Bilger, 2000) is playing an important role in clarifying the limits of flamelet modelling validity and the development of new modelling concepts.

Figure 7 shows a substantial revision of the usual premixed turbulent flame structure diagram (Bray, 1996) as recently proposed by Chen and Bilger (2000) on the basis of measurements with advanced laser diagnostics. Here d_{th} is the "thermal slope thickness" of an unstrained planar laminar flame defined from the maximum temperature gradient in the flame, S_L is laminar burning velocity for the unstrained planar laminar flame and q' is the rms velocity fluctuation of the turbulence and L_I its integral length scale. The Karlovitz number, Ka, is defined by $\mathrm{Ka} \equiv \frac{q' d_{th}}{l S_L}$, where l is the Taylor microscale for the turbulence defined such that $e = 15 n \left(\frac{q'}{l}\right)^2$, and the Damkohler number Da is defined by $\mathrm{Da} \equiv \frac{L_I S_L}{q' d_{th}}$. The nominal flame thickness, d, is defined as d ° v/S_L and is much smaller than d_{th}. Figure 7 is constructed for $d_{th} S_L/n = d_{th}/d = 10$, a typical value in laboratory flames.

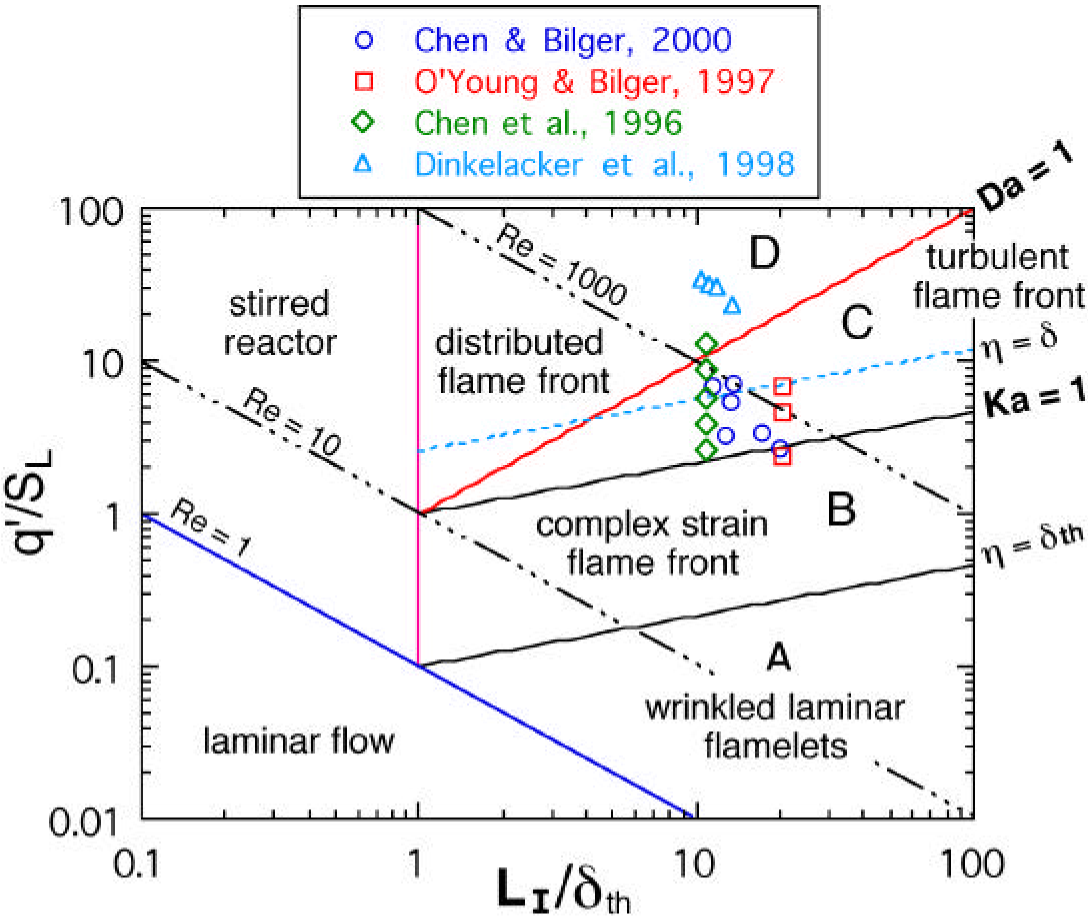

Figure 7. Regime diagram for turbulent premixed combustion as proposed by Chen and Bilger (2000).

A major departure from the usual diagram of this sort is that the limit of the wrinkled laminar flamelet regime, A, is at the well-known Klimov-Williams criterion, but for $d_{th}/h = 1$, rather than $d/h = 1$. This makes a considerable difference, as can be seen in Fig. 7, and means that most turbulent premixed flames in practical systems are not validly modelled by laminar flamelet models. In addition, a new regime, B, with flame fronts subject to complex strain fields is proposed for the region between d_{th}/h = 1 and Ka = 1. In this regime the flame structure appears to be that of a wrinkled thin flame but there are strong departures from relationships to the progress variable, C, that pertain in stretched laminar flames. Measurements with planar Rayleigh scattering (O'Young and Bilger, 1997; Chen and Bilger, 2000) show that magnitudes of the scalar dissipation $a\nabla C \cdot \nabla C$ and scalar diffusion $a\nabla^2 C$ are considerably altered (usually much reduced). Measurements of the slip velocity (the difference in the conditional average velocity in the products and reactants, Bray, 1996) by joint particle imaging velocimetry (PIV) and PLIF for OH (Frank *et al*, 1999; Kalt *et al*, 1998) are much below those for stretched laminar flames. Furthermore, OH concentrations measured by PLIF (Chen and Bilger, 2000) are found to increase from subflamelet values to superflamelet values in this region.

In the turbulent flame front regime, eddies of the order of the interaction length scale, l_m, thicken and contort the local instantaneous flame front which is wrinkled by eddies of larger scale. Here, $l_m / d_{th} = \left(q' / S_l \right)^{3/2} \left(L_I / d_{th} \right)^{-1/2}$. When the interaction length scale grows to be the same order as L_I then Da≈1 and above this bound the instantaneous flame front will occupy essentially all of the volume of the turbulent flame brush.

Further work is required to fully explore and validate the criteria proposed in this new flame regime diagram. It is likely that there will be other regimes embedded within those described here within which the turbulence enters into the fuel consumption zone and may even under some conditions cause extinction. It may be that significantly different regime diagrams are needed for systems with markedly different boundary conditions such as those that produce strong shear or large mean .pressure gradients.

5. CONCLUSIONS

It is concluded that advanced laser diagnostics have not yet fulfilled their early promise but are close to doing so in some areas. Their use in routine combustor development is close to being feasible for reciprocating engine development in the automotive industry. Advanced laser diagnostics are playing a very important role in providing accurate data bases for validating combustion models for predicting pollutant emissions via CFD style codes. These are close to being of direct use in combustor development. Advanced laser diagnostics are now capable of resolving issues of flame structure for turbulent premixed flames. Such issues are important in the development of improved combustion models for premixed systems.

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