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Sandia Cooperative Group on the Aerothermochemistry of Turbulent Combustion

(Discussion Record of Fourth Meeting, General Electric Corporate Research
and Development Center, October 8-9, 1984. Supported by the United
States Department of Energy, Office of Basic Energy Sciences)

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SANDIA COOPERATIVE GROUP ON THE AEROTHERMOCHEMISTRY OF TURBULENT COMBUSTION

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ABSTRACT

A turbulent reacting flow working group has been established through the Department of Energy/Office of Basic Energy Sciences. The purpose of this group is to establish and maintain a strong interaction and active dialogue between workers currently involved in modeling turbulent reacting flows and those involved in related experiments. One objective of this collaboration is to develop an increased understanding of the fundamental interaction between the chemical and fluid dynamical processes occurring in chemically-reacting flows and to utilize this understanding to improve predictive capabilities for turbulent combustion.

Regular members, who represent academia, private industry, and national laboratories, and guests participate in the meetings. Several guests are invited to each meeting to provide an influx of different ideas and opinions to the discussions.

This document is a summary of the discussion that took place during the fourth meeting, which was held at General Electric Corporate Research and Development Center on October 8-9, 1984.

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INTERMITTENCY, CONDITIONAL SAMPLING AND TURBULENT COMBUSTION

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Intermittency arises in those turbulent shear flows involving an external stream or ambient, the situation in many cases of turbulent combustion, and leads to a distinct structure to the time history of the fluid mechanical variables at a fixed spatial location, a structure overlooked in the early descriptions of such flows and ignored in most current predictive methods. The most obvious manifestation of intermittency occurs when the turbulent fluid is tagged with a scalar such as temperature. In this case the signals from a thermometer or other sensor indicate a constant temperature when in the external medium and the usual randomness when inside the turbulent fluid. In an idealized sense the probability density function of the scalar involves a definite value a certain fraction of the time and a continuous distribution the remainder of the time. Such signals can therefore be used to condition the output from one or more anemometers so that the statistical behaviour within the two fluids can be separately determined. This technique has been developed and extended during the past fifteen years and is now widely used in experimental turbulence. Although relatively seldom used, there exists a theoretical counterpart of this technique leading to predictions of the features of intermittent turbulence.

Because special scalar variables play essential roles in the most soundly based theories for turbulent combustion, both nonpremixed and premixed, it is not surprising that in recent years conditional sampling has been applied to experiments involving such combustion and to theoretical descriptions thereof. Improvements in both our perspective of the aerothermochemistry involved and in the modeling of various processes arising in the theory have resulted from consideration of the variables within two separate, identifiable gases. The most obvious example of such improvements relates to the Bray-Moss-Libby model for the aerothermochemistry of premixed turbulent combustion. Application of the theory which results from application of conditional averaging to reactants and products has exposed new processes of countergradient diffusion, nongradient diffusion and turbulent production within premixed turbulent flames. In addition the theory is found by experimentalists to provide a useful framework for the presentation and interpretation of the results of their measurements in such flames. Recent work on this model relates to extensions to a two-point, two-time generalization which incorporates information on the length and time scales of the scalar field and to nonisenthalpic flows which can arise in a variety of circumstances, e.g., in the case of a lean premixed flame discharging into air.

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Aerothermochemistry of Turbulent Combustion

CONDITIONAL MODELING IN TURBULENT SHEAR FLOWS

S. B. Pope

The phenomenon of intermittency in shear flows has been known for over forty years, but only in the last ten years have modellers paid it attention. Since the turbulent fluid is highly rotational while the nonturbulent fluid is irrotational, the fluid behavior can be expected to be significantly different in these two states. Experiments confirm this expectation. It can also be expected that a model that explicitly accounts for the different behavior of turbulent and nonturbulent fluid can be more accurate than one that makes no such distinction.

A modeled joint probability density function (pdf) equation has been solved to calculate the one-point statistical properties of a self-similar plane jet¹. The equation solved is for the joint pdf of the three velocity components $\underline{U}(\underline{x}, t)$ and a conserved passive scalar $\phi(\underline{x}, t)$. With θ being the nondimensional, cross-stream variable, the joint pdf is $f(\underline{V}, \psi; \theta)$, where $\underline{V} \equiv V_1, V_2, V_3$, and ψ are the independent variables corresponding to \underline{U} and ϕ . The conserved scalar $\phi(\underline{x}, t)$ is zero in the irrotational ambient fluid and is positive within the turbulent jet. Thus the condition $\{\phi(\underline{x}, t) > \psi^*\}$ (where the threshold ψ^* is a small positive number) can be used to distinguish between turbulent and nonturbulent, irrotational fluid. In the joint pdf equation, conditional modeling is used: that is, different models are used depending upon whether the fluid is locally turbulent or nonturbulent.

The modeling of the interactions between turbulent and nonturbulent fluid centers on the rate of entrainment g , the rate of momentum exchange \dot{M} , and the rates of energy transfer \dot{E}_T and \dot{E}_N . According to the models, momentum is transferred at a rate proportional to the turbulent frequency ω and proportional to the velocity difference $(\underline{U}-\bar{U})$. Similarly, the rate of energy transfer is proportional to $\omega(u_1''u_1''-u_1'u_1')$. (In both cases, the direction of the transfer is such as to decrease the difference in momentum and energy.)

The calculated intermittency factor and unconditional mean velocity and Reynolds stresses agree well with the three available sets of experimental data. The calculated conditional mean velocity is in agreement with Gutmark and Wagnanski's² measurements, but the agreement with the conditional Reynolds stresses does not appear to be so good. The calculated ratio of nonturbulent to turbulent velocity fluctuations is in the range of values measured in shear flows.

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The microstructure approach to conserved scalar pdf models

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Abstract

A parametric expression for the conserved scalar probability density function (pdf) is derived on the basis of a physical interpretation of the turbulent signal. The scalar signal is split into three parts: a fully turbulent part, a superlayer part, and an outer flow part. Each part is represented by a different form of the pdf. The composite pdf which is obtained by adding these parts together has four parameters in addition to the intermittency factor. It can be integrated so that algebraic relations between these parameters and the first four moments are obtained. Application of the formulation to LaRue's and Libby's measurements in the plane turbulent wake indicates the existence of transitions that are interpreted as internal superlayers far inside the turbulent flow. An interesting result of these measurements is that the mean of the turbulent part of the signal remains constant. This is related to the occurrence of large structures.

Slow Chemistry Effects in a Turbulent Mixing Layer

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The overall chemical rate in the hydrogen-fluorine-nitric oxide chemical system was varied by changing the concentration of nitric oxide while keeping the hydrogen and fluorine concentrations fixed. The temperature field in the mixing layer responds to reduced chemical rate by three main effects.

[1] reduction of mean temperature rise profile

[2] symmetrizing of mean temperature profile

[3] lessening of "ramp-like" features within a given large structure

The results are interpreted by comparison to chemical reactions in liquid mixing layers.

RAYLEIGH SCATTERING FOR DENSITY MEASUREMENTS IN PREMIXED FLAMES
ONE POINT, TIME SERIES DATA

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ABSTRACT

Rayleigh scattering measurements for molecular number density in turbulent, premixed CH_4 -air flames are discussed, and data for both flamelet passage time distributions and power spectral density functions are reported and compared to the recent predictions of Bray, Libby and Moss [5]. Measurement problems associated with variations in mixture-averaged Rayleigh scattering cross section, index of refraction fluctuations, finite spatial and temporal resolution and with scattering from particles are discussed. It is concluded that these effects are relatively minor in the reported experiments. Correction procedures are suggested for the effects of cross section variation and of finite resolution.

Passage time and spectral data support the Bray, Libby and Moss hypothesis for the passage time distribution function. Furthermore, model predictions for the variation across the flame brush of mean passage times for both reactant and product eddies are in reasonable agreement with experiment except on the edges of the flame brush. Finally, the data suggest that these mean times scale in part with \bar{U} and λ in the reactant flow.

RECENT MEASUREMENTS IN TURBULENT JET FLAMES AT SANDIA COMBUSTION RESEARCH FACILITY

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OUTLINE

1.A Conditional Sampling of Velocity Probability Distributions in Mixing Flows Resulting From LDV Seed Particle Origin.

1.B Reconstruction of Unconditional Probability Distribution of Velocity from Conditional Sampling of Velocity and Scalars.

2. Two Dimensional Imaging of C₂ Fluorescence as an Indicator of Flame Front Position.

A brief abstract of each topic follows:

1.A Conditional Sampling of Velocity Probability Distribution in Mixing Flows Resulting From LDV Seed Particle Origin: Laser-Doppler Velocimetry (LDV) has achieved widespread use, particularly in combustion flows, where high temperatures limit the use of conventional probes, such as hot wires and Pitot probes. The LDV measures the velocity of individual particles, which also represent the fluid velocity and which are, in most cases, artificially added to the flow. From an ensemble of such individual realizations of velocity, a probability distribution of velocity $P(u, v)$ is generated. In mixing flows, such as that of a jet of gaseous fuel into coflowing air, the measured probability distribution $P(u, v)$ is sensitive to the number density of particles in each flow. In this investigation, we establish the limits of this potential bias by measuring the velocity distribution when only the fuel is seeded $P_{fuel}(u, v)$ and then when only the air flow is seeded $P_{air}(u, v)$. In addition to establishing these limits, we present a data reduction strategy which will generate the unbiased probability distribution $P(u, v)$.

1.B Reconstruction of Unconditional Probability Distribution of Velocity from Conditional Sampling of Velocity and Scalars: Our strategy relies upon the measure-

ment of the joint probability distribution of velocity and mixture fraction $P(u, v, f)$. The mixture fraction, which is unity in the fuel stream and zero in the coflow air stream, is a quantitative measure of the extent of mixing. The mixture fraction is determined from the vibrational Raman scattering from a single laser pulse which is triggered from the LDV event. Figure 1 is a schematic of the simultaneous LDV-laser-Raman-scattering apparatus. Using this apparatus, we determine the joint probability distribution $P(u, v, f)$. Since we trigger the pulsed laser shortly after the LDV event, we obtain a probability distribution of the mixture fraction which is conditioned by the LDV event and, thus, by the origin of the seed particle. Comparison of the velocity and scalar probability distributions obtained from the two experiments are clearly different. This difference is illustrated in Figure 2, where the mean radial velocities, i. e. the first moment of the velocity probability distribution, are compared.

Accurate determination of the true velocity probability distribution is the central topic of our investigation. In brief, we argue that the unbiased probability distribution $P(u, v)$ can be constructed from a linear combination of the two limiting probability distributions $P_{air}(u, v)$ and $P_{fuel}(u, v)$:

$$P(u, v) = \gamma P_{fuel}(u, v) + (1 - \gamma) P_{air}(u, v) \quad (1)$$

Both $P_{air}(u, v)$ and $P_{fuel}(u, v)$ have been measured; however, γ remains undetermined. The factor γ is determined by an analogous equation for the mixture fraction:

$$P(f) = \gamma P_{fuel}(f) + (1 - \gamma) P_{air}(f) \quad (2)$$

The unbiased probability distribution of the mixture fraction can be determined by operating the laser Raman scattering system independently of the LDV system. Since all three probability distributions in Equation 2 are measured, γ can be determined and then inserted into Equation 1 to obtain the unbiased probability distribution of velocity $P(u, v)$. Comparison of various moments of the unbiased distribution with moments of the biased distributions shows the potential for bias when using LDV in mixing flow experiments.

2. Two Dimensional Imaging of C_2 Fluorescence as an Indicator of Flame Front Position: In the course of our investigations into turbulent nonpremixed methane flames, we encountered a strong fluorescent interference with our spon-

taneous Raman point measurements and with our two dimensional Ramanography. The interference is laser induced fluorescence from diatomic carbon, C_2 .

We optimized this fluorescence intensity by tuning the CRF dye laser to $\lambda = 512$ nm which is essentially the bandhead of C_2 ($\lambda = 516.5$ nm). The resulting fluorescence intensity is comparable to the Raman scattering intensity from nitrogen in room air. Images of this fluorescence were readily obtained with the the Ramanography system by simply changing an optical interference filter from a Raman wavelength to the wavelength of most intense Stokes fluorescence ($\lambda = 565$ nm).

The resulting images, see Fig. 3, show a thin zone of C_2 on the fuel rich side of the flame front. At a jet Reynolds numbers of less than 20,000, the image of C_2 fluorescence is always connected. At higher Reynolds numbers, the C_2 zone is often disconnected; the flame blows out at Reynolds numbers greater than 30,000. It appears that a disconnected flame is a precursor to flame blowout; however this assumes that the disconnected nature of the C_2 fluorescence is a consequence of local flame extinction rather than of the existence of a flame front which has no detectable C_2 fluorescence (see footnote). Our tentative impression is that C_2 fluorescence is a superb marker of the flame front position; better than, for example, OH fluorescence because the C_2 molecule is short lived transient that is generated and consumed in a thin zone near the flame front whereas the OH molecule is a much longer lived species that appears in a broad zone which spans from the fuel rich side to the fuel lean side of the flame front.

Footnote: Our investigations after this meeting show us that C_2 fluorescence is associated with the flame front until flame extinction.

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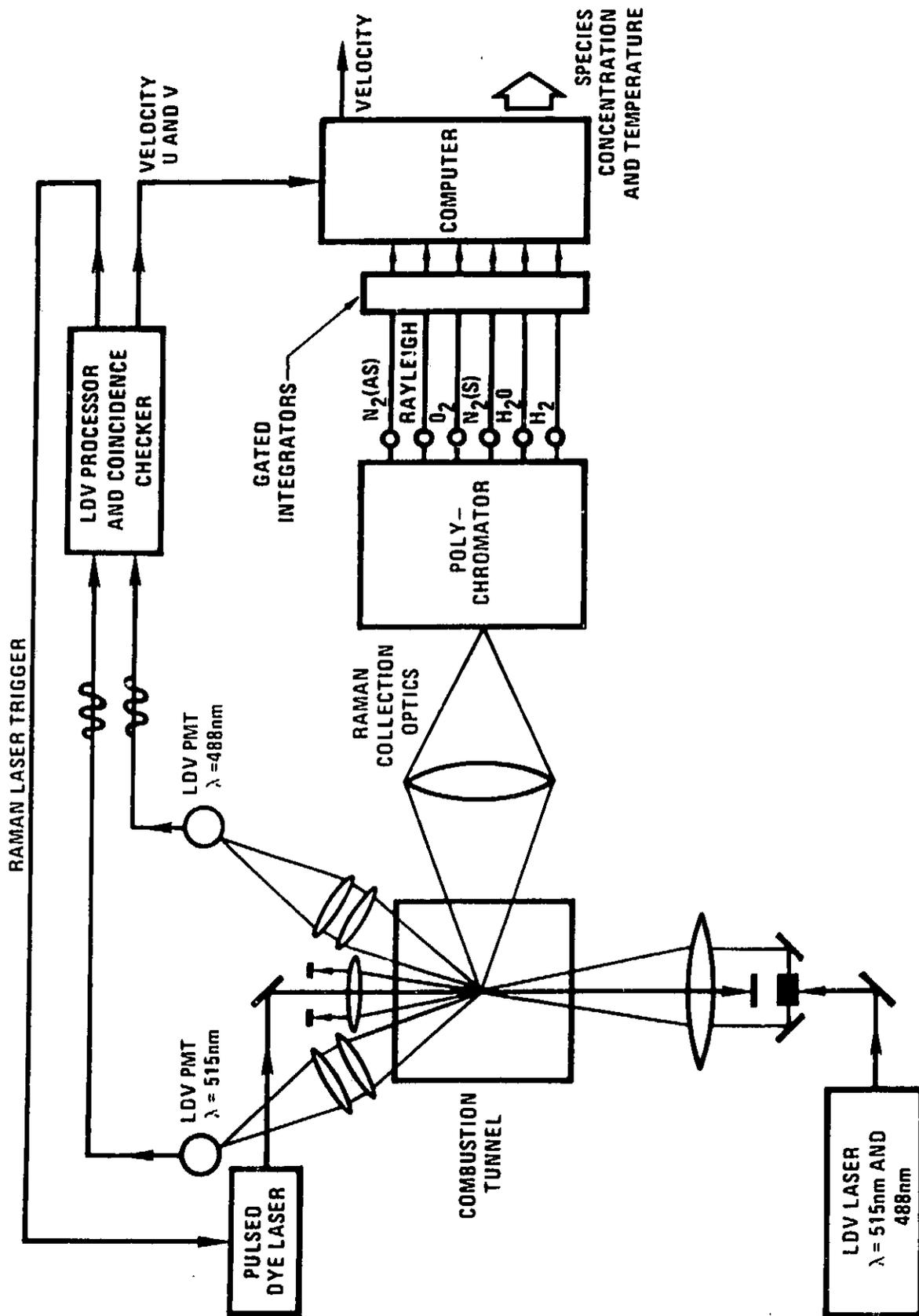


Figure 1. The key components of the simultaneous LDV-laser-Raman-scattering apparatus are schematically illustrated.

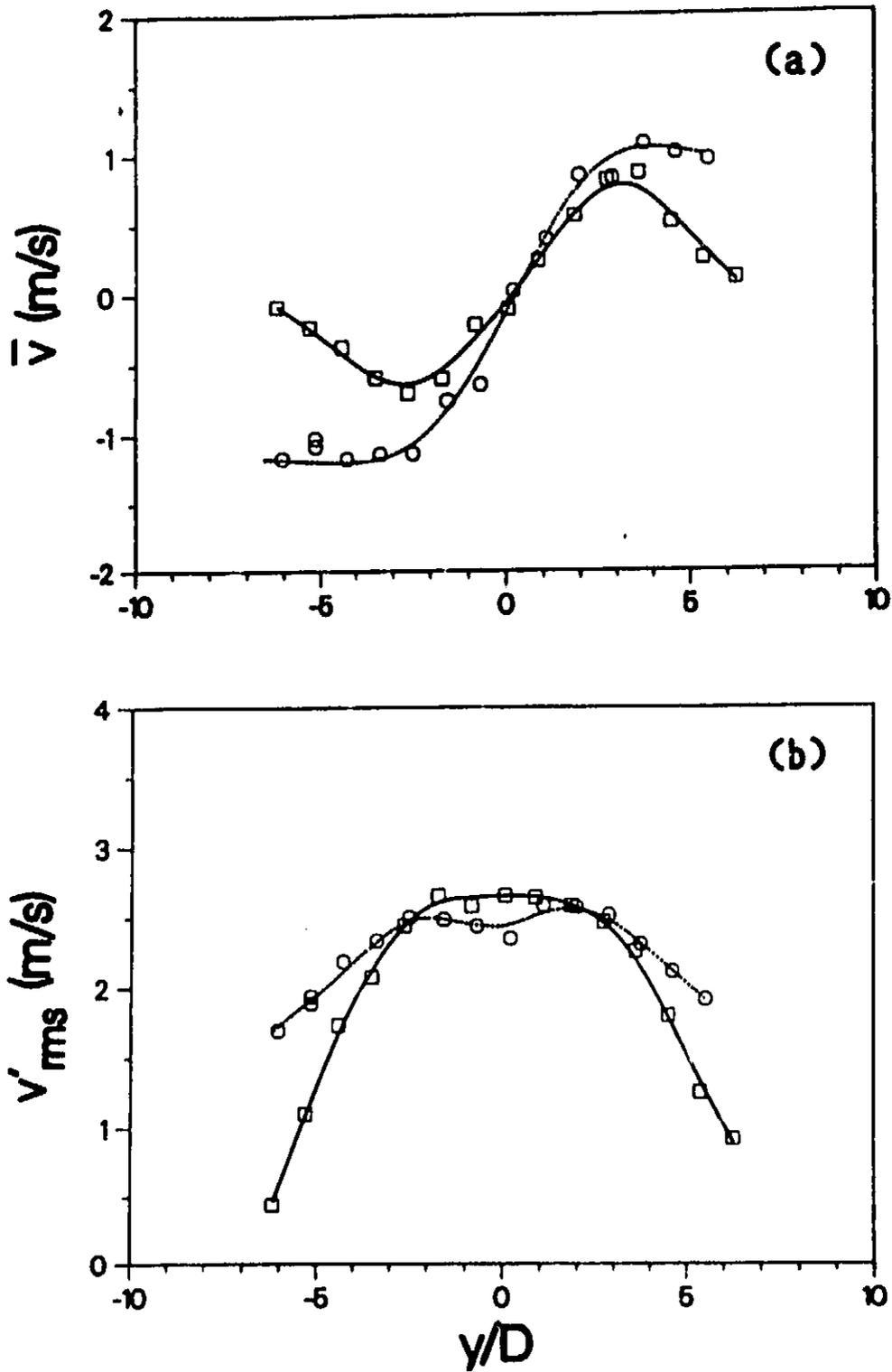


Figure 2. Radial profiles for a nonreacting jet at an axial location of $x/D=50$. Bulk jet velocity=108 m/s; coflowing air velocity=9.2 m/s. Solid line through squares indicates data collected with LDV seed added to the coflowing air stream only; dotted line through circles indicates data collected with LDV seed added to the fuel jet stream only. (a) Radial profiles of mean radial velocity; (b) Radial profiles of radial velocity fluctuations.



Figure 3. These simultaneous 2-dimensional images of C_2 fluorescence (lower image) and Rayleigh scattering (top image) were collected 30 diameters downstream from the nozzle exit in a nonpremixed turbulent flame of a fuel consisting of 30 percent hydrogen in methane. For this flame, the jet Reynolds number is 20,000. In both images, the signal intensity spans from dark blue (zero intensity) to red (maximum intensity).

ASSESSMENT OF SUPERLAYER CONTRIBUTION TO THE CONSERVED
SCALAR PDF IN A HYDROGEN TURBULENT JET DIFFUSION FLAME

W. Shyy, M.C. Drake and R.W. Pitz

For non-premixed flames in a turbulent flow, the concept of intermittency is important because of the highly nonlinear relationship between mixture fraction and local thermodynamic state. Recently Pitz and Drake [1] have demonstrated via their experimental data that the conventional treatment of modeling the turbulent part of probability density function (pdf) as a Gaussian distribution is not a good approximation in the region close to the edge of the jet. Effelsberg and Peters [2] have explained this phenomenon by including a third zone - the viscous superlayer - a viscous layer between the turbulent and nonturbulent zones. Effelsberg and Peters have proposed a composite pdf model for the conserved scalar pdf which includes three fluid states: fully turbulent, superlayer, and laminar. This model is adopted here to assess the contribution of the superlayer to the composite pdf. The hydrogen jet diffusion flame data of Drake and Pitz [3] were used to supply the necessary information i.e., the first four moments of the conserved scalar variable. The results, at four different axial locations, are shown in Fig. 1. Several characteristics can be observed from this assessment.

1. A large contribution of the superlayer to the composite pdf is seen in the region close to the edge of the jet.

2. The peak contribution of the super layer occur at the radial position of about 1.6 times half radii of the conventionally-averaged mixture fraction.
3. The peak contribution of the superlayer doesn't appear to change along the axial direction.
4. The region where the superlayer effects are observable widens along the downstream direction.
5. Peak contribution of the superlayer in this jet flame (80%) is larger than that in the nonreacting wake flow behind a heated cylinder of LaRue and Libby [4] studied by Effelsberg and Peters (60%).

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H₂ jet diffusion flame

- Re = 8000
- Fully Turbulent
- Superlayer
- Laminar

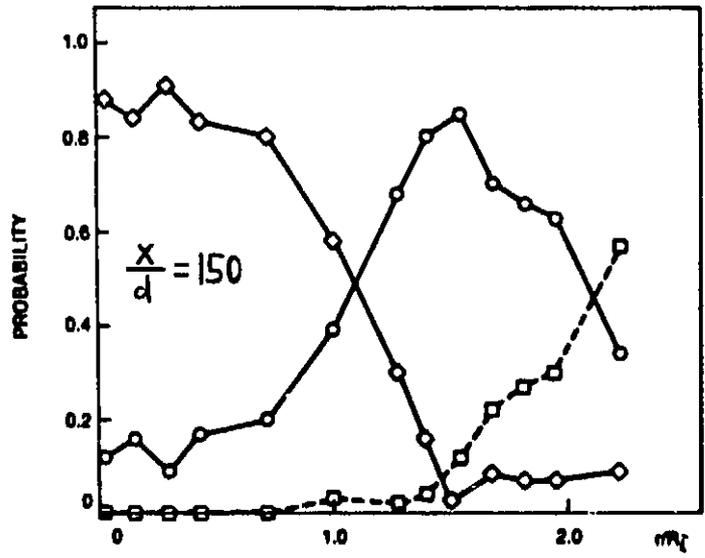
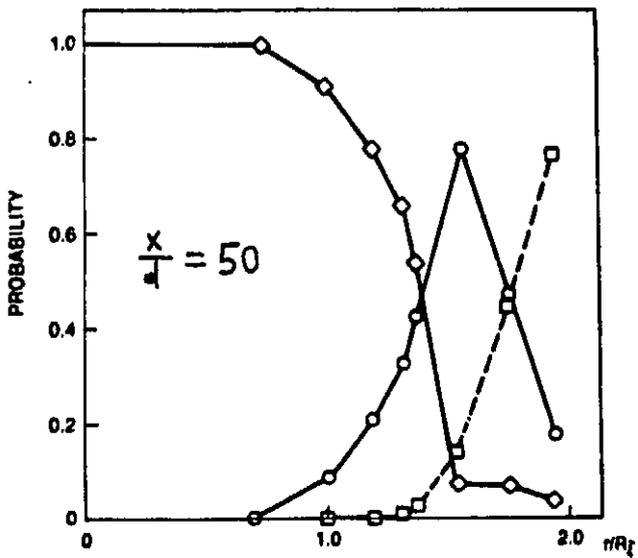
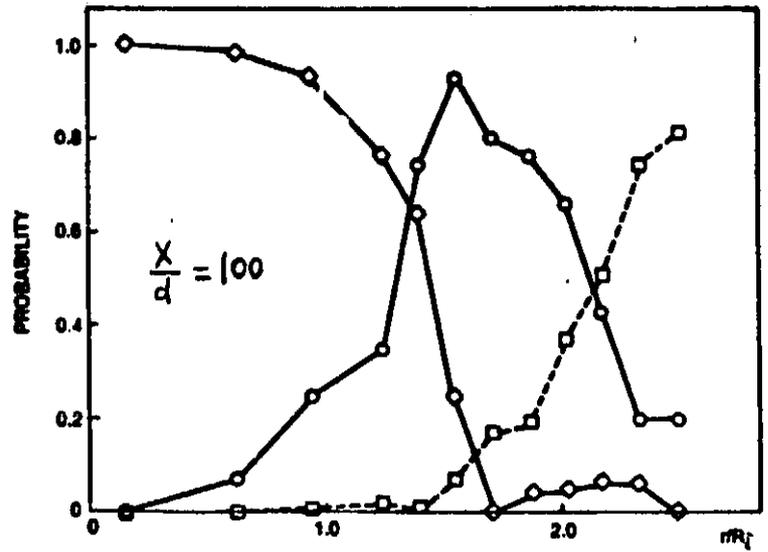
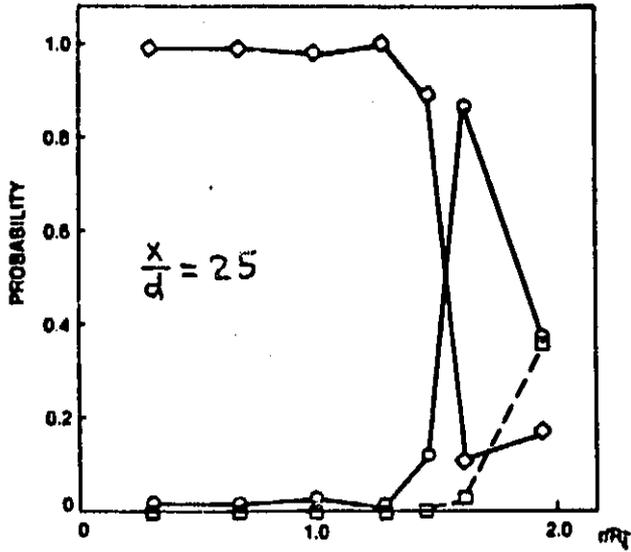


Fig 1

BLOWOUT OF TURBULENT DIFFUSION FLAMES

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ABSTRACT

A simple description has been formulated of the mechanisms governing the stability of turbulent diffusion flames. It is based upon the nature of the large scale motions that have been observed in turbulent jets and includes a process for maintaining a stable flame. An analysis, based on the proposed model, leads to a single parameter which determines the blowout velocity of pure fuels and of fuels diluted with air and with CO_2 . The parameter is the ratio of two times: a characteristic chemical reaction time and a time associated with the mixing of reentrained hot products into fresh reactants. The agreement with a set of experimental observations for both pure and diluted gases is good.

**Strong Turbulence Chemistry Interaction in a
Piloted Turbulent Jet Diffusion Flame**

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Experiments are being carried out on a turbulent jet diffusion flame burner specially designed to produce intense turbulent mixing rates in the shear layer well downstream of the nozzle where the turbulence is fully developed. The main fuel jet diameter, D_j , is 7.5 mm and this is surrounded by a premixed pilot flame to an outer diameter of 18 mm. The pilot is stoichiometric combustion products of a mixture of C_2H_2/H_2 and air which have the same carbon to hydrogen ratio as the main fuel - methane/natural gas or propane/LPG. The main findings, so far, are:

1. Blow-off occurs at high jet velocities leaving the pilot flame alight. Incipient extinction occurs at a blue neck region $20 D_j$ from the nozzle.
2. Shadowgraphs indicate that the turbulence is three-dimensional and "fully-developed" in the blue neck region.
3. Below extinction jet velocities, the electrical connectedness between the jet nozzle and a grid of fine wires at $x/D_j = 70$ becomes intermittent and finally continuously broken. There is no visible or audible indication of incipient blow-off under these conditions.
4. Mean temperature measurements made by thermocouples indicate that the peak mean temperature in the radial profile at x/D_j drops to below $500^\circ C$.
5. Sample probe measurements of composition indicate large amounts of oxygen on the centreline and overlaps of oxygen and fuel near stoichiometric mean composition that are too large to be explained by turbulent fluctuations of a continuous flame sheet. At lower jet speeds, the overlap is more consistent with such a model.

It is concluded that the flame near extinction has considerable patches of unburnt mixture indicating holes in the flame sheet. A preliminary report was given on the experiments under way at Sandia to use the Diana laser-Raman system to make instantaneous composition measurements in this flame. Problems of fluorescences from C_2 and other species were outlined. These results, in a simple parabolic flow, will provide a good test of our ability to model strong turbulence/chemistry interactions.

NON-EQUILIBRIUM EFFECTS IN TURBULENT DIFFUSION FLAMES

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ABSTRACT

The interaction between non-equilibrium chemistry and turbulence may be described by the statistics of two parameters: the mixture fraction and the instantaneous scalar dissipation rate. The hypothesis of statistical independence of these two parameters is discussed. Calculation methods for the marginal distributions are reviewed. It is shown how local quenching of diffusion flamelets leads to a reduction of burnable flamelets. However, there are burnable flamelets in a turbulent flame which are not reached by an ignition source. This phenomenon is described by percolation theory. Finally, criteria for the stabilization of lifted turbulent flames are derived.

Vortex Simulation of V-Shaped Flame

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The premixed flame under investigation is called a v-shaped flame for its appearance: placing a wire normal to a turbulent flow creates two flame sheets. Two recent experimental investigations have shown the effect of low intensity turbulence on a premixed flame. In the first experiment Rajan, Smith and Rambach measured density along a line through the flame brush and showed that flame thickness remains at its laminar value. The apparent thickening of the flame is due to the flapping motion of the thin laminar flame. In the second experiment, Cheng (LBL) seeded the flow with oil droplets and solid particles in order to measure conditioned velocity statistics; i.e., he split the velocity data into burnt and unburnt values.

Stimulated by this new experimental information, I have made a discrete vortex simulation of the v-shaped flame, in which the turbulence intensity is created in a stochastic fashion by adding discrete vortices to the freestream flow. The flame is assumed to be of zero thickness, its location is described by its x,y coordinates in terms of arc length, and the flame speed is a defined function of flame curvature. Discrete volume sources are located along the flame in order to generate the proper density change. While the modeling assumptions are many, the dynamic motion of the flame produces velocity statistics which are in good agreement with Cheng's experimental values.

Examination of the mean velocities in the flame region shows that the hot products move faster than the cold reactants and the angle of the flow is towards the midplane for products and away from the midplane for reactants. The conditioned turbulence quantities do not show the large rise in the flame region as is found in the unconditioned signals. It is the intermittent motion of the flame which generates the apparent turbulence. Therefore, time-averaged Eulerian information obtained without knowledge of the flame location is very misleading and the flame appears turbulent. Lagrangian information with respect to the flame would reveal the dual nature of the flow. We now see that previous measurements of velocity have mislead time-average turbulence models.

We now describe in more detail the effects of the flame motion on the velocities at a fixed space location. Figure 1 presents a time record of the two velocity components along with an indicator signal which has the value of unity when the probe location is in the burnt gas and the value zero when unburnt. A long time average of the indicator signal at this location yields a burnt fraction of seventy percent. In this short time record there are seven passings of the flame front, which are determined by the indicator changing from zero to one. The flow direction velocity (solid line) shows a ramp-type increase followed by a sharp drop which from the indicator signal can be seen to be correlated with flame motion. Thus,

when the probe is close to the flame on the burnt side, it has the largest U velocity magnitude. When it is close to the flame on the unburnt side, it has the smallest U velocity. The other velocity component V (dash line) is not as ramp-like, but tends to be either negative or positive, and is again correlated with the flame location and its passage: flow is away from the midplane when unburnt and towards the midplane when burnt. From this velocity record we see the strong effect of volume expansion.

Figure 2 is a scatter plot made from a similar time record of velocity at one location. For each discrete time-step a dash line is plotted in U, V velocity space. The dash is horizontal if the gas is burnt and vertical if unburnt. In the scatter plot we see that the burnt and unburnt signals divide into two regions. The tic-marks along the axes represent conditioned and unconditioned velocity averages. With respect to the unconditioned mean, the burnt gas has a larger U velocity and a smaller V velocity with the opposite true for the unburnt gas. From the scatter plot, we see that the data falls mostly into the second and fourth quadrants formed by the unconditioned mean velocities. A cross correlation of all the data yields the unconditioned turbulent shear stress $u'v'$, and from the data location this shear stress will be negative. This result is in agreement with Cheng's experimental value and as he points out, implies counter-gradient transport since the sign of both mean velocity gradients produce a positive shear stress.

As in Cheng's results, the conditioned shear stresses are an order of magnitude smaller than the unconditioned; Figure 3 presents the profile of shear stress across the flame brush region.

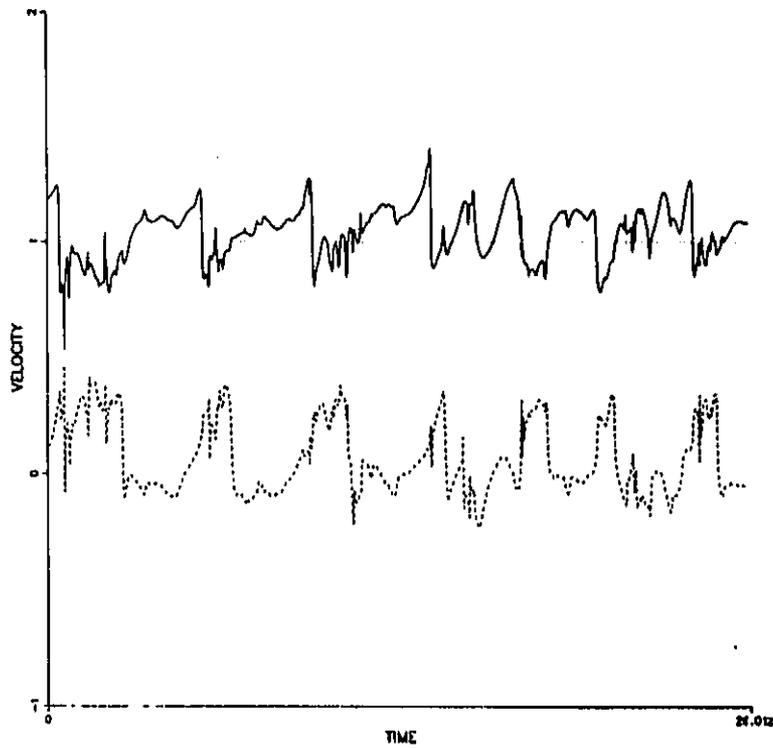


Figure 1. Sample velocity time record at a location which is burnt seventy percent of the time. U velocity is solid line, V velocity is dash line and the indicator signal (dotted line) is zero for unburnt and unity for burnt.

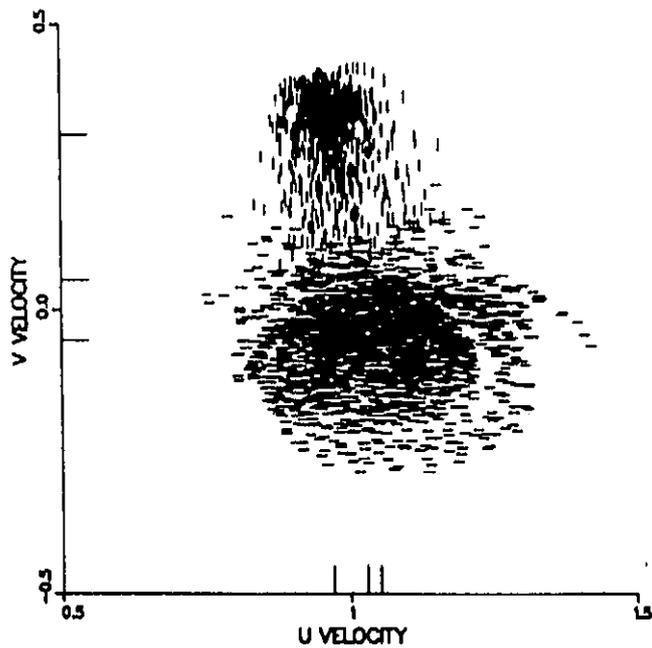


Figure 2. Scatter plot of burnt (horizontal dash) and unburnt (vertical dash) velocity signals. Tic-marks along the axes represent conditioned and unconditioned velocity averages.

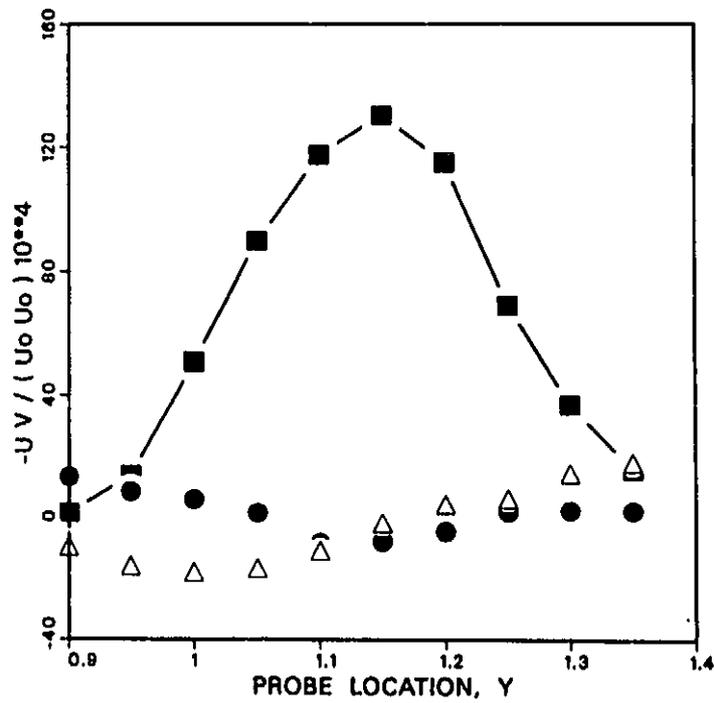


Figure 3. Time-average turbulent shear stress across the flame brush region: unconditioned (solid squares), unburnt (solid circles) and burnt (triangles).

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