Investigation of subgrid-scale mixing and turbulence-chemistry interaction in turbulent partially premixed flames using experimental data

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INVESTIGATION OF SUBGRID-SCALE MIXING AND TURBULENCE-CHEMISTRY INTERACTION IN TURBULENT PARTIALLY PREMIXED FLAMES USING EXPERIMENTAL DATA

A Dissertation
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the Graduate School of
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In Partial Fulfillment
of the Requirements for the Degree
Doctor of Philosophy
Mechanical Engineering

by
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Accepted by:
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Abstract

The filtered mass density function (FMDF) of mixture fraction, temperature and species used in large eddy simulation (LES) of turbulent combustion is studied experimentally using line images obtained in turbulent partially premixed methane flames (Sandia flames D and E). Cross-stream filtering is employed to obtain the FMDF and other filtered variables. The mean of the FMDF conditional on the subgrid-scale (SGS) scalar variance at a given location are found to vary from unimodal to bimodal, corresponding to quasi-equilibrium distributed reaction zones and laminar flamelets (including extinguished flamelets), respectively. The conditionally filtered mixture fraction dissipation for small SGS variances has a relatively weak dependence on the mixture fraction, and is not sensitive to temperature for extinguished samples. For large SGS variance the large dissipation is concentrated in the cliffs and increases with decreasing temperature. The conditionally filtered temperature dissipation for small SGS variances is the highest for intermediate temperature. For large SGS variance the dependence is more complex and the pilot gas appears to be playing an important role. The conditionally filtered scalar and temperature diffusion for small SGS variance have a simple structure. For large SGS variance the diffusion structure is much more complex, with the pilot and local extinction also playing important roles. The results show that it is important that mixing models for filtered density function methods be able to account for the different SGS mixture fraction and temperature structures for small and large SGS variance. The different SGS mixture fraction structures for small and large SGS variances, as reflected by the unimodal and bimodal FMDF, have a strong impact on the small-scale mixing and turbulence-chemistry interaction, as reflected by the results for the conditionally filtered dissipation rates and diffusion. The results have implications for understanding and modeling multiple reactive scalar SGS mixing.

Scalar dissipation rate is an important quantity in turbulent mixing and combustion. Its measurement depends on two opposite trends, noise and resolution effects, making their separation
and accurate corrections difficult. A major task in dissipation rate correction, therefore, is to isolate each effect. A conditional sampling-based method for correcting noise and resolution effects for scalar dissipation rate measurements is developed. The conditional-sampling method uses instantaneous local scalar mean and variance as conditioning variables, and is based in part on Kolmogorov’s refined similarity hypotheses. It ensures selection of instantaneous fully resolved local scalar fields, which are analyzed to determine the measurement noise. Noise correction is applied to potentially under-resolved local scalar fields, also selected using the conditional-sampling procedure, effectively separating the effects of noise from those of resolution. The error function is used as a model for the potentially under-resolved local scalar fields to evaluate their dissipation length scales and to make corrections for the dissipation rate. The present method uses local instead of spectral analysis; therefore, can be applied to the mean scalar dissipation rate conditional on the scalar values. Applications of the method to scalar dissipation rate in a slightly heated turbulent jet and turbulent flames show excellent results, validating the method.
Dedication

To my mother
I owe my deepest gratitude to my supervisor, Prof. Tong, whose encouragement, guidance and support from the initial to the final level enabled me to develop an understanding of the subject. I would like to thank Dr. Lin Ma, Prof. Richard S. Miller and Prof. Chanseok Park for serving on my advisory committee.

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This thesis would not have been possible without my mother, who supports and encourages me and to whom this dissertation is dedicated.
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Chapter 1

Introduction

Combustion is the most common energy generating method, providing about 85 percents of the world’s energy needs. Through oxidation of high heating value fuels, chemical energy is converted into heat, which can be directly used or further converted into other forms of energy. In industrial application, combustion process generally occurs in high Reynolds number therefore in turbulent environments. Due to the enhanced mixing by turbulence, chemical reactions are increased compared to laminar flames, resulting in high energy density[33].

In turbulent flows and turbulent flames, velocities and scalars such as temperature and species concentrations are random and fluctuating quantities[38]. They also contain a wide range of spatial and time scales. For this reason, direct simulation of high Reynolds number turbulent flows and flames in engineering application are not possible in the near future[48]. Therefore, it is necessary to develop computational models. Computational prediction of turbulent flow is an active research topic. Several modelling approaches have been developed and are widely used. Among these method, Large Eddy Simulation (LES) has several attractive attributes and is the most promising LES computes the instantaneous large, resolvable scales, and model the effects of small, subgrid scales (SGS). Therefore instant time dependent flow structures are available which are not accessible from Reynolds-averaged Navier-Stokes (RANS).

In the past decade, much effort was devoted to developing LES for turbulent reacting flows[20, 37, 11, 23, 19, 41, 35]. In LES of turbulent combustion, a major task is to compute the filtered chemical source term. Though the chemical source term is a deterministic function of scalars such as species and enthalpy, the functional dependence is highly nonlinear due to the complexity of
reaction mechanism. When reaction zone thickness is smaller than the filter size, which is generally
the case, there are large variations of scalars within subgrid scales. Coupled with the nonlinear
dependence, such variations cause the filtered chemical source term to differ from an approximation
based on the lower-order scalar statistics. For example, the filtered reaction rate is different from the
reaction rate evaluated using the filtered scalar values. In general, the computation of the filtered
chemical source term requires the SGS scalar distribution i.e. the filtered density function (FDF) of
the reactive scalars, which is not available in moment closure.

To overcome the problem with the chemical source term, Pope [37] proposed an extension of
the probability density function (PDF) method, the filtered density function (FDF) approach. Unlike
PDFs used in RANS type modelling approach, the FDF used in LES is not a statistical property and
requires averaging, because it comes from a single realization. In this approach, the FDF transport
equation for the species mass fraction and enthalpy is solved and the chemical reaction terms appear
in closed form, while the SGS advection and mixing needs modelling. Therefore, main challenge in
FDF methods is to develop mixing models that can correctly describe the evolution of scalar FDF
shapes due to molecular diffusion and chemical reaction.

The most frequently modelled mixing term is scalar diffusion. The conditionally filtered
diffusion appears as unclosed term in FDF equations. Therefore a model for the conditionally
filtered diffusion is needed in simulation. One of the simplest models for conditionally filtered
diffusion is the interaction by exchange with the mean (IEM) model[16]. The model is linear in
composition space. To take into count the effect of scalar mixing time scale changes due to various
scalar spectrum distributions, the model introduces a parameter to describe the mixing time. The
difficulty of IEM model is to determine the mixing time. The deficiency of IEM model is that, in
a statistically homogeneous scalar field, the IEM model preserves the shape of PDF, therefore the
scalar PDF does not relax to Gaussian form.

Another representation of molecular mixing in the FDF transport equation is the condi-
tionally filtered scalar dissipation rate[35]. The scalar dissipation rate measures the rate of decay
of scalar fluctuations due to molecular mixing and determines the mixing time scale. For infinitely
fast chemistry, the combustion process is mixing controlled. The mean burning rate is proportional
to the scalar dissipation rate of mixture fraction. For finite rate chemistry, a higher dissipation
rate corresponds to a smaller scalar local mixing time scale. When the mixing time scale becomes
comparable to the chemical time scale, local flame extinction occurs. Therefore, the dissipation rate
is employed as a parameter for modelling mixing in combustion models such as the laminar flamelet.

When the reaction rates are finite, there is an interaction between turbulence and chemistry. Such coupling can affect the stability of turbulent flames and the flame structures as well as the formation of pollutants. In engineering combustion applications, compact combustion chambers with high air/fuel flow rates are used to achieve for higher power density. In such combustors, high mixing rate (scalar dissipation rate) must be maintained, resulting in turbulent mixing time scales comparable to the chemical time scales. There is a strong interaction between turbulence and chemistry and the flame is close to extinction. To maintain stable combustion and to be able to control the combustion process, the designers need a simulation tool that can accurately predict local extinction, reignition and pollutant formation. Therefore understanding of mixing and turbulence-chemistry interaction is essential for modelling mixing in turbulent combustion.

Conventional understanding of turbulent scalar mixing is largely based on the Kolmogorov-Obukhov-Corrin theory. When Schmidt number is close to unit, the smallest mixing scale is of the same order as the Kolmogorov scale[38]. Therefore, at sufficient high Reynolds numbers, statistics in the inertial scales are expected to be universal. Therefore, for an inertial-range filter size, the SGS scalar is expected to have self-similar distributions. However, several recent studies [45] [52] on the conserved scalars in nonreacting jets and flame showed that the SGS scalar have qualitatively different distributions and structures, depending on the instantaneous SGS scalar variance. When the SGS variance is small compared to its mean value, the SGS scalar has a close to Gaussian distribution. This indicates a well-mixed SGS scalar field. However, when the SGS variance is large compared to its mean value, the SGS scalar on average has a bimodal distribution, indicating highly segregated SGS scalar fields. Such distinct scalar field structures can have strong influences on the flame structures. For well-mixed SGS scalar fields, the scalar fluctuations at the dissipation scales must be larger than the reaction zone width in the mixture fraction space to support the laminar flamelets. For the highly nonpremixed scalar fields, the fuel and oxidant are segregated by a thin layer smaller than dissipation scale, which results in laminar flamelets.

Previous studies on the flame structures are based on the statistics of in combustion conditioning on conservative scalars[52]. In this dissertation, joint statistics of conservative scalar (i.e. mixture fraction) and reactive scalar (e.g. temperature and species mass fraction) are presented. Chapter 2 includes the FMDFs and conditionally filtered dissipations in partially premixed piloted flames. The results on conditionally filtered diffusion are included in Chapter 3. Results on con-
ventional conditional statistics are included in Chapter 4. Conditionally filtered statistics involving reactive species are included in Chapter 5. Chapter 6 presents a novel noise correction and resolution inference algorithm for conditionally filtered mixture fraction dissipation rate. Its application in combustion is presented in Chapter 7. The data reduction procedures for three-stream mixing experiments are included in Chapter 8.
Chapter 2

FMDF and Dissipation Rate in Turbulent Non-premixed Piloted Jet Flame

As discussed in Chapter 1, FDF is needed to maintain a closed form of filtered chemistry source term in turbulent combustion simulation. In combustion process, the temperature varies within a large range, density variation should be considered. Density weighted form of FDF is FMDF. In this chapter, results of FMDF and conditionally filtered dissipation rates in turbulent partially premixed pilot flames are presented.

The joint filtered mass density function of mixture fraction and temperature is defined as

\[
F_{\xi TL}(\hat{\xi}, \hat{T}; x, t) = \int \rho(x', t) \delta[\hat{\xi} - \xi(x', t)] \delta[\hat{T} - T(x', t)] G(x' - x) \, dx'.
\]

(2.1)

where \(\xi\) and \(T\) are the mixture fraction and temperature respectively, and \(\hat{\xi}\) and \(\hat{T}\) are their sample space variables, \(G(x' - x)\) is the filter, \(\rho\) is the density and \(\delta[x]\) is delta function. Integration is taking over all the space.

Unlike a PDF, the FMDF is a random variable, therefore must be characterize statistically. We use the approach by Tong [45] which computes their conditional averages. In this approach, the
Favre filtered mixture fraction,
\[ \langle \xi \rangle_L = \frac{\langle \rho \xi \rangle_t}{\langle \rho \rangle_t} \]  
(2.2)
and Favre SGS scalar variance,
\[ \langle \xi''^2 \rangle_L = \frac{1}{\langle \rho \rangle_t} \int F_{\xi'}(\xi; x, t) \left( \xi - \langle \xi \rangle_L \right)^2 d\xi = \frac{\langle \rho \xi''^2 \rangle_t}{\langle \rho \rangle_t} - \langle \xi \rangle_L^2 \]  
(2.3)
are used as conditioning variables. The filtered mixture fraction is set to the stoichiometric mixture fraction \( \xi_s = 0.35 \), to maximize the probability of the SGS field containing reaction zones.

### 2.1 Experimental Data

The experimental data provided by Dr. Robert Barlow were obtained in turbulent partially premixed piloted jet flames at Sandia National Laboratory [2, 28, 3]. Measurements were made in a series of six flames of increasing Reynolds numbers, named Flames A to F. Flame D(Re=22400) has a small degree of local extinction, Flame E(Re=33600) has more local extinction and downstream reignition.

The main jet consists of 25% CH\textsubscript{4} and 75% air by volume. The pilot is premixed flame of C\textsubscript{2}H\textsubscript{2}, H\textsubscript{2}, air, CO\textsubscript{2}, and N\textsubscript{2} having nominally the same equilibrium composition and enthalpy as CH\textsubscript{4}/air. The pilot is operated lean, \( \phi = 0.77 \), and the flow rate is scaled in the Flames C to F to maintain the pilot at \( \sim 6\% \) of the power of the main flame. The stoichiometric mixture fraction is 0.35. Reaction zone width \( \Delta \xi_R (\approx 0.23) \) in mixture fraction space defined by the lean and rich limits that correspond to 10\% of the peak CO oxidation reaction rate in mildly strained laminar flames[18].

Line images of experimental data are taken at several downstream locations. The center of the images is approximately at the location where the mean mixture fraction stoichiometric. The measurement employed combined Rayleigh scattering, Raman scattering and laser-induced CO fluorescence. With this combination, the concentrations of the major species (CH\textsubscript{4}, CO, CO\textsubscript{2}, H\textsubscript{2}, H\textsubscript{2}O, N\textsubscript{2} and O\textsubscript{2}) are measured simultaneously. Concentration of CO is measured from both Raman scattering and laser-induced fluorescence (LIF). Since the LIF is superior to Raman scattering for measurement of CO, the LIF results of CO is used. Mixture fraction is calculated using a variation of Bilger’s definition, from major species without O\textsubscript{2}[2]. This definition reduces the sensitivity of
measurement noise and interferences between O\textsubscript{2} and other species.

Line images are used to analyze local flame structure. Each image has 30 pixels with a pixel size of 0.2 mm. The actual measurement resolution is larger (\approx 0.22 mm) due to the blurring effects of the optical system and data processing\cite{54}. Therefore, the measured mean scalar dissipation rate is fully resolved for flame D and is slightly under-resolved for flame E at \( x/D = 7.5 \)\cite{54}. However, this resolution might still under-resolve very large dissipation fluctuations, thereby under-estimating the conditionally filtered dissipation rate in cliffs (see Chapter 7). Our analysis (see Chapter 7) shows that for both flame D and E the conditionally filtered dissipation rates (computed from the gradient component along the line images) are well resolved using fourth-order finite difference for small SGS variance. For large SGS variance, a sixth-order finite difference stencil is capable of resolving over 97\% of the dissipation. Further increasing the order of schemes has little contribution to the resolution. Therefore we use sixth-order central difference to compute the dissipation rates.

### 2.2 Data processing

In flames the dependence of molecular diffusivity on temperature is important due to large variations of temperature. We use the temperature dependence of mixture fraction diffusivity suggested by Karpetis and Barlow\cite{27}, which is a fit from a strained laminar partially premixed CH\textsubscript{4}/air flame calculation.

\[
D_\xi = -0.12013 + 0.74818 \left( \frac{T}{1000} \right) + 1.1631 \left( \frac{T}{1000} \right)^2 \text{ (cm}^2/\text{s}) \quad (2.4)
\]

The temperature dependence of thermal diffusivity suggested by Bilger\cite{4} and recently used by Wang \textit{et al}\cite{57} is given as

\[
D_T = 2 \times 10^{-5} \left( \frac{T}{300} \right)^{1.8} \text{ (m}^2/\text{s}) \quad (2.5)
\]

Within the flame temperature range (300 \sim 2300 K), the difference between the dependence given by Equation 2.4 and 2.5 are small.

Filtering is performed in one dimension using the line images. Previous studies showed that scalar filtered density function (FDF) obtained from one dimensional filters is similar to that from two dimensional filters, which is a good approximation of three dimensional filters. Only one filter size (3 mm) is considered within this study, previous studies showed that changing filter size to
(6mm) does not affect the conclusion on transit from unimodal to bimodal.

Conditional statistics are computed in two steps. In the first step, we select conditional samples near the stoichiometric mixture fraction \((0.3 < \langle \xi \rangle_L < 0.4)\). Then in the second step, data samples are partitioned according to their scalar SGS variance \(\langle \xi'^2 \rangle_L\). To balance the resolution and statistical convergence, we use five bins of equal size for the logarithm of SGS variance. The bin width \(\Delta \ln(\langle \xi'^2 \rangle_L)\) is approximately 1.3. The number of SGS images in each bin ranges from several hundred to slightly above one thousand. Since increasing the bin width generally results in averaging of the FDFs for the nearby SGS variance values, a wider bin will underestimate the bimodality for the FDF. Therefore, the conclusions obtained here regarding the bimodalities are somewhat conservative.

To achieve better statistical convergence, conditionally filtered variables conditioning on temperature and mixture fraction are computed using kernel methods\[49\]. Gaussian kernels are employed. The choice of kernel size depends on the density of the data points. Large kernel sizes are used when the data is sparse, where as small sizes are used when data points are clustered.

2.3 Result and discussion

2.3.1 The conditional mixture fraction-temperature FMDF

The conditional mixture fraction FMDF, \(\langle F_{\xi T} | \langle \xi \rangle_L, \langle \xi'^2 \rangle_L \rangle\), for flame D and E at \(x/D = 7.5, 15\) and 30 are shown in figure 2.1, 2.2, 2.3, 2.4, 2.5 and 2.6 respectively.

For flame D at \(x/D = 7.5\), (figure 2.1) there is little local extinction and the FMDF for both small and large SGS variance is concentrated not far from the equilibrium values. For small SGS variance, e.g. \(\langle \xi'^2 \rangle_L \approx 0.0012\) (figure 2.1a), the conditional FMDF is unimodal. The peak of the FMDF (most samples) is near the equilibrium values. Due to the well mixed SGS scalar the SGS reactions are expected to be in the quasi-equilibrium reaction zones regime. For flame E (figure 2.4a), there is some local extinction as reflected by the low temperature but the results are otherwise similar to those for flame D.

As the SGS variance increases, the FMDF for \(x/D = 0.75\) becomes bimodal (figure 2.1b) with the bimodality stronger for larger SGS variance. The peaks are at \(\xi = 0.17\) and 0.62, indicating that the rich and lean mixtures in the SGS field (i.e., a grid cell) are essentially segregated. Furthermore, there is a sharp interface (diffusion-layer) separating the two regions, across which there
is a large scalar value jump (also see the discussion on the conditionally filtered scalar dissipation rate below). For flame D although most samples are still far from extinction, but the temperature near $\xi = 0.4$ is lower than that for the small SGS variance. For a bimodal FMDF the difference between the $\xi$ values for its peaks is often larger than the reaction zone width in the $\xi$ space for these methane flames, $\Delta \xi_R (\approx 0.23)$, defined by the lean and rich limits that correspond to 10% of the peak CO oxidation reaction rate in mildly strained laminar flames[18]. Therefore, such a mixture fraction structure will limit the reaction zones in thin diffusion layers, thereby resulting in laminar flamelets. By contrast, for the well-mixed SGS mixture fraction field, the turbulence cascade is likely to dominate and the dissipation-scale scalar fluctuations largely follow the Kolmogorov-Obukhov-Corrsin predictions. Therefore, such a SGS scalar is likely to result in distributed reaction zones. For flame E the FMDF values near equilibrium are lower than for flame D and there is a relatively large probability of local extinction due to the large scalar dissipation rate with temperature as low as 1000K. These results are consistent with the mixture fraction FMDF in previous study[52].

At $x/D = 15$, there are more extinguished samples for both flame D and E (figure 2.2 and 2.5). For small SGS variance (e.g. $\langle \xi''^2 \rangle_L \approx 0.003$ figure 2.2a), the FMDF shape is similar to that at $x/D = 7.5$. For large SGS variance (e.g. $\langle \xi''^2 \rangle_L \approx 0.069$ 2.2b), the FMDF peak on the rich side is broader due to the increased temperature variations, therefore the peak value is lower. The amount of local extinction in flame E is approximately 5 times that in flame D.

At $x/D = 30$, the probability of local extinction is approximately 2-3 times lower than at
Figure 2.2: FMDF of Flame D at $x/D = 15$

$x/D = 15$ because the scalar dissipation is reduced as the flames evolve downstream. For large SGS variance (figure 2.3b and 2.6b), the peak is narrower than at $x/D = 15$, indicating the flame is near quasi-equilibrium.

The filter scale is an important parameter in LES and it is important to understand how the FMDF varies with it. Our previous results have shown that increasing the filter scale does not alter the shape of the FMDF[52]. The results in the present study are consistent with this finding.
Figure 2.3: FMDF of Flame D at $x/D = 30$

Figure 2.4: FMDF of Flame E at $x/D = 7.5$
Figure 2.5: FMDF of Flame E at $x/D = 15$

Figure 2.6: FMDF of Flame E at $x/D = 30$
2.3.2 The conditionally filtered scalar dissipation rate

The conditionally filtered scalar dissipation rate, $\langle \langle \chi | \xi, T \rangle | \xi \rangle_L \langle \xi^2 \rangle_L$, for the same conditions are shown in figure 2.7, 2.8, 2.9, 2.10, 2.11 and 2.12 respectively. We limit the domains of the conditioning variables $\xi$ and $T$ to those of the corresponding FMDF shown in previous subsection.

![Figure 2.7](image1.png)  
(a) $\langle \xi^2 \rangle_L = 0.0012$  
(b) $\langle \xi^2 \rangle_L = 0.066$

Figure 2.7: The conditionally filtered scalar dissipation rate of Flame D at $x/D = 7.5$

![Figure 2.8](image2.png)  
(a) $\langle \xi^2 \rangle_L = 0.0030$  
(b) $\langle \xi^2 \rangle_L = 0.069$

Figure 2.8: The conditionally filtered scalar dissipation rate of Flame D at $x/D = 15$

At $x/D = 7.5$, flame D (figure 2.7) has little local extinction. For small $\langle \xi^2 \rangle_L$ it has a relatively weak dependence on $\xi$, consistent with the conditional FMDF being unimodal. However,
higher dissipation rate generally corresponds to lower temperature. The observed temperature-scalar-dissipation correlation for a fixed mixture fraction is consistent with the expectation that in quasi-equilibrium distributed reaction zones the temperature decreases as the scalar dissipation increases[4].

In flame E the samples close to equilibrium have a similar dependence on ξ and T. However, flame E already has significant amount of local extinction but the scalar dissipation near the stoichiometric mixture fraction at lower temperature (1250-1750K) does not depend strongly on temperature.

For large \((\langle \xi''^2 \rangle)_L\), the conditionally filtered dissipation in flame D (figure 2.7b) is generally large near ξ = 0.4 to 0.45, where the maximum gradient in the ramp-cliff structure is located[52]. The maximum value increasing with the SGS variance value. Near the equilibrium values the scalar dissipation is generally larger for lower temperature, consistent with strained laminar flamelets. Again, at \(x/D = 7.5\), flame D has little local extinction; therefore the conditional dissipation does not extend to very low temperatures. For flame E, the samples close to equilibrium are similar to those in flame D. Further away from equilibrium at lower temperatures the dissipation rate is larger and there is a significant amount of local extinction. The highest value (one component) of approximately 700s\(^{-1}\), which well exceeds the extinction dissipation rate for a steady laminar flamelets, occurs at very low temperature (approximately 750K). Considering the reduced diffusivity at these temperatures, the high dissipation rate is likely caused by very high strain rates. Because
the SGS scalar contains ramp-cliff structure, these samples are most likely extinguished laminar flamelets.

At \( x/D = 15 \) flame D (figure 2.8) has a larger number of extinguished samples with very low temperatures (< 1300K) and the dissipation is qualitatively similar to those for flame E at \( x/D = 7.5 \). When the SGS variance is small, the dissipation rate increases with decreasing temperature for the burning samples. The dependence is insensitive to the \( \xi \) values, similar to the results shown in figure 2.10a. For the extinguished samples the peak conditional dissipation rate is approximately 150s\(^{-1}\), below the extinction rate for steady laminar flamelets (\( \approx 400s^{-1} \))[27]. Therefore these might be samples extinguished upstream. As they are advected downstream to the measurement location the scalar dissipation rate has reduced but they have not yet mixed with high temperature parcels to reignite. Therefore, their temperatures remain low. The results for Flame E show a similar trend.

For large SGS variance both flame D and E have extinguished samples, with the latter having approximately 5 times more but the scalar dissipation results are similar to those at \( x/D = 7.5 \). The maximum conditionally filtered dissipation rate is reduced to 500s\(^{-1}\) for both flames.

At \( x/D = 30 \) (figure 2.9 and 2.12), there is significant amount of reignition and the probability for extinguished samples is reduced. For small SGS variance, the dependence of the dissipation on \( \xi \) is weaker compared to \( x/D = 7.5 \) and 15. For large SGS variance the maximum conditionally filtered dissipation rate remains approximately 500s\(^{-1}\) for both flames. However, the probability of occurrence for the large variance is smaller compared to the upstream locations, consistent with the
Figure 2.11: The conditionally filtered scalar dissipation rate of Flame E at $x/D = 15$

(a) $\langle \xi''^2 \rangle_L = 0.0028$

(b) $\langle \xi''^2 \rangle_L = 0.064$

reignition and the reduced degree of local extinction.
Figure 2.12: The conditionally filtered scalar dissipation rate of Flame E at $x/D = 30$

(a) $\langle \xi''^2 \rangle_L = 0.0018$

(b) $\langle \xi''^2 \rangle_L = 0.044$
2.3.3 The conditionally filtered thermal dissipation rate

The results in previous subsection indicate that the different structures of the SGS mixture fraction fields for small and large SGS variances result in different conditionally filtered scalar dissipation. Through interaction with combustion chemistry, the SGS mixture fraction fields will result in qualitatively different temperature dissipation structure. We now examine the conditionally filtered temperature dissipation.

The conditionally filtered scalar dissipation rate, \( \langle \langle \chi_T | \xi, T \rangle \rangle_{L}, \langle \xi^2 \rangle_{L} \), for the same conditions are shown in figure 2.13, 2.14, 2.15, 2.16, 2.17 and 2.18. We limit the domains of the conditioning variables \( \xi \) and \( T \) to those of the corresponding FMDF shown before.

In flame D at \( x/D = 7.5 \) the temperature is close to the equilibrium values for small SGS variance (figure 2.13a). Near \( \xi = 0.45 \) the flame reaches the local maximum temperature, leading to the lowest temperature dissipation. Away from \( \xi = 0.45 \) the temperature dissipation is small near the equilibrium values and increases with decreasing the temperature. There is some similarities between the conditional temperature dissipation and the conditional scalar dissipation samples for the rich and lean mixtures because for these mixtures there exists correlation between \( \xi \) and \( T \) near the equilibrium curve

\[
\chi_T = D_T \left( \frac{dT}{dx} \right)^2 \approx D_\xi \left( \frac{d\xi}{dx} \right)^2 \cdot \left( \frac{dT}{d\xi} \right)^2 = \chi \left( \frac{dT}{d\xi} \right)^2
\]  

(2.6)
Figure 2.14: The conditionally filtered thermal dissipation rate of Flame D at $x/D = 15$

where $\frac{dT}{d\zeta}$ is positive for $\zeta < 0.4$ and negative for $\zeta > 0.4$. Therefore, the temperature dissipation increases with the scalar dissipation for these mixture fraction values. In flame E there are some non-burning samples with higher $\chi_T$ but the results are otherwise similar to those for flame D.

For large SGS variance, flame D is still close to fully burning (figure 2.13b). For the samples not far from equilibrium, large temperature dissipation values occur in rich mixtures with $\xi$ values ranging from 0.5 to 0.65, but not in the lean mixtures. This is a result of the strained laminar flamelet structure. For a flamelet far from extinction $T = T(\xi, \chi_s)$ and $\frac{\partial T}{\partial y} = \frac{\partial T}{\partial \xi} \frac{\partial \xi}{\partial y}$, where $\chi_s$ is the scalar dissipation rate at the stoichiometric mixture fraction. Because $\frac{\partial T}{\partial \xi}$ is V-shaped with a minimum (zero) near $\xi = 0.45$ and at the same time $\frac{\partial \xi}{\partial y}$ is bell-shaped with its peak value located near $\xi = 0.5$, large values of $\frac{\partial T}{\partial \xi} \frac{\partial \xi}{\partial y}$ and the temperature dissipation occur for $\xi$ values ranging from 0.5 to 0.65. Further away from equilibrium, there are some large $\chi_T$ values on both the rich and lean side of the flame. An examination of the line images indicates that these large $\chi_T$ values come from images that contain straight lines in the $\xi - T$ space, running from $\xi_s$ to the lean or the rich sides, indicating that the samples are being mixed but not burning. At this location a significant portion of the SGS stoichiometric mixture for large SGS variance may be the pilot flame gas, suggesting that the high temperature dissipation values are largely due to the mixing of the pilot gas with the lean and rich mixtures. Because the scalar dissipation rate is high, mixing is much faster than reaction, resulting a mixing line (mixing without reaction). This observation suggests that each of these laminar flamelets is split by the pilot gas, effectively forming two flamelets, one lean and one
The results for the near equilibrium samples in flame E are similar except that the largest $\chi_T$ comes from the mixing of the pilot and the lean mixtures (figure 2.16). For the extinguished samples at much lower temperature ($<1200K$) the line images in the $\xi - T$ space include ones running from near stoichiometric mixture to both sides as well as straight lines running from the lean side to the rich side of the equilibrium curve, consistent with extinguished laminar flamelets.

At $x/D = 15$ a number of extinction events occur for both small and large SGS variance values. In flame D for small SGS variance the samples close to equilibrium have similar temperature dissipation structures to those at $x/D = 7.5$ with low $\chi_T$ near $\xi = 0.45$ (figure 2.14a). The extinguished samples with very low temperatures ($<1300K$) generally have small temperature dissipation because the temperature gradient is reduced by mixing. In addition, lower diffusivities resulted from the reduced temperature can also contribute to the lower dissipation rates. The samples with intermediate temperatures (1300-1600K) have the highest temperature dissipation which results from mixing between the burning and extinguished samples. The dependence on the mixture fraction is relatively weak compared to samples with higher temperature because $T$ and $\xi$ no longer follow the equilibrium relationship. Therefore, these samples have high $\chi_T$ but relatively low $\chi$.

For large SGS variance (figure 2.14b), $\chi_T$ for the burning samples (close to equilibrium) is similar to that at $x/D = 7.5$ with large values near $\xi = 0.55$. Away from equilibrium the situation is different. The dissipation is maximum near $\xi = 0.5$ and $T = 1600K$. An examination of the line
images going through this region in the $\xi - T$ space shows that the lean sides of the images still have the shape of strained laminar flamelets, indicating that the lean sides of the laminar flamelets are still nearly fully burning. However, the rich sides are essentially straight lines in the $\xi - T$ space, running from $\xi_s$ to the rich sides, indicating that these samples are being mixed but not burning. At this location, we expect that the proportion of pilot gas at the stoichiometric mixture to be much smaller compared to $x/D = 7.5$, but apparently there is still a sufficient amount to form a mixing line on the rich side. Therefore, the high temperature dissipation is largely due to the rapid mixing of the pilot gas with the rich mixtures. The mixing is faster than the reactions, resulting a mixing line. Again, the results suggest that each of these laminar flamelet is split by the pilot gas to form two flamelets with one on the lean side burning and the one on the rich side extinguished. Again, for the samples at much lower temperature ($< 1200K$) the line images in the $\xi - T$ space are straight line from the lean to the rich side, consistent with extinguished laminar flamelets. There is no apparent evidence of the pilot separating the lean and rich side. This is probably because the pilot gas is already mixed with the rest of the fluid due to large $\chi$ in these flamelets. The results for flame E are similar.

At $x/D = 30$ for small SGS variance (figure 2.15a), $\chi_T$ is low for high temperatures and is higher for intermediate temperatures (1500-1800K). Due to reignition there are fewer samples with temperature below 1500K. For large SGS variance (figure 2.15b), $\chi_T$ has two peaks near $\xi = 0.3$ and 0.5 and $T = 1600K$ although the peak values are smaller. These are again due to mixing of
Figure 2.17: The conditionally filtered thermal dissipation rate of Flame E at $x/D = 15$ near stoichiometric mixture with lean and rich mixtures. The dissipation rate is approximately the same for both peaks whereas at $x/D = 7.5$ and 15 one peak dominates.

The temperature dissipation results indicate that for small SGS variance, which corresponds to distributed reaction zones, there is temperature mixing in the absence of significant mixture fraction mixing. On the other hand, for large SGS variance, mixture fraction mixing and temperature mixing proceed simultaneously according to laminar flamelets. These qualitatively different properties of SGS mixing must be reflected by mixing models.

\[(a) \langle \xi'^2 \rangle_L = 0.0028 \quad (b) \langle \xi'^2 \rangle_L = 0.064\]
Figure 2.18: The conditionally filtered thermal dissipation rate of Flame E at $x/D = 30$

(a) $\langle \xi'' \rangle_L = 0.0018$

(b) $\langle \xi'' \rangle_L = 0.044$
Chapter 3

Conditionally Filtered Diffusion of Mixture Fraction and Temperature

3.1 Introduction

Turbulent mixing and turbulence-chemistry interaction are key processes in turbulent combustion. Accurate predictions of turbulent flames depend critically on correct modeling of these processes. In large-eddy simulation (LES) of turbulent combustion mixing by the large, resolved scales is computed while the effects of the subgrid scales are modeled. Specifically, the subgrid-scale (SGS) scalar mixing and the resulting instantaneous distribution of scalar values in each grid volume, which is the species filtered joint mass density function (FMDF), must be faithfully represented in order to accurately predict the chemical reaction rate\cite{37,11}. Modeling the FMDF, therefore, is the main challenge in LES and requires knowledge of SGS mixing and its interaction with chemistry.

Our recent studies ([45, 39, 50, 53, 51, 52]) have shown that the SGS mixture fraction at a fixed location has qualitatively different filtered density function (FDF) shapes and structures depending on the instantaneous SGS scalar variance. When the SGS variance is small compared to its mean value, the distribution of the SGS scalar is close to Gaussian, indicating well mixed SGS scalar fields. When the SGS variance is large compared to its mean value, distribution is bimodal, indicating highly nonpremixed SGS scalar fields. In a flame this mixing scenario would indicate that the fuel lean and rich regions of the SGS fields are highly segregated. There is a sharp
interface separating the two regions, across which there is a large scalar value jump (can be as large as the integral-scale fluctuations). The conditional SGS structure on average resembles that of a counter-flow diffusion flame, which is a model for laminar flamelets.

The well-mixed and the highly-nonpremixed SGS mixture fraction fields have strong influences on the flame structure. The former is likely to result in distributed reaction zones while the latter supports laminar flamelets\cite{52, 10}. The mixture fraction-temperature filtered mass density function (FMDF) and the conditionally filtered dissipation rates of the mixture fraction and the temperature also are consistent with distributed reaction zones and laminar flamelets, respectively. Here we use the term “flamelets” to describe the thin physical flame structure rather than any modeling approach; therefore, we simply refer to them as flamelets hereafter. In this study we investigate the effects of the SGS mixture fraction structure on the conditional scalar diffusion and the temperature diffusion in turbulent partially premixed flames, which evolve the FMDF of mixture fraction and temperature:

\[
F_{\xi TL}(\xi, \hat{T}; x, t) = \langle \rho(x, t) \delta(\xi - \hat{\xi}) \delta(T - \hat{T}) \rangle_L = \\
\int \rho(x', t) \delta(\xi - \hat{\xi}) \delta(T - \hat{T}) G(x - x') dx',
\]

where \(\xi, T, \hat{\xi}, \text{ and } \hat{T}\) are the mixture fraction, temperature, and their sample-space variables, respectively. \(\rho\) is the fluid density. The subscripts \(\ell\) and \(L\) denote conventional and Favre filtered variables, respectively. The knowledge of these diffusion terms is a first step in understanding the SGS turbulence-chemistry interaction and an important step toward understanding the SGS mixing of multiple reactive scalars.

### 3.2 Experimental data and processing procedures

We use experimental data obtained in piloted turbulent partially premixed methane with a 1:3 ratio of CH\(_4\) to air by volume (Sandia flame D and E, see Ref.\cite{28, 2}). Their measurements employed combined line-imaging of Raman scattering, Rayleigh scattering, and laser-induced CO fluorescence. Simultaneous measurements of major species (CO\(_2\), O\(_2\), CO, N\(_2\), CH\(_4\), H\(_2\)O, and H\(_2\)), mixture fraction (obtained from all major species), temperature, and the radial component of scalar
dissipation rate were made. The mixture fraction is calculated using a variation of Bilger’s definition, which has been modified by excluding the oxygen terms. The length of the imaging line is 6.13 mm with a resolution of 0.2044 mm.

Measurements of the filtered density functions require spatial filtering of scalar fields. In this work one-dimensional filtering is employed. In LES filtering is generally performed in three dimensions. Our previous results [50] have shown, however, that the FDF obtained with a one-dimensional filter is qualitatively the same as those with a two-dimensional filter, which has been shown to be a very good approximation of three-dimensional filters, with errors of approximately 5% for the rms resolvable- and subgrid-scale variables[47]. For similar bimodality the corresponding SGS variance is somewhat larger for a one-dimensional filter. For conditional diffusion (and dissipation), the primary effect of a one-dimensional filter is a somewhat higher SGS variance. But the increase is much smaller than the change needed to affect the shape of the conditional diffusion. Consequently, one-dimensional filters are expected to yield similar results. To ensure that the results are relevant to LES the filter sizes ∆ employed in this work (3.0 mm and 4.9 mm) are significantly larger than the dissipative (Corrsin) scales (0.065 - 0.106 mm[54]), such that the subgrid scales contain sufficient fluctuations to interact with chemistry, allowing the physics of the SGS mixing and its interaction with chemistry to be related to inertial-range dynamics.

3.3 Results

The scalar diffusion and temperature diffusion are analyzed using their conditional samples. We use the Favre filtered mixture fraction, $\langle \xi \rangle_L = \langle \rho \xi \rangle_{\ell} / \langle \rho \rangle_{\ell}$, and the Favre SGS scalar variance,

$$
\langle \xi'^2 \rangle_L \equiv \frac{1}{\langle \rho \rangle_{\ell}} \int F_{\xi L}(\hat{\xi}; \mathbf{x}, t)(\xi - \langle \xi \rangle_L)^2 d\xi = \langle \rho \xi^2 \rangle_{\ell} / \langle \rho \rangle_{\ell} - \langle \xi \rangle_L^2, \quad (3.2)
$$

as conditioning variables.

The conditionally filtered scalar and temperature diffusion conditional on both the mixture fraction and temperature, $\langle \langle \partial_{xy} (\rho D \xi) \rangle \xi, T \rangle_{\ell} | \langle \xi \rangle_L, \langle \xi'^2 \rangle_L \rangle$ and $\langle \langle \partial_{xy} (\rho D T) \xi, T \rangle_{\ell} | \langle \xi \rangle_L, \langle \xi'^2 \rangle_L \rangle$ are shown in Figs. 1-5. In the FMDF equation these variables appear in the terms transporting the FMDF in the $\xi$ and $T$ spaces, respectively; therefore, they are the two components of the diffusion
velocity of the FMDF in the $\xi - T$ space. In the present study we use streamlines and isocontours to represent the direction and the magnitude of the diffusion velocity, respectively. The diffusion terms are calculated using tenth-order central differencing. The mixture fraction diffusion and the temperature diffusion are normalized by the filtered scalar dissipation rate, the SGS variance, and the maximum values of the mixture fraction (1.0) and temperature (2300 K), respectively.

The results for Flame D at $x/D = 7.5$ is shown in Fig. 1. For small SGS variance, the streamlines appear to move first towards a manifold close to the ridgeline of the FMDF, in the direction perpendicular to the ridgeline. They then move along the manifold towards a stagnation point near $\xi \approx 0.4$ and $T = 2000 K$. The velocity magnitude decreases as it approaches the ridgeline. The ridgeline, therefore, appears to be a one-dimensional manifold in a two-dimensional scalar space, to which the streamlines first approach. After approaching the ridgeline the diffusion becomes one-dimensional in scalar space. The magnitude of the diffusion velocity decreases upon approaching the manifold; therefore, the diffusion towards the manifold is a fast process whereas diffusion along the manifold is a slow process.

This streamline pattern can be understood in terms of the SGS mixture fraction structure for small SGS variance and the resulting quasi-equilibrium distributed reaction zones (QEDR) proposed by Bilger [4]. Because the SGS mixture fraction is well mixed, diffusion of the SGS mixture fraction is towards its local mean. With the dissipation-scale mixture fraction fluctuations smaller than the reaction zone width [52], the well-mixed SGS mixture fraction results in QEDR. In such reaction
zones the temperature depends on the mixture fraction and the (local) scalar dissipation rate. This situation is different from flamelets, in which the temperature depends on the mixture fraction and the scalar dissipation rate at the stoichiometric mixture fraction. Assuming unity Lewis number, the temperature diffusion in a QEDR, therefore, depends on these fields as:

$$\frac{1}{\rho} \frac{\partial}{\partial x_i} (\rho D \frac{\partial T}{\partial x_i}) = \frac{\partial^2 T}{\partial \xi^2} \chi + \frac{1}{\rho} \frac{\partial T}{\partial \xi} \frac{\partial}{\partial x_i} (\rho D \frac{\partial \xi}{\partial x_i}) + \frac{\partial^2 T}{\partial \xi \partial \chi} \frac{\partial \xi}{\partial x_i} \frac{\partial T}{\partial \chi} + \frac{1}{\rho} \frac{\partial T}{\partial \chi} \frac{\partial}{\partial x_i} (\rho D \frac{\partial \chi}{\partial x_i}), \quad (3.3)$$

where $\chi = D \frac{\partial \xi}{\partial x_i} \frac{\partial \xi}{\partial x_i}$ and $\chi_\chi = D \frac{\partial \chi}{\partial x_i} \frac{\partial \chi}{\partial x_i}$ are the scalar dissipation rate and the dissipation rate of $\chi$, respectively. In a QEDR, which is not far from equilibrium, the first term is always negative, with the magnitude diminishing towards the equilibrium temperature. This trend is inconsistent with the sign change in the temperature diffusion shown in Fig. 1. The second term is close to zero near the local average mixture fraction, $\langle \xi \rangle_L$, because the scalar diffusion is small. The third term is more complex but may be small due to the mixed dissipation rate. The sign of the fourth term is determined by $\frac{\partial^2 T}{\partial \chi^2}$, which is chemistry dependent. For the simple chemistry model used by Bilger[4], the perturbation of a progress variable from its equilibrium value is given as $\sim -\chi^{1/2}$. If we assume $T - T_e \sim -\chi^{1/n}$, then $\frac{\partial^2 T}{\partial \chi^2}$ is positive, where $T_e$ is the equilibrium temperature, and $n > 1$, reflecting a nonlinear reaction rate. While $\chi_\chi$ may increase when $\chi$ increases ($T$ decreases), $\frac{\partial^2 T}{\partial \chi^2}$ decreases. Thus, the fourth term also is likely to be inconsistent with the trend in Fig. 1.

In the last term, $\frac{\partial T}{\partial \chi}$ is negative. Our previous study[39] shows that the dissipation rate diffusion term in a well-mixed scalar field is similar to the mixture fraction dissipation, being generally positive for $\chi > \chi_L$ and negative for $\chi < \chi_L$, where $\chi_L$ is the local average of $\chi$. The contribution of the last term to the temperature diffusion, therefore, is positive for temperatures above the local mean where $\chi < \chi_L$, and is negative for temperatures below the local mean where $\chi > \chi_L$, resulting in convergence of the streamlines to a manifold. Thus, it appears that only this term is consistent with the observed streamline pattern. Physically, since the temperature field in a QEDR is closely related to the scalar dissipation rate (in addition to the mixture fraction), the temperature diffusion is controlled partly by the diffusion of the scalar dissipation rate.

The observed diffusion velocity streamline pattern has some similarities to three-scalar mixing in a non-reacting flow. In our recent study of three-scalar mixing in a co-axial jet, which will be published in a separate paper, the three scalars are introduced by a center jet, an annular flow,
and co-flow air, with the second scalar initially separating the first and the third. The resulting diffusion velocity streamline pattern in this jet is qualitatively similar to that in Fig. 1a. There is a manifold to which the streamlines converge quickly. They then move at a slower velocity on the manifold. During the convergence the diffusion of the second scalar is faster than the first, analogous to the fast diffusion of temperature shown in Fig. 1a. In this jet the three scalars have a similar spatial relationship to that among the mixture fraction, the temperature, and the co-flow air in a nonpremixed flame; therefore, the temperature in the QEDR has a similar physical space structure as the annulus flow, separating the other two scalars. Such a structure is different from three scalar mixing cases where the three scalars are arranged symmetrically in physical space [24].

For large SGS variance (Fig. 1b) the streamlines for very rich ($\xi > 0.6$) and lean ($\xi < 0.2$) mixtures generally move in the direction of the ridgeline of the FMDF (see Ref. [10]) towards the stoichiometric mixture fraction. Our previous results have shown that for large SGS variance the SGS flames are strained flamelets. Here the mixture fraction profiles have approximately error-function profiles (ramp-cliff structure). Thus, the diffusion of the mixture fraction is towards the center of the profiles (appears to be near $\xi = 0.45$). For very rich and lean mixtures the temperature depends approximately linearly on the mixture fraction; therefore, its diffusion is proportional to the mixture fraction diffusion, resulting in straight diffusion streamlines along the ridgeline.

Near the peak temperature the mixture fraction diffusion is small because this region is close to the center of the error-function profiles where the curvature of the profiles is zero. The temperature diffusion is negative due to the negative curvature of the temperature profiles as a function of the mixture fraction and the approximately linear mixture fraction profiles. Consequently, the streamlines starting from the equilibrium curve near $\xi = 0.45$ move nearly vertically towards lower temperatures. As the streamlines move towards lower temperatures, the scalar dissipation rate increases, corresponding to more strongly strained flamelets with stronger diffusion. The largest magnitude of the diffusion velocity vector occurs for temperatures near 1600-1800K. Below this temperature range the temperature profiles become broader in the mixture fraction space with smaller curvatures, resulting in lower temperature diffusion. There appears to be a stagnation point at $\xi \approx 0.4$ and $T = 1300K$. Note that although this point appears to be the “center” of diffusion, it does not correspond to the conditional mean temperature for this mixture fraction value.

The streamlines starting from the very rich and lean regions move up along the ridgeline and turn near $\xi \approx 0.27$ and $T = 1600K$ and near $\xi \approx 0.55$ and $T = 1600K$, respectively, towards
the stagnation point. The temperature diffusion changes sign near these points, where the inflection points of the temperature profiles are located. This result is consistent with our previous study [10] which shows that the temperature dissipation rate is largest in this region. Below these points the diffusion is dominated by mixing whereas above it the diffusion is strongly influenced by both mixing and reaction. This streamline pattern is also consistent with the structure of flamelets.

Figure 1b also shows that in the very rich and lean regions the streamlines generally first approach the FMDF ridgeline and then move along it. One possible reason for this trend is the diffusion among flamelets in the direction along the iso-mixture fraction surfaces. Because the ridgeline represents the flamelets with the highest probability of occurrence, the flamelets nearby tend to diffuse towards the ridgeline. Another possibility is that in the SGS fields with large SGS variance, in addition to the ramp-cliff structure, there are also “background” mixture fluctuations, which are generally well mixed and tend to have smaller dissipation time scales, causing diffusion streamlines to converge to those of the flamelets. There also appears to be two diffusion processes involved: in the fast process the streamlines approach a one-dimensional manifold and in the slow process they move along the manifold.

At $x/D = 15$ the results for small SGS variance (Fig. 2a) are similar to those at $x/D = 7.5$ for the samples with temperatures higher than 1900K, where the mixing of temperature is dependent on the mixture fraction, the scalar dissipation rate, and the chemistry. There is, however, a second manifold with a stagnation point near $\xi = 0.4$ and $T = 1600K$, probably due to the mixing between the burning and extinguished samples, which have temperatures as low as 1000K. The mixing process
at these temperatures is different from that at higher temperatures. Here the reaction rate has decreased significantly due to local extinction. The temperature no longer strongly depends on the scalar dissipation rate and the chemistry. Its mixing (e.g., Ref. [42]), therefore, becomes similar to that of a non-reactive scalar. In addition, because the SGS mixture fraction is well mixed, the mixing process is similar to three-scalar mixing in a homogeneous scalar field. The fast convergence to the manifold in the direction of temperature suggests that the mixing of temperature is faster than that of mixture fraction.

To understand this streamline pattern further, we compute the conditionally filtered diffusion with the Favre filtered temperature as a third conditioning variable, in addition to the Favre filtered mixture fraction and the Favre SGS scalar variance. The samples used to obtain Fig. 2a are separated into two groups, one with $\langle T \rangle_L > 1800$ K and the other with $\langle T \rangle_L < 1800$ K. The streamline pattern for the former (Fig. 3a) is similar to that at $x/D = 7.5$. There is one manifold, to which the streamlines converge. The streamlines for the latter (Fig. 3b) converge to approximately 1600K, corresponding to the second stagnation point in Fig. 2a. The diffusion vector pattern shown in Fig. 2a, therefore, can be viewed as a superposition of two different states of the SGS flames: mixing in nearly fully burning distributed reaction zones and mixing between fully burning and extinguished distributed reaction zones. Between the stagnation point near $\xi = 0.4$ and $T = 1600$ K and the one near 2000K, there appears to be a saddle point (or a saddle line) separating the two regions. The location of the saddle point probably depends on the relative strength of the two stagnation points.

For large SGS variance (Fig. 2b) the overall diffusion pattern for burning samples are similar.
to that at \( x/D = 7.5 \). For the lean mixtures the streamlines turn towards the stagnation point as early as \( \xi \approx 0.15 \) and \( T = 1300K \). There are more extinguished samples, for which the streamlines move primarily in the direction of mixture fraction towards \( \xi \approx 0.4 \), with only modest increases in temperature. These trends indicate that for these samples the mixture fraction diffusion is initially much faster than the temperature diffusion. An examination of the instantaneous profiles in the scalar space shows straight lines running from the lean side to the rich side, largely in the same direction of the diffusion vectors; therefore, these lines are extinguished flamelets, hence the smaller temperature diffusion. For these extinguished flamelets, temperature diffusion can occur in the direction of the mixture fraction gradient as well as along the iso-mixture fraction surface. The latter is diffusion among burning and extinguished flamelets (flamelet-flamelet interaction). Near \( \xi = 0.4 \) the scalar is close to the center of the error-function profiles (ramp-cliff structure) where mixture fraction diffusion is zero; therefore, the streamlines move largely in the direction of temperature.

For rich samples there are a significant number of nearly straight streamlines running from very rich region (\( \xi \approx 0.9, T \approx 500K \)) towards the region corresponding to the pilot. These streamlines may be due to the pilot flame separating the rich and lean mixtures, and are essentially a result of mixing between the pilot and the fuel/air streams without reactions. The pilot flame, therefore, appears to have a strong influence on the diffusion. Our previous results \([10]\) have shown that it also has a strong influence on the temperature dissipation. These streamlines turn near \( \xi = 0.5 \) and \( T = 1600K \) towards the stagnation point, a result of the strained flamelets. Similar to the results at \( x/D = 7.5 \), the rich samples close to equilibrium diffuse first towards a manifold (the ridgeline of the FMDF) and then follow the manifold. The approach to the manifold is faster than at \( x/D = 7.5 \). In the low temperature region the temperature diffusion is faster than for the lean samples.

At \( x/D = 30 \) the results for small SGS variance (Fig. 4a) are similar to those at \( x/D = 15 \). For large SGS variance (Fig. 4b) the influence of the pilot is much less evident with the streamlines from the rich side with temperature below 1200K moving in a direction much closer to the horizontal direction toward \( \xi \approx 0.4 \), indicating that the SGS mixing has progressed much further and that there is little pure pilot gas left. These streamlines are a result of mixing along scalar profiles running from the rich to the lean side (extinguished flamelets). Note that at \( x/D = 15 \) the streamlines in this region are closer to the direction of the mixing line between the pilot and the fuel stream, suggesting that the influence of the pilot on the diffusion is stronger than the effects of the extinguished flamelets.

The results for flame E (Fig. 5) are qualitatively similar to those for flame D. Due to the
Figure 3.4: The mean conditionally filtered scalar diffusion and temperature diffusion conditional on both the mixture fraction and temperature for $\Delta = 3.0$ mm and $\langle \xi \rangle_L = \xi_s$ at $x/D = 30$ in flame D. (a) $\langle \xi''^2 \rangle_L = 0.0019$; (b) $\langle \xi''^2 \rangle_L = 0.059$.

higher Reynolds number, flame E already has a significant amount of local extinction at $x/D = 7.5$, with the largest amount occurring at $x/D = 15$. For small SGS variance, the temperature decreases to as low as 1000K at $x/D = 7.5$ and $x/D = 15$. The amount of local extinction is also much larger than in flame D. The diffusion streamlines at $x/D = 15$ is similar to those for flame D. But the lower stagnation point occurs at a slightly lower temperature. In addition, the stagnation point near 2000K appears to be weaker, which may be due to the stronger stagnation point near 1600K resulting from the larger amount of local extinction.

For large SGS variance, the streamline patterns also are generally similar to those for flame D. At $x/D = 7.5$ the streamlines for the extinguished samples are approximately symmetric with respect to $\xi = 0.4$. These streamlines become asymmetric at $x/D = 15$, again perhaps due to the influence of the pilot flame. They become more symmetric at $x/D = 30$.

The results for the diffusion streamlines in Figs. 1a & 2a suggest that the SGS mixing processes for small SGS variance can be modeled in a way similar to non-reactive scalars. For QEDRs, which have temperatures not far from the equilibrium values, the mixing can be modeled through the mixing of mixture fraction and the scalar dissipation rate, due to the strong influence of the latter on the temperature. The similarities of the streamline pattern to those of three-scalar mixing in a co-axial jet suggest that the mixing process needs to be modeled in a way that reflects the separation of two of the scalars (the mixture fraction and the co-flow) by the third (the scalar dissipation rate) in physics. For SGS fields with lower temperature (e.g., $\langle T \rangle_L < 1800K$), the SGS mixing can be modeled as the mixing of mixture fraction and the non-reactive temperature due to
Figure 3.5: The mean conditionally filtered scalar diffusion and temperature diffusion conditional on both the mixture fraction and temperature for $\Delta = 3.0$ mm and $\langle \xi \rangle = \xi_s$ in flame E. (a), (c), and (e): $x/D = 7.5, 15$ and $30$ respectively. Small SGS variance ($\langle (\xi')^2 \rangle_L = 0.0011, 0.0028$, and $0.0018$); (b), (d), and (f): the same locations. Large SGS variance ($\langle (\xi')^2 \rangle_L = 0.081, 0.064$, and $0.044$).
the decoupling of temperature from the chemistry and the scalar dissipation rate as a result of much reduced reaction rate. In contrast to the mixing in QEDRs, the mixing process for these SGS fields resembles three-scalar mixing in a homogeneous scalar field, therefore can be modeled as such. For large SGS variance, mixing models need to incorporate the physics of the more complex diffusion velocity pattern resulting from the flamelet structure and local extinction.
Chapter 4

Conditional Statistics Condition on Mixture Fraction and Temperature

We also investigated the conditional statistics without filtering using joint mass density functions (JMDF) of mixture fraction and temperature, conditional mixture fraction and temperature dissipation rates condition on mixture fraction and temperature as well as streamline plots of mixture fraction and temperature diffusion condition on mixture fraction and diffusion.

4.1 Joint Mass Density Functions

For Flame D at $x/d = 7.5$, the joint PDF is shown in Fig. 4.1a. The mean mixture fraction of the data is $\langle \xi \rangle = 0.34$. The JMDF has a ridge which is close the equilibrium curve. The JMDF has a peak centered near $\xi = 0.30$ and $T = 1800K$. The JMDF on rich side is broader than lean side. At this location, there is little extinction as indicated by the extremely low probability below 1500K near the stoichiometric mixture fraction.

Moving downstream to $x/d = 15$ (Fig. 4.1b), significant amount of local extinction is observed as shown as the higher probability for low temperature. The JMDF ridge is also close to equilibrium curve. The JMDF retains single peak, but the peak value is reduced.

Further downstream at $x/d = 30$ (Fig. 4.1c), the amount of local extinction is reduced by approximately 50% indicating reignition. The ridge is close the equilibrium curve. The JMDF on
Figure 4.1: Joint mass density function for Flame D at different downstream locations

rich side is broader than lean side. The JMDF has one peak centered near $\xi = 0.45$ and $T = 2050$K.

The JMDF for Flame E (Fig. 4.2a, 4.2b and 4.2c) is similar to Flame D, except that there is already a significant amount of local extinction at $x/d = 7.5$. The amount of extinction drops slightly when move to $x/d = 15$, but still approximately three times the amount in Flame D at the same location. Reignition further reduces extinction at far downstream ($x/d = 30$).
4.2 Conditional mean mixture fraction dissipation

In general, the mixture fraction dissipation is higher near $\xi = 0.5$, where the peak gradient of mixing layer is located. The dissipation rate near equilibrium curve is higher for lower temperature, which can be explained as flamelets with higher strain rates. At $x/d = 7.5$ (Fig. 4.3a), though the JMDF does not extend to lower temperatures due to little local extinction, the peak dissipation still reaches over $500s^{-1}$. Such a high dissipation rate is likely to initiate local extinction, therefore, the flame at this location is probably maintained by the pilot.

Moving downstream to $x/d = 15$ (Fig. 4.3b), the JMDF extends to lower temperatures
due to local extinction. The dissipation is higher for $\xi$ near 0.4 to 0.5 as predicted by ramp-cliff structure. Along the equilibrium curve, the dissipation shows similar trends as upstream but with lower values. Away from the equilibrium curve, the dissipation rate increases for lower temperature, which is consistent with the characteristics of flamelets. For the extinguished samples ($T < 1400K$), the dissipation is over $100s^{-1}$. This dissipation rate is much less than the dissipation of upstream, due to both reduced diffusivity at lower temperature and a reduced strain rate.

Further move downstream to $x/d = 30$ (Fig. 4.3c), the dissipation structure is similar as upstream, except dissipation rate is lower than at the upstream locations. This trend is consistent with the smaller amount of local extinction and the occurrence of reignition.

Generally, Flame E has more local extinction than Flame D, which gives more extended dissipation. At $x/d = 7.5$ (Fig. 4.4a), away from the equilibrium curve, Flame E gives more extinction with the dissipation much less than Flame D ($100 \sim 200s^{-1}$ compared to $200 \sim 400s^{-1}$), this may come from less portion of pilot when Flame E has higher flow rate.

### 4.3 Conditional mean temperature dissipation

For Flame D at $x/d = 7.5$ (Fig. 4.5a), the temperature dissipation is higher for intermediate temperature, which is consistent with temperature structure of flamelet near equilibrium. The highest peak is near $\xi = 0.62$ and $T = 1600K$. This corresponds to the local peak in mixture fraction dissipation. This shows that near equilibrium curve, temperature is a function of mixture fraction, therefore, temperature dissipation is proportional to mixture fraction dissipation. Similarly at intermediate temperature ($1300 < T < 1800K$), temperature dissipation increases as mixture fraction dissipation except near stoichiometric mixture fraction where temperature reaches local maximum. The temperature dissipation has two weaker peaks near $\xi = 0.45$ and 0.23, $T = 1700K$ while at the same location mixture fraction only has a moderate dissipation rate $\chi_\xi \sim 100s^{-1}$. An examination of the line images shows that this is due to direct mixing between pilot and rich or lean gases without reaction.

At $x/d = 15$ (Fig. 4.5b), the temperature dissipation is higher for intermediate temperature. Near equilibrium, the temperature dissipation increases with mixture fraction dissipation, which consistent with flamelet structure. The temperature gives small dissipation for $T > 1900K$ due to reaching its local maximum. This indicates that temperature layer becomes unstable when
mixture fraction dissipation increases, this generates local extinction. Though at high temperature $T > 1500$K, the mixture fraction has a ramp-cliff structure similar to upstream, due to less effects of pilot, the mixture fraction dissipation induces thinner temperature mixing layer. As a result, thermal energy diffuses much faster than species and temperature decreases quickly to form local extinction. Such temperature structure gives different temperature structure from burning flamelets at $x/d = 7.5$. The deviation from burning flamelets is observed by the disappearing of the dissipation valley near stoichiometric mixture fraction at $x/d = 7.5$. At very low temperature $T < 1500$K, the temperature dissipation is very small due to reduced thermal diffusivity and less temperature
At $x/d = 30$ (Fig. 4.5c), the temperature dissipation is largely reduced due to mixing process. The dissipation is larger for intermediate temperature. Along the equilibrium curve, the temperature follows from flamelet prediction. The high temperature dissipation region near $\xi = 0.65$ corresponds to high mixture fraction dissipation. There appears a peak near $\xi = 0.25$, $T = 1400K$ corresponding to the high mixture fraction dissipation at the same location, which results from direct mixing between pilot gas and lean mixture.

Flame E (Fig. 4.6a, 4.6b and 4.4c) generally has similar result except for more local extinc-
tion at $x/D = 7.5$.

Figure 4.5: Conditional mean temperature dissipation rate for Flame D at different downstream locations

(a) $x/D = 7.5$
(b) $x/D = 15$
(c) $x/D = 30$

4.4 Conditional mean diffusion streamline

For $x/d = 7.5$ (Fig. 4.7a), near equilibrium, the mixtures first converges to a manifold corresponds to the ridge of the JMDF. Along the manifold, the magnitude of diffusion vector is small. Then the diffusion vectors follow the manifold toward the reaction zone. Mixtures coming from outside reaction zones will first go up to 1700K, then moving towards low temperature. During this process, the mixture fraction always diffuses toward intermediate value, in this case approximately
Figure 4.6: Conditional mean temperature dissipation rate for Flame E at different downstream locations

0.4. The turnover position is $\xi = 0.3$ and 0.5, $T = 1800K$. Within the reaction zone, mixture with temperature beyond the manifold first diffuse toward then cross the manifold in almost vertical direction. This shows that the dominant mixing is between mixture with different temperature but close mixture fraction. However, when crossing the manifold, diffusion streamlines are distorted by the manifold. Compare to our previous results, these distortion is a result of additive horizontal diffusion vectors from strong mixing of mixture fraction but relatively weak mixing of temperature. These additional diffusion vectors are consistent with the distributed reaction zones prediction as shown in small SGS variance case. Near $\xi = 0.4$ the scalar is close to the center of ramp-cliff structure,
therefore the mixture fraction diffusion is zero, the mixing between different temperatures results in a vertical converging manifold. The diffusion vector gives highest magnitude at $\xi = 0.4, T = 1800K$.

At $x/d = 15$ (Fig. 4.7b), there are two dominant converging manifolds indicated by the small magnitude of diffusion vectors, one is along the equilibrium curve, the other one is vertical near $\xi = 0.4$ and low temperature. For the rich mixtures near equilibrium, the mixtures quickly converge to the converging manifold along the equilibrium curve, and then move towards reaction zone along this manifold. The situation is similar for the lean mixtures except that the manifold seems to be unstable, as the streamlines quickly deviate from the manifold after crossing. Within the reaction zone at high temperature, the distorted streamlines reflect the composition of two types of mixing vectors depending on local mixture fraction fluctuations. For large local mixture fraction fluctuations, the mixture fraction has the ramp-cliff structure, the high temperature region is a result of burning flamelets. In this case, the mixture fraction the mixing vectors are almost vertical as well as large magnitude. There appears a stagnation point near $\xi = 0.4$ and $T = 1550K$.

At $x/d = 30$ (Fig. 4.7c), the diffusion streamlines near equilibrium quickly converge to the equilibrium curve. Along the equilibrium curve the magnitude is small. Below the equilibrium curve, the converging streamlines are almost perpendicular, our pervious results show that this is because less effect of pilot.
Figure 4.7: Streamline plot of Conditional mean mixture fraction and temperature diffusion for Flame D at different downstream locations
Figure 4.8: Streamline plot of Conditional mean mixture fraction and temperature diffusion for Flame E
Chapter 5

Filtered Statistics Condition on Mixture Fraction, Temperature and Species

In order to study the impact of different mixing regimes on the reactive species, we studied the FMDF of and conditionally filtered dissipation rates condition on mixture fraction, temperature and one of the species. The FMDF is defined as

\[ F_{\xi Y_i}(\xi, \hat{T}, \hat{Y}_i; x, t) = \langle \rho \delta(\xi - \hat{\xi}) \delta(T - \hat{T}) \delta(Y_i - \hat{Y}_i) \rangle_{t} \]

\[ = \int \rho(x', t) \delta(\xi(x', t) - \hat{\xi}) \delta(T(x', t) - \hat{T}) \delta(Y_i(x', t) - \hat{Y}_i) G(x - x') dx' \]  

The dissipation rate is defined as

\[ \chi_{\xi} = D_{\xi} \frac{\partial \xi}{\partial x_i} \frac{\partial \xi}{\partial x_i} \]

\[ \chi_T = D_T \frac{\partial T}{\partial x_i} \frac{\partial T}{\partial x_i} \]

\[ \chi_s = D_s \frac{\partial Y_s}{\partial x_i} \frac{\partial Y_s}{\partial x_i} \]  

The diffusivity of the sth species \( D_s \) is taken to be the same of mixture fraction diffusivity at the same temperature, which is equivalent to unity Lewis number assumption.
5.1 Reduced methane reaction mechanism

Peters and Williams [34] considered three steps reduced reaction mechanism by assuming steady state of all radical species and quasi-equilibrium of reactions involving radicals.

\[
\begin{align*}
\text{CH}_4 + \text{O}_2 & \rightarrow \text{CO} + \text{H}_2 + \text{H}_2\text{O} \quad (5.6) \\
\text{CO} + \text{H}_2\text{O} & \rightleftharpoons \text{CO}_2 + \text{H}_2 \quad (5.7) \\
\text{O}_2 + 2\text{H}_2 & \rightarrow 2\text{H}_2\text{O} \quad (5.8)
\end{align*}
\]

5.2 FMDF and dissipation rates condition on $\xi$, $T$ and $\text{CH}_4$

5.2.1 FMDF condition on $\xi$, $T$ and $Y_{\text{CH}_4}$

For flame D at $x/D = 7.5$, the FMDF of $\text{CH}_4$ is unimodal at small SGS variance (Fig. 5.1a), with peak located at $0.4, 2000\text{K}, 0.004$ on the equilibrium curve. The majority of the FMDF is located at high temperature with very little amount of $\text{CH}_4$ showing very few amount of local extinction. At large SGS variance (Fig. 5.4a), the FMDF concentrates along the equilibrium curve showing little local extinction. The FMDF has two branches, the branch at lean mixture showing little $\text{CH}_4$ while the branch at rich mixture shows the $\text{CH}_4$ accumulates linearly with mixture fraction. The FMDF has two peaks, a strong peak is formed at lean mixture with $\xi = 0.14, T = 1200\text{K}$. The $\text{CH}_4$ is completely consumed in this situation. A weaker peak is located at $\xi = 0.66, T = 1430\text{K}$.

For flame D at $x/D = 15$, the FMDF of $\text{CH}_4$ is unimodal for small SGS variance (Fig. 5.2a), with peak located at $0.32, 1900\text{K}, 0$ on the equilibrium curve. The FMDF concentrates along a two dimensional manifold showing that the mass fraction of $\text{CH}_4$ can be approximated well using mixture fraction and temperature. This indicates the heat releasing reactions immediately take place after $\text{CH}_4$ dissociation. This supports large Damkohler number assumption. This ridge-surface of the FMDF is curved to lower temperature due to the buildup of CO.

For large scalar SGS variance (Fig. 5.5a), the FMDF of $\text{CH}_4$ is bimodal, consistent with our previous results. The peak at lean mixture is located at $\xi = 0.15, T = 1300\text{K}, Y_{\text{CH}_4} = 0$, the other peak is located at $\xi = 0.65, T = 1350\text{K}$ and $Y_{\text{CH}_4} = 0.055$. Both peaks are on the equilibrium curve. Since both peaks are outside the reaction zones, this FMDF resembles the structure of laminar flamelets. There is few local extinction as shown in low amount of low temperature probability.
within the reaction zone.

Further downstream to $x/D = 30$ (Fig. 5.3a and 5.6d), the amount of local extinction is reduced indicates reignition.

### 5.2.2 Dissipation rates condition on $\xi$, $T$ and $\text{CH}_4$

For flame D at $x/D = 7.5$, when scalar SGS variance is small, the conditionally filtered mixture fraction dissipation rate ($\frac{\langle \chi|\xi, T,Y_{\text{CH}_4} \rangle |\langle \xi \rangle_L, \langle \xi'^2 \rangle_L }{\langle \xi \rangle_L}$) has little dependency on $\xi$, but increases as temperature drops (Fig. 5.1c). This is consistent with our previous conclusions on being quasi-equilibrium distributed reaction zones. The scalar dissipation rate has no dependency on $\text{CH}_4$ in lean mixture, but weakly increases in rich mixture. This shows that as dissipation rate increases, the first reaction for $\text{CH}_4$ consumption becomes incomplete.

The temperature dissipation rate (Fig. 5.1c) is small for peak temperature because $dT/d\xi = 0$. Away from the peak temperature near equilibrium curve, temperature linearly depends on mixture fraction, thereby, the temperature dissipation rate resembles the structure of mixture fraction dissipation.

On the lean side the $\text{CH}_4$ dissipation rate (Fig. 5.1d) is very small and comparable to noise contributions, it also shows little dependency on mixture fraction and temperature. Considering the low level of $\text{CH}_4$ mass fraction (less 1% in mass fraction), $\text{CH}_4$ is almost fully burned. On the rich side the $\text{CH}_4$ dissipation is larger for higher $\text{CH}_4$ mass fraction. This is consistent with distributed reaction zones theory.

For large scalar SGS variance, the mixture fraction dissipation rate (Fig. 5.4d) is smaller for lean and rich mixture and larger for intermediate $\xi$, this is consistent with laminar flamelets. Dissipation rate reaches local maximum near $\xi = 0.45$ where the sharpest mixing layer is located. Near equilibrium, the dissipation rate increases as temperature drops, which is consistent with strained laminar flamelets. Within the reaction zone, the dissipation rate is larger for higher $Y_{\text{CH}_4}$ showing that higher dissipation rate are more likely to extinguish the flame. The peak dissipation is over $400 \text{s}^{-1}$ which higher than critical dissipation rate, therefore, the local extinction is likely to happen first in flamelets.

The temperature dissipation is small for intermediate mixture fraction (Fig. 5.4c), which is consistent with temperature reaching maximum in strained laminar flamelets. It has two peaks, one is located at $\xi = 0.3, T = 1650 \text{K}, Y_{\text{CH}_4} = 0$, the other one is located at $\xi = 0.53, T = 1680 \text{K}$,
$Y_{CH_4} = 0.038$. Near the peak in lean mixture, the temperature dissipation rate decreases with $Y_{CH_4}$ while the dependency is reversed near the peak in rich mixture.

The CH$_4$ dissipation is very small in lean mixtures which is consistent with total consumption (Fig. 5.4d). Near equilibrium curve, the CH$_4$ dissipation rate varies with decreasing temperature. This is because in strained laminar flamelets reactive species is uniquely determined by mixture fraction and stoichiometric mixture fraction dissipation. Comparing to mixture fraction dissipation, the CH$_4$ dissipation peak shifted out of the reaction zone, because firstly, within reaction zone CH$_4$ is largely consumed by reaction but outside reaction zone CH$_4$ linearly increases with mixture fraction, secondly due to the structure of laminar flamelet, the mixture fraction dissipation rate is higher for intermediate mixture fraction.

At $x/D = 15$, when scalar SGS variance is small the mixture fraction dissipation (Fig. 5.2b) is generally similar to the upstream for burning samples. There is more extinguished sample as shown in temperature below 1300K. However, since peak the dissipation is less than 150s$^{-1}$, the extinguished samples come from upstream and not mix with high temperature parcel yet. The mixture fraction dissipation has little dependency on mixture fraction but increases weakly as temperature increases.

The temperature dissipation is similar to upstream for burning regime (Fig. 5.2c). For extinguished samples, temperature dissipation is small because the temperature gradient is reduced by mixing and lower diffusivity. The temperature dissipation increases with temperature up to its peak at approximately 1500K, which is a result of locally mixing between burning and extinguished samples. At lower temperature, temperature dissipation dependence on mixture fraction and CH$_4$ is relatively weak because $T$ is out of dependence of $\xi$ when deviates from equilibrium.

The CH$_4$ dissipation (Fig. 5.2d) is also similar to upstream for burning regime. Away from burning samples, the CH$_4$ dissipation shows the structure of temperature dissipation. This is consistent with reduced heat release due to CH$_4$ accumulation.

### 5.3 FMDF and dissipation rates condition on $\xi$, $T$ and $Y_{CO}$

#### 5.3.1 FMDF condition on $\xi$, $T$ and $Y_{CO}$

For Flame D at $x/D = 7.5$, the FMDF of mixture, temperature and CO mass fraction for small scalar SGS variance is shown in Fig. 5.13a. The FMDF is unimodal. The figure shows FMDF
largely concentrates along equilibrium curve with strong CO mass fraction dependency on mixture fraction. This is consistent with quasi-equilibrium distributed reaction zones. The ridge line of FMDF is along the equilibrium curve and peak is located on the equilibrium. Further downstream to $x/D = 15$ (Fig. 5.14a) and $x/D = 30$ (Fig. 5.15a), the FMDF is still unimodal except significant amount of local extinction is observed for $x/D = 15$ and less extinction is reduced at $x/D = 30$ due to reignition.

Increasing scalar SGS variance, the FMDF becomes complicated (Fig. 5.16d). The FMDF becomes bimodal. At $x/D = 7.5$ the flamelets are close to fully burning. Both CO and temperature decreases nearly proportionally with increasing the mixture fraction on the rich branch. The fractional variations of CO mass fraction near the stoichiometric mixture fraction appear to be larger than those of temperature. Moving away from the stoichiometric mixture fraction on the lean branch the CO mass fraction decreases rapidly to very small values due to the high rate of the CO oxidation whereas temperature decreases much more slowly. At $\xi = 0.3$ the CO mass fraction is very small and the lean branch becomes nearly horizontal. CO mass fraction reaches its peak near $\xi = 0.5$ where $Y_{CO}$ also shows the largest variation. On the rich branch ($\xi > 0.5$), $Y_{CO}$ increases with temperature. This shows that on the rich branch the dominant heat releasing reaction is the oxidation of CH$_4$ to CO. On the lean branch and within the reaction zone, $Y_{CO}$ increases with decreasing temperature near equilibrium, showing the effect of additional heat release from CO oxidation.

At $x/D = 15$ the FMDF is more complex. Due to the local extinction events, the FMDF extends to a region in scalar space much larger than at $x/D = 7.5$. The extinguished samples are distributed largely in two mixing planes, one formed by the three points near ($\xi = 0$, $T=300K$, $Y_{CO} = 0$), ($\xi = 0.3$, $T = 1900K$, $Y_{CO} = 0$), and ($\xi = 0.52$, $T = 2000K$, $Y_{CO} = 0.07$), and the other formed by the points near ($\xi = 0.3$, $T = 1900K$, $Y_{CO} = 0$), ($\xi = 0.5$, $T = 2200K$, $Y_{CO} = 0.075$), and ($\xi = 0.9$, $T = 500K$, $Y_{CO} = 0$). These four points are the vertices of a tetrahedron forming the boundary of the allowable scalar values in the scalar space. When local extinction events occur the CO consumption on the lean side of the laminar flamelets decreases, causing the CO level to rise. SGS mixing then begins to mix these samples in the former mixing plane. One of the boundary lines of the allowable scalar values in this plane is the line running from the peak CO mass fraction ($\xi = 0.52$, $T = 2000K$, $Y_{CO} = 0.07$) to the oxidizer stream ($\xi = 0$, $T = 300K$, $Y_{CO} = 0$). The mixture on this boundary then starts to mix with the mixtures near the rich side of the equilibrium curve, essentially in the latter mixing plane. This boundary also separates the SGS mixtures in the
two planes in physical space. Consequently, SGS mixing between two sides must go through it.

5.3.2 dissipation rates condition on $\xi$, $T$ and $Y_{CO}$

For Flame D at $x/D = 7.5$, when SGS variance is small, the mixture fraction dissipation rate condition on $\xi$, $T$ and $Y_{CO}$ is shown in Fig. 5.13b. It has little dependency on CO mass fraction which is consistent with previous conclusion that mixture fraction dissipation has little dependency on $\xi$ for distributed reaction zone while the CO mass fraction is determined on mixture fraction near equilibrium. The temperature dissipation also shows little dependency on CO (Fig. 5.13c). The CO dissipation (Fig. 5.13d) is small for lean mixture because of low concentration. In rich mixture, the CO dissipation depends largely on temperature but weakly on mixture and CO.

For large SGS variance, near equilibrium curve, mixture fraction dissipation rate is small (Fig. 5.16b). The dissipation rate decreases with temperature, which is consistent with strained laminar flamelets. On the lean branch, the dissipation increases with $Y_{CO}$ near equilibrium curve, while this trend is reversed on the rich branch. Within the reaction zone, mixture fraction dissipation shows little dependency on $Y_{CO}$. This shows that on the lean branch an increasing strain rate reduces CO oxidation, on the rich branch an increasing strain rate reduces CO formation, while within the reaction zone, the CO variation mostly comes from water-gas reaction which contributes little to heat release. The peak dissipation rate is higher than its critical value and occurs at over one half of peak CO mass fraction, showing that the flame is stabilized by pilot.

The temperature dissipation rate (Fig. 5.16c) generally has little dependency on $Y_{CO}$. Its dependency on $\xi$ and $T$ is similar to previous results.

The CO mass fraction dissipation rate (Fig. 5.16d) is small outside the reaction zone. Such small dissipation rate on the rich branch is a result of linear dependence of $Y_{CO}$ and $\xi$ and small dissipation of mixture fraction. Small dissipation rate on lean branch near equilibrium curve is a result of total consumption but increases with $Y_{CO}$ because of increasing strain rate in laminar flamelet. Within the reaction zone near equilibrium curve, the dissipation is larger because of strong sensitivity of $Y_{CO}$ on mixture fraction. The peak appears at intermediate $Y_{CO}$ where both $|dY_{CO}/d\xi|$ and $\chi_\xi$ are large.

Moving to $x/D = 15$, for small SGS variance, the mixture fraction dissipation rate (Fig. 5.14b) shows similar result as upper stream for burning samples. The peak dissipation samples have
relative low temperature and $Y_{CO}$ but with the dissipation value below critical value ($\sim 400 \text{s}^{-1}$). Therefore these might be samples from extinguished upstream but not yet mixed with high temperature to reignite.

The temperature dissipation rate is shown in Fig. 5.14c. For burning samples it is small because $dT/d\xi \sim 0$ as temperature reaches its peak value. The temperature dissipation is larger for intermediate temperature because of mixing between burned and extinguished samples. This is also confirmed by its dependency on $Y_{CO}$.

The $Y_{CO}$ dissipation (Fig. 5.14d) shows similar trends as upper stream near equilibrium curve. For extinguished samples represented by lower temperature, the dissipation has a weak peak for intermediate $\xi$, $T$ and $Y_{CO}$, but little dependency otherwise. This indicates that CO mass fraction field is not well mixed though $\xi$ field is.

For large SGS variance, the mixture fraction dissipation rate in burning samples is similar to upper stream (Fig. 5.17b). For extinguished samples the mixture fraction dissipation rate is larger for $\xi \sim 0.5$, this is where the peak dissipation of a ramp-cliff structure located. The dissipation rate increases with decreasing temperature, consistent with laminar flamelets. The dissipation rate also increases with $Y_{CO}$ for lower temperature, which may because dissipation rate affects more on $\text{H}_2$ oxidation causing CO accumulation. The peak dissipation rate is higher than critical dissipation rate.

The temperature dissipation for extinguished sample is small, consistent with extinguished flamelets (Fig. 5.17c). There appears a temperature dissipation peak at $\xi = 0.5$, $T = 1600 \text{K}$ and $Y_{CO} = 0.03$. Because of its low CO concentration, this peak is a result of direct mixing between pilot and fuel without reaction.

The CO dissipation is shown in Fig. 5.17d. For burning samples it is similar to upper stream. For extinguished samples, the CO dissipation rate is very small which is consistent with extinguished flamelets.

Further downstream to $x/D = 30$, the dissipation rates show similar trend as $x/D = 15$ except that the dissipation rate is reduced due to reduced strain rate and reignition is observed (Fig. 5.15b, 5.15c, 5.15d, 5.18b, 5.18c and 5.18d).
Figure 5.1: Filtered mass density function and dissipation rates for Flame D at $x/D = 7.5$ $(\xi''^2)_L = 0.0012$. The contours are obtained at $\xi = 0.20, 0.32, 0.43, 0.55$ respectively.
Figure 5.2: Filtered mass density function and dissipation rates for Flame D at $x/D = 15 \langle \xi'^2 \rangle_L = 0.0030$. The contours are obtained at $\xi = 0.20, 0.32, 0.43, 0.55$ respectively.
Figure 5.3: Filtered mass density function and dissipation rates for Flame D at $x/D = 30 \langle \xi'^2 \rangle_L = 0.0019$. The contours are obtained at $\xi = 0.20, 0.32, 0.43, 0.55$ respectively.
Figure 5.4: Filtered mass density function and dissipation rates for Flame D at $x/D = 7.5$ $(\xi''^2)_L = 0.066$. The contours are obtained at $Y_{CH_4} = 0.0008, 0.0256, 0.0504, 0.0752$ and $0.1000$ respectively.
Figure 5.5: Filtered mass density function and dissipation rates for Flame D at $x/D = 15$ $\langle \xi'^2 \rangle_L = 0.069$. The contours are obtained at $Y_{\text{CH}_4} = 0.0008, 0.0256, 0.0504, 0.0752$ and $0.1000$ respectively.
Figure 5.6: Filtered mass density function and dissipation rates for Flame D at $x/D = 30$ ($\xi''_L = 0.059$. The contours are obtained at $Y_{CH_4} = 0.0008, 0.0256, 0.0504, 0.0752$ and $0.1000$ respectively.
Figure 5.7: Filtered mass density function and dissipation rates for Flame E at $x/D = 7.5$ $(\xi^{(r)})_L = 0.0011$. The contours are obtained at $\xi = 0.20, 0.32, 0.43, 0.55$ respectively.
(a) FMDF
(b) Mixture fraction dissipation
(c) Temperature dissipation
(d) CH$_4$ mass fraction dissipation

Figure 5.8: Filtered mass density function and dissipation rates for Flame E at $x/D = 15$ $(\xi'^2)_L = 0.0028$. The contours are obtained at $\xi = 0.20, 0.32, 0.43, 0.55$ respectively.
Figure 5.9: Filtered mass density function and dissipation rates for Flame E at $x/D = 30$ $(\xi'^2)_L = 0.0018$. The contours are obtained at $\xi = 0.20, 0.32, 0.43, 0.55$ respectively.
Figure 5.10: Filtered mass density function and dissipation rates for Flame E at $x/D = 7.5$ $\langle \xi'^2 \rangle_L = 0.081$. The contours are obtained at $Y_{CH_4} = 0.0008, 0.0256, 0.0504, 0.0752$ and 0.1000 respectively.
Figure 5.11: Filtered mass density function and dissipation rates for Flame E at $x/D = 15$ ($\xi''^2)_L = 0.064$. The contours are obtained at $Y_{\text{CH}_4} = 0.0008, 0.0256, 0.0504, 0.0752$ and $0.1000$ respectively.
Figure 5.12: Filtered mass density function and dissipation rates for Flame E at $x/D = 30$ $\langle \xi'^2 \rangle_L = 0.044$. The contours are obtained at $Y_{CH_4} = 0.0008, 0.0256, 0.0504, 0.0752$ and $0.1000$ respectively.
Figure 5.13: Filtered mass density function and dissipation rates for Flame D at $x/D = 7.5$ $(\xi''^{2})_{L} = 0.0012$. The contours are obtained at $Y_{CO} = 0.001, 0.016, 0.031, 0.046$ and 0.061 respectively.
Figure 5.14: Filtered mass density function and dissipation rates for Flame D at $x/D = 15$ $\langle \xi'^{2} \rangle_L = 0.0030$. The contours are obtained at $Y_{CO} = 0.001, 0.016, 0.031, 0.046$ and 0.061 respectively.
Figure 5.15: Filtered mass density function and dissipation rates for Flame D at $x/D = 30$ $\langle \xi''^2 \rangle_L = 0.0019$. The contours are obtained at $Y_{CO} = 0.001, 0.016, 0.031, 0.046$ and $0.061$ respectively.
Figure 5.16: Filtered mass density function and dissipation rates for Flame D at $x/D = 7.5$ \(\langle \xi'^2 \rangle_L = 0.066\). The contours are obtained at $Y_{CO} = 0.001, 0.016, 0.031, 0.046$ and $0.061$ respectively.
Figure 5.17: Filtered mass density function and dissipation rates for Flame D at $x/D = 15 \langle \xi'^2 \rangle_L = 0.069$. The contours are obtained at $Y_{CO} = 0.001, 0.016, 0.031, 0.046$ and $0.061$ respectively.
Figure 5.18: Filtered mass density function and dissipation rates for Flame D at $x/D = 30$ $(\xi''^2)_L = 0.059$. The contours are obtained at $Y_{CO} = 0.001, 0.016, 0.031, 0.046$ and $0.061$ respectively.
Figure 5.19: Filtered mass density function and dissipation rates for Flame E at $x/D = 7.5$ ($\xi^{\prime 2})_L = 0.0011$. The contours are obtained at $Y_{CO} = 0.001, 0.016, 0.031, 0.046$ and $0.061$ respectively.
Figure 5.20: Filtered mass density function and dissipation rates for Flame E at $x/D = 15$ \langle \xi'^2 \rangle_L = 0.0028. The contours are obtained at $Y_{CO} = 0.001, 0.016, 0.031, 0.046$ and 0.061 respectively.
Figure 5.21: Filtered mass density function and dissipation rates for Flame E at $x/D = 30$ $\langle \xi''^2 \rangle_L = 0.0018$. The contours are obtained at $Y_{CO} = 0.001, 0.016, 0.031, 0.046$ and 0.061 respectively.
Figure 5.22: Filtered mass density function and dissipation rates for Flame E at $x/D = 7.5$ ($\xi'^2)_L = 0.081$. The contours are obtained at $Y_{CO} = 0.001, 0.016, 0.031, 0.046$ and 0.061 respectively.
Figure 5.23: Filtered mass density function and dissipation rates for Flame E at $x/D = 15$ $(\xi'^2)_L = 0.064$. The contours are obtained at $Y_{CO} = 0.001, 0.016, 0.031, 0.046$ and $0.061$ respectively.
Figure 5.24: Filtered mass density function and dissipation rates for Flame E at $x/D = 30$ $\langle \xi'^2 \rangle_L = 0.044$. The contours are obtained at $Y_{CO} = 0.001, 0.016, 0.031, 0.046$ and $0.061$ respectively.
Chapter 6

Noise and Resolution Corrections for Scalar Dissipation Rate

6.1 Introduction

The scalar dissipation rate is an important variable characterizing turbulent mixing. It is the rate at which the variance of scalar fluctuations is reduced by molecular mixing. It is also a key variable in studying and modeling turbulent nonpremixed/partially premixed flames [4, 33]. Therefore, much effort has been devoted to measurements of the scalar dissipation rate. Because the scalar dissipation rate in a turbulent flow comes primarily from the smallest scalar length scales, its measurements require high spatial resolution. At the same time, the scalar fluctuations at these scales are generally much smaller than the energy-containing fluctuations, requiring low measurement noise to achieve an adequate signal/noise ratio for dissipation rate measurements. In practice, however, none of the two requirements are guaranteed. Often the resolution of the measurement system is comparable to the smallest length scales and the noise contributions to the dissipation rate are significant, potentially resulting in significant errors in the measured dissipation rate.

Resolution and noise have different effects on dissipation rate measurements. The measured scalar dissipation rate decreases with measurement resolution. Measurement noise, however, is usually additive to the measured scalar; therefore the noise contribution to the measured mean dissipation is always positive. The contribution generally increases with resolution (or smaller sam-
ple spacing) because the distance over which the derivatives are taken is reduced while the noise differences are generally independent of (or even increase with) the resolution. Because the noise and resolution effects are generally present at the same time, the opposite trends of resolution and noise effects make correction difficult. Therefore, a major task in noise and resolution corrections is to separate their effects.

Previous studies generally focused on one of the issues or considered the combined effects. The effects of the probe resolution on the dissipative scale turbulent velocity and scalar fluctuations were first studied by Wyngaard [59, 60, 61]. Using the spectral models of Corrsin[12] and Pao[21] he analyzed the attenuation of the dissipative scale velocity, vorticity, and scalar spectra due to the finite probe size. He found that a temperature resistance wire (cold wire) must have a length comparable to or smaller than the scalar dissipation length scale to resolve 98% of the mean scalar dissipation rate. Brown et al. [6], Atonia and Mi [1], Mi and Nathan[31] examined the effects of the probe separation when using two cold wires to measure the scalar dissipation rate. Tong and Warhaft [46] found that a probe separation of one scalar dissipation length scale is needed to measure accurately the scalar derivative kurtosis, which is strongly influenced by large derivative fluctuations. For smaller separations the noise contribution becomes significant. These studies provided the understanding of the effects of noise and resolution, but the effects are not separated. The studies also highlighted the need for separating the two effects in order to make accurate correction for noise and resolution effects.

To evaluate the resolution effects the scalar dissipation length scale is needed. One way to evaluate the resolution and the dissipation length scales is to measure the dissipation rate with a range of resolutions to determine whether the measured mean dissipation rate is approaching an asymptotic value when the resolution is increased[1, 31]. However, in such measurements noise is also present and the its contribution increases with resolution. Therefore, for high-resolution measurements the noise contributions become significant, making it difficult to evaluate the length scales.

Using spectral analysis Wang et. al.[56] considered the overall impact of a measurement system. They considered the effects of optical blurring, pixel size, numerical schemes, and noise. Wang and Barlow[55] used the method to evaluate the dissipation length scales in turbulent nonpremixed flames. In such spectral approaches for evaluating resolution and noise, if the spatial resolution and the signal-to-noise ratio are sufficiently high, the noise spectrum can often be determined because it
is generally constant with respect to the wavenumber (i.e., white noise) and dominates the measured spectrum at wavenumbers higher than the signal cutoff wavenumber. However, when the scalar is not fully resolved or the signal-to-noise ratio is low, there are significant contributions from both the signal and noise. Consequently, it is generally not possible to separate the noise spectrum. Instead, a model spectrum with the noise contribution added to it needs to be used to fit the measured spectrum by varying the length scale and the relative noise contribution to the model spectrum. These parameters are then regarded as the length scale and the noise contribution.

A limitation of spectral approaches is that it cannot be applied to the conditional scalar dissipation rate, \( \langle \chi | \phi \rangle \), where \( \chi \) and \( \phi \) are the scalar dissipation rate and the scalar value respectively. The conditional dissipation rate is a key mixing term evolving the scalar probability density function. Its value near the stoichiometric mixture fraction largely determines the reaction rate in nonpremixed flames\[4, 33\]. It is also a key variable in several models for nonpremixed and partially premixed turbulent combustion. Therefore, it is essential that a correction method is applicable to the conditional dissipation rate. Another limitation of the spectral method is that it is a global analysis method. In turbulent passive scalar fields as well as in nonpremixed and partially premixed turbulent flames the so-called ramp-cliff scalar structure\[46, 50, 39, 51, 52\] is usually present. The cliff is a highly local structure generating large local dissipation rate but do not necessarily contribute significantly to the spectrum. Furthermore, the spectrum calculated depends on the ratio of the length of the signal record to the thickness of the cliff. Therefore, spectral analyses are generally not suitable for characterizing scalar fields containing the ramp-cliff structure.

In the present work we develop a local analysis approach which uses conditional sampling to evaluate the noise contributions (see Sec. 6.2 and Ref.\[45, 50, 51\] for the conditional sampling procedures). This method does not rely on spectral analysis and allows conditioning of the dissipation rate on the scalar value at the same location. The most important aspect of the method is the conditional sampling procedure, which is based on Kolmogorov’s refined similarity hypotheses\[29\] (see Sec. 6.3 for details). It is used to select fully resolved (verified a posteriori) local scalar fields, effectively separating the noise effects from the resolution effects. The fully resolved local scalar fields are then used to determine the measurement noise. Because the conditional sampling procedure makes use of the properties of turbulent scalar fields, it can essentially guarantee selection of fully resolved local scalar, even when the whole scalar field is not fully resolved. The experimentally determined noise is applied to potentially under-resolved conditional local scalar fields for noise
correction. The noise-corrected dissipation rate is then used to evaluate the scalar dissipation length scales (relative measurement resolution) and to make corrections to the scalar dissipation for under-resolution.

In this method we make use of the different spectral response (or resolution) of finite difference schemes (or numerical stencils) of different order in determining the measurement noise and evaluating the measurement resolution. Therefore, unlike some of the previous methods, this method does not rely on varying the measurement resolution (or the sample spacing) to evaluate dissipation length scale and only one resolution is needed. This local analysis method has several advantages over previous methods: 1) The use of conditional sampling allows separation of noise from the resolution effects to evaluate the noise contribution and the dissipation length scales. 2) It is applicable to the conditional dissipation rate. 3) it can capture the effects of the ramp-cliff structure, which is not well represented in spectral correction methods. In the following we first describe conditional sampling procedure followed by discussions of the finite difference schemes and its role in determining measurement noise and evaluating the dissipation length scales (relative resolution). Application of the method to measurements of temperature dissipation in a slightly heated turbulent jet is discussed in Sec. 6.3.

6.2 Description of the method

6.2.1 Conditional sampling

We use the conditional sampling technique that we developed to study the subgrid-scale (SGS) scalar mixing[45, 50, 39, 53, 51, 52]. The technique uses two conditioning variables: the filtered (locally averaged) scalar

\[ \langle \phi \rangle_L = \int \phi(x') G(x - x') dx' \]  \hspace{1cm} (6.1)

and the SGS scalar variance (or local scalar variance)

\[ \langle \phi'^2 \rangle_L = \int (\phi(x') - \langle \phi \rangle_L(x))^2 G(x - x') dx' \]  \hspace{1cm} (6.2)

The conditional sampling method makes use of the properties of the turbulent scalar fields.
Our previous studies\cite{45, 50, 39, 53, 51} have shown that for small SGS variance (smaller than mean SGS variance) the SGS scalar is well mixed. The statistics of such (conditional) fields are well described using Kolmogorov-Obukhov-Corrsin theory. The locally averaged scalar dissipation rate and the scalar variance spectral transfer rate are lower than the mean scalar dissipation rate. In the spirit of the Kolmogorov’s refined similarity hypotheses, the local conditional Peclet number is expected to be lower than that based on the unconditioned statistics; therefore, the scalar dissipation length scales for these fields are expected to be larger than the mean scalar dissipation length scale. By choosing sufficiently small SGS variance values, one can select local scalar fields with sufficiently large dissipation length scales so that they are well resolved by the measurement apparatus. This property of the local turbulent scalar fields is demonstrated by the experimental results (Figs. 6.2 and 6.11a).

For large SGS variance, the locally averaged conditional scalar dissipation rate and the spectral transfer are larger than their mean values. In addition, the SGS scalar is highly segregated and contains the so-called ramp-cliff structure\cite{46, 50, 39, 51}. The scalar dissipation rate is very large inside the cliffs. At the same time, the cliffs in the SGS scalar are likely to have smaller length scales. Using conditional sampling with large (much larger than the average SGS variance) SGS variance values, one can select local scalar fields that are potentially under-resolved to evaluate their dissipation length scales. These fields will be analyzed to determine the dissipation length scales and to correct for any under-resolution.

6.2.2 Finite difference schemes for calculating scalar derivative

To obtain the scalar dissipation rate numerical (usually finite difference) schemes are needed to calculate the derivatives because experimental data are generally discrete samples. Different schemes involve different numbers of samples and different weights to the samples. Consequently, the calculated scalar dissipation rate and the noise contribution are scheme dependent. Here we discuss the finite different schemes used.

A generalized form of a one-dimensional equidistant central finite difference scheme for the first derivative is

\[ h \cdot \frac{d\phi}{dx} = a_1(\phi_1 - \phi_{-1}) + a_2(\phi_2 - \phi_{-2}) + a_3(\phi_3 - \phi_{-3}) + a_4(\phi_4 - \phi_{-4}) + \ldots \]  

(6.3)
where $h$ and $\frac{d\phi}{dx}$ are the distance between adjacent samples and the estimation of first derivative respectively. Selected schemes and their orders are listed in table 6.1.

Table 6.1: Central finite difference scheme for first derivative

<table>
<thead>
<tr>
<th>order</th>
<th>$a_1$</th>
<th>$a_2$</th>
<th>$a_3$</th>
<th>$a_4$</th>
<th>$a_5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>1/2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>8/12</td>
<td>-1/12</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>6</td>
<td>45/60</td>
<td>-9/60</td>
<td>1/60</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>8</td>
<td>672/840</td>
<td>-168/840</td>
<td>32/840</td>
<td>-3/840</td>
<td>0</td>
</tr>
<tr>
<td>10</td>
<td>2100/2520</td>
<td>-600/2520</td>
<td>150/2520</td>
<td>-25/2520</td>
<td>2/2520</td>
</tr>
</tbody>
</table>

All finite difference schemes have numerical errors. One way to quantify the errors is to examine the spectral responses of the schemes, which we discuss briefly. For more detailed discussions, see Ref. [30]. Here we focus on explicit central finite difference schemes. Using Fourier transform, a suitable function $\phi(x)$ can be represented as a superposition of a series of harmonic basis functions, $e^{i\kappa x}$, where $\kappa$ is the wavenumber. The maximum wavenumber that can be represented by a set of discrete samples is $\kappa_{max} = \pi/h$, the Nyquist wavenumber, and higher wavenumbers will be aliased to those below $\phi/h$, where $h$ is the distance between adjacent samples. It is, therefore, useful to analyze finite difference schemes in the wavenumber domain.

We examine the behavior of schemes by assigning $\phi$ to a harmonic function $\phi = \phi_m e^{i\kappa x}$, its first derivative is $\frac{d\phi}{dx} = i\kappa \phi_m e^{i\kappa x}$. The response of finite difference scheme can be represented as a function of the non-dimensional wavenumber $h\kappa$ ($0 \leq h\kappa \leq \pi$). From (6.3) the estimated first derivative is

$$\frac{\tilde{d\phi}}{dx}h = \sum_{n=-N}^{N} a_n\phi(x + nh)$$  \hspace{1cm} (6.4)

$$= \sum_{n=1}^{N} a_n\phi_m(e^{i\kappa(x+nh)} - e^{i\kappa(x-nh)}) \quad \text{(note that } a_n = -a_{-n})$$  \hspace{1cm} (6.5)

$$= 2i\sum_{n=1}^{N} a_n\phi_m \sin(nkh)e^{i\kappa x}$$  \hspace{1cm} (6.6)

$$= iR(\kappa h)\phi_me^{i\kappa x}$$  \hspace{1cm} (6.7)

where

$$R(\kappa h) = \sum_{n=1}^{N} 2a_n \sin(nkh)$$  \hspace{1cm} (6.8)
is the response at wavenumber $\kappa$. In the limit that $N \to \infty$, $\mathcal{R}(\kappa h) \to \kappa h$. Also note that the response of a central finite difference scheme is a real function of wavenumber.

The wavenumber responses of several one-dimensional finite difference schemes have been discussed by Lele [30]. Figure 6.1 shows the spectral response of the schemes given in Table 6.1. All numerical differentiation schemes except spectral methods attenuate the wavenumbers near $\pi/h$. Lower-order schemes generally attenuate more severely than higher-order ones. For example, the second-order scheme results in a 36.3% reduction at one half of the Nyquist wavenumber whereas the tenth-order scheme attenuates 1.375%.

The spectral responses of the different schemes can be used to evaluate the measurement resolution and the scalar dissipation length scales. When a scalar field is fully resolved, the scalar derivative and the scalar dissipation rate obtained by all the schemes are identical. For an under-resolved scalar field, higher-order schemes result in higher dissipation rates. Convergence of the dissipation rate as the scheme order increases would indicate that the scalar field is fully resolved by schemes of certain order or higher but not by the lower-order ones, providing an estimate of the length scale of the dissipation scale scalar. If no convergence is observed, the different dissipation rate values can be compared to a model with known length scale to infer the scalar dissipation length
To illustrate the effect of spectral response, we approximate the scalar profile as an error function with width $w$

\[
\phi(x) = \text{erf} \left( \frac{x}{w} \right) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt
\] (6.9)

The dissipation rate is calculated at $\phi = 0.5$ where it is at its maximum. A comparison between selected schemes is shown in Fig. 6.9. For a given scheme, as the distance between adjacent samples ($h$) increases, the calculated dissipation rate decreases. For a fixed $h$, higher-order schemes have better resolution. A very high-order scheme will approach the spectral method. However, when noise is present in the samples, higher-order schemes generally result in higher noise contributions because these schemes involve more samples. As a result, without noise correction lower-order schemes tend to underestimate the dissipation rates, while higher-order ones tend to overestimate it. Therefore, it is essential to correct the noise effects before evaluating the resolution effects.

### 6.2.3 Effect of noise on dissipation rate measurement

The following discussion is based on the assumption that noise at different measurement locations (be it different samples from a single probe or pixels of an imaging device) are independent random variables additive to measured quantities.

\[
\phi = \phi^* + n
\] (6.10)

where $\phi^*$, $\phi$ and $n$ are the true scalar value without noise, the measured value and the noise respectively. To correct for noise contributions to the measured dissipation rate the noise variance needs to be determined. The noise variance is in general a function of $\phi$

\[
\langle n^2 \rangle = \sigma_n^2(\phi)
\] (6.11)

For the temperature dissipation rate measurement considered here, the noise from the resistance-wire temperature sensor (or cold-wire) is independent of the temperature signal and has a constant variance.

By applying this noise model to the finite difference scheme in Equation (6.3), the estimated
First derivative is
\[
\frac{h \cdot \tilde{d} \phi}{dx} = a_1(\phi_1 - \phi_{-1}) + a_2(\phi_2 - \phi_{-2}) + a_3(\phi_3 - \phi_{-3}) + a_4(\phi_4 - \phi_{-4}) + \ldots
\] (6.12)

\[
= a_1(\phi^*_1 - \phi^*_{-1}) + a_2(\phi^*_2 - \phi^*_{-2}) + a_3(\phi^*_3 - \phi^*_{-3}) + a_4(\phi^*_4 - \phi^*_{-4}) + \ldots
\] (6.13)

\[
+ a_1 n_1 - a_{-1} n_{-1} + a_2 n_2 - a_{-2} n_{-2} + a_3 n_3 - a_{-3} n_{-3} + a_4 n_4 - a_{-4} n_{-4} + \ldots
\] (6.14)

where \( \tilde{\frac{d\phi}{dx}} \) is the estimated derivative without noise. Note that such an estimated first derivative is dependent on the scheme used due to the different spectral response. Then the measured mean dissipation rate is

\[
\langle \tilde{\chi} \rangle = \left\langle 2D \left( \frac{\tilde{d} \phi}{dx} \right)^2 \right\rangle
\] (6.15)

\[
= \left\langle 2D \left( \frac{\tilde{d} \phi^*}{dx} \right)^2 \right\rangle + \left\langle \frac{2D}{h^2} \sum_{i=-N}^{N} a_i^2 n_i^2 \right\rangle
\] (6.16)

\[
= \left\langle 2D \left( \frac{\tilde{d} \phi^*}{dx} \right)^2 \right\rangle + \frac{2(D)}{h^2} \left\langle \sum_{i=-N}^{N} a_i^2 n_i^2 \right\rangle
\] (6.17)

\[
= \left\langle 2D \left( \frac{\tilde{d} \phi^*}{dx} \right)^2 \right\rangle + \frac{2(D)}{h^2} \sum_{i=-N}^{N} a_i^2 \langle n^2 \rangle
\] (6.18)

\[
= \left\langle 2D \left( \frac{\tilde{d} \phi^*}{dx} \right)^2 \right\rangle + \frac{2(D)}{h^2} C_N \langle n^2 \rangle
\] (6.19)

where \( D, C_N = \sum_{i=-N}^{N} a_i^2 \langle \phi_i T_i \rangle \) and \( 2D \left( \frac{\tilde{d} \phi^*}{dx} \right)^2 \) are the diffusivity, a scheme dependent factor and an estimation of dissipation rate without noise.

When all the schemes can resolve the turbulence scalar field, the mean dissipation rate \( \left\langle 2D \left( \frac{\tilde{d} \phi^*}{dx} \right)^2 \right\rangle \) does not depend on the scheme. Therefore, the plot of mean dissipation rate vs. \( C_N \) is a straight line, with a slope of \( \frac{2k(D)}{h^2} \) and an intercept equal to the noise-corrected dissipation rate. This linear relationship can be used to determine the noise variance \( \langle n^2 \rangle \).

When the resolution is reduced, the measured dissipation rate by the second-order scheme will fall below the straight line first because it is the least capable of resolving the dissipation rate. As the resolution is further reduced the fourth- and higher-order schemes will deviate from the linear
relationship. On the other hand, as long as the eighth- and tenth-order schemes follow this straight line the dissipation is still fully resolved. The $\langle \chi \rangle - C_N$ plot, therefore, can be used to determine whether the scalar dissipation is fully resolved. In the following we employ the conditional-sampling method to select fully resolved local scalar fields and determine the noise variance according to Eq. 6.19. The noise variance is used to correct the dissipation rate for potentially under-resolved local scalar fields. The noise-corrected dissipation rates from the different schemes then are analyzed to evaluate the scalar dissipation length scales and to correct for the resolution effects.

6.3 Application to a slightly heated turbulent jet

In this section the previous discussed noise and resolution correction method is applied to scalar dissipation rate of passive temperature fluctuations in a slightly heated turbulent jet[45, 50, 39, 51]. The experimental data used in the present study were obtained in a heated turbulent jet. The jet facility was housed in a large, air conditioned room. The jet assembly was mounted vertically. A collection hood at a downstream distance of 260 nozzle diameters (3.9 m) minimizes the effects of the ceiling on the jet. Jet air supply was heated with a pipe heater before entering the plenum chamber, producing an excess temperature (above the ambient) of 20°C at the nozzle exit.

Measurements were made for a jet exit velocity $U_j$ of 40 m/s, which gives a jet Reynolds number $Re_j$ of 40 000. The nozzle diameter $D_j$ was 15 mm. Data were collected at a downstream distance of $x/D_j = 80$ on the jet centerline. The effects of the initial jet-to-air density ratio $\approx 0.93$ on the properties of the jet, such as the spreading rate and the rms fluctuations of velocity and temperature, were small.[30] Thus, in our measurements the temperature fluctuations were dynamically passive.

One-dimensional streamwise filtering was employed to compute the filtered scalar and the SGS scalar variance. The filtering was performed by invoking Taylor’s hypothesis. Filter widths ranging from 5 to 40 mm were used, corresponding to $\Delta/\eta = 31$ to 250. Here $\eta = 0.16 mm$ is the Kolmogorov scale. The scalar dissipation (or Obukhov-Corrsin) scale, $\eta_\phi$, is 0.22 mm. The filter widths were chosen to be much larger than the dissipation scales.

Temperature fluctuations were measured with a platinum resistance wire of 0.6 mm in length and 0.625 $\mu$m in diameter, which has a frequency response up to 5 kHz. Details of the devices are given in Ref. [39]. The temperature signals were low-pass filtered at 5 kHz and amplified by Krohn-
Hite 3364 filter/amplifiers. The signals were digitized at 10 000 samples/second by a 12 bit National Instrument analog to digital converter (PCI-6071E). This sampling rate corresponds to a sample interval of 0.307 mm. The streamwise component of the scalar dissipation rate is measured using Taylor’s hypothesis. In the following analyses we use data collected on the jet centerline where the mean velocity is 3.07 m/s. Only the fluctuating temperature is used, which is normalized by its rms values.

6.3.1 Conditional local scalar field

We first use small SGS variance values to select well-resolved local scalar fields, from which the conditionally filtered dissipation rates are calculated using the central difference schemes. As the scheme order increases, the conditionally filtered dissipation rate increases. We plot the conditional dissipation rate at $\phi'' = 0$ for a filter size of 20 mm ($\Delta/\eta = 125$). Figure 6.2 shows that for $\langle \phi \rangle_L = 0.0$ and $\langle \phi''^2 \rangle_L = 9.67 \times 10^{-4}$, $\langle \langle \chi | \phi'' \rangle_L | \langle \phi \rangle_L, \langle \phi''^2 \rangle_L \rangle$ as a function of $C_N$ follows a straight line, indicating that for small SGS variance the local scalar fields are well resolved by all the schemes. The noise variance determined from this figure is $6.96 \times 10^{-4}$. Note that the intercept of the straight line ($\sim 0.02 s^{-1}$) is much lower than the dissipation rate calculated using the second-order scheme ($\sim 0.17$), indicating that even when using second-order scheme the noise contribution is greater than the true dissipation rate.

As the SGS variance value increases to $\langle \phi''^2 \rangle_L = 6.34 \times 10^{-3}$ (Fig. 6.3), the conditionally filtered dissipation rates obtained using the fourth- and higher-order schemes form a straight line while the dissipation rate using the second-order scheme is below this line, indicating that the higher-order schemes are capable of resolving the smallest scalar length scales in this case but second-order scheme is not. The slope of the line is very close to that in Fig. 6.2, indicating that the noise variance is determined accurately. In this case the noise-corrected conditionally filtered dissipation (the intercept ) is of the same order of magnitude as (or smaller than) the noise contributions for the second- and fourth-order schemes, indicating that the conditional sampling and the use of the varying spectral response of the finite difference schemes of different orders allow accurate determination of the noise variance even when the noise contribution is greater than the dissipation rate.

For large SGS variance, $\langle \phi''^2 \rangle_L = 4.34$ (Fig. 6.4), the conditionally filtered dissipation rates using the eighth- and lower-order schemes are below the straight line going through the data point for the tenth-order scheme and having the same slope as that in Fig. 6.2, indicating that the
Figure 6.2: Measured conditionally filtered dissipation rate \( \langle \chi' | \phi'' \rangle_L \langle \phi \rangle_L \langle \phi' \rangle_L \rangle \) vs \( C_N \) for \( \langle \phi'' \rangle_L = 9.67 \times 10^{-4} \). Circles with increasing \( C_N \) values represent the second- to tenth-order schemes. The filter size is 20 mm and the scalar value \( \phi \) is 0.0. The straight line is the best fit of the data points.

The straight line intercept of \( \sim 150 s^{-1} \), indicating that even without correcting for noise these schemes are underestimating the dissipation rate. There is, however, no evidence to show that whether the tenth-order scheme is capable of fully resolving the scalar scales. A model for the scalar dissipation rate profile, therefore, is needed to evaluate the resolution.

### 6.3.2 Noise correction and resolution evaluation

The conditionally filtered dissipation rate for a range of scalar fluctuations obtained using the schemes for three SGS scalar variances, \( \langle \phi'' \rangle_L = 9.67 \times 10^{-4}, 6.26 \times 10^{-3}, \) and 4.34, are given in Figs. 6.5(a), 6.6(a), and 6.7(a) respectively. All the figures show that the calculated dissipation rates increase as the order of schemes increases. The increases come from both noise and better resolution of higher-order schemes. In Figs. 6.5(b), 6.6(b), and 6.7(b) we show the results after subtracting the noise contributions determined in the previous subsection.

For small SGS scalar variance (Fig. 6.5), the noise-corrected dissipation rate values calculated
using second- to tenth-order schemes largely overlap, indicating that all the schemes are capable of resolving the scalar dissipation length scale and the noise correction is accurate. Increasing the SGS scalar variance to \( \langle \phi'^2 \rangle_L = 6.26 \times 10^{-3} \) (Fig. 6.6), the conditionally filtered dissipation rates using fourth- or higher-order schemes overlap, consistent with Fig. 6.3, indicating that these schemes are sufficient to resolve all the scalar length scales and noise contributions have been removed.

For large SGS scalar variance (Fig. 6.7), the conditionally filtered dissipation rates for different schemes still show differences near \( \phi'' = 0 \) after the noise correction, indicating that the resolution requirement depends on the scalar value. The increase of the calculated dissipation rate from the second order to fourth order is large, indicating that the second-order scheme is far from having sufficient resolution. The differences between eighth- and tenth-order schemes are much smaller, indicating that the dissipation rates calculated using these schemes are close to the true dissipation rate. After correcting for the noise, the measured dissipation rate is only affected by the measurement resolution, which is expected to be worst when the SGS scalar variance is large due to the steep cliffs present in the SGS scalar. Because the length scales of these cliffs are not known a priori, we need to use experimental data to infer them. In the present study, the Obukhov-Corrsin scale is estimated from the Kolmogorov scale. In a more complex flow (e.g., a turbulent flame) it is generally not possible to estimate accurately the local scalar dissipation length scale. In any case,
the scales of the cliffs are not known. Comparing the measured scalar spectrum to a model spectrum can provide an estimate of the average length scale, but not those of the cliffs dominating the scalar dissipation rate for large SGS variance.

To estimate the length scales of the cliffs we use the error function [Eq. 6.9] as a model for the ramp-cliff structure, and calculate its dissipation rate using different schemes with a range of sample intervals (spatial resolutions). The error-function profile is the canonical solution of the diffusion equation with an advective-diffusive balance. Tong and Warhaft [46] found experimentally that there is a distribution of the cliff thickness ranging from the Kolmogorov scale to the Taylor microscale, with the average thickness scaling with the Taylor microscale, suggesting that they are a result of the balance between the large-scale strain rate and the molecular diffusivity. Buch and Dahm [7, 8] showed experimentally that in general the dissipation layers have errorfunction profiles. The results in the present study (see below) are also consistent with the error-function profile, providing further evidence supporting the use of the error function as a profile for the ramp-cliff structure.

In order to infer the scalar dissipation scale we use the ratios of the dissipation rates calculated using schemes of different orders. By equating the ratios from the measurements and from the model, a scalar dissipation length scale can be inferred. The results are shown in Fig. 6.8.
horizontal axis is the ratio of sample interval to the scalar profile width, $h/w$. Here the ratios for the conditional dissipation rate at $\phi'' = 0.0$ are shown because at this scalar value the dissipation is the highest, corresponding to the smallest scalar length scale. These measured ratios are compared to the error-function model predictions to infer the length scale. For example, the ratio of the second order to the tenth order is approximately 0.84, giving a $h/w$ of 0.54. This $h/w$ value corresponds to 0.324 times the full width at half maximum (FWHM) of the scalar dissipation rate profile, which is $0.307/0.324=0.948$ mm. The scales inferred from the other schemes also agree very well, indicating the overall success of the noise correction and resolution/length scale evaluation. The $h/w$ value can be used to correct for underresolution. Figure 6.9 shows the fraction of the dissipation resolved by the schemes for a range of $h/w$ values. With a sample interval of $h/w = 0.54$ the second- to the
Figure 6.7: Conditionally filtered dissipation rates before and after noise correction for $\langle \phi''^2 \rangle_L = 4.34$.

Figure 6.8: Estimation of the scalar dissipation length scale by comparing the ratio of dissipation rates obtained using different schemes from the data and the model. Curves are ratios of dissipation rates using different schemes. Solid squares are the ratios calculated from the data.

tenth-order schemes underestimates the conditionally filtered dissipation rate by 17%, 5%, 2%, 1.1%, and 0.7%, respectively. Thus, sample interval of approximately $0.5w$ combined with a sixth- and higher-order finite difference scheme is able to resolve the dissipation rate with sufficient accuracy. Note that the peak conditionally filtered dissipation rate for large SGS variance comes from very large dissipation rate fluctuations and is much larger than the mean dissipation rate ($4.20s^{-1}$).

The choice of filter size in the conditional-sampling method is not critical. Generally, it should be large compared to the dissipation length scale so that the Kolmogorov-C Obukhov-Corrsin theory applies to the conditional local scalar fields with small SGS variance. Here we use experimental data to show that the results are not sensitive to the filter size. Figure 6.10 shows the estimated scale ($h/w$) for the ramp-cliff structure for filter sizes, 5 and 40 mm, corresponding to $\Delta/\eta = 31$ and
Figure 6.9: Estimation of the percentage of the resolved dissipation rates of the error-function scalar profile using different finite difference schemes.

Figure 6.10: Estimation of resolved dissipation length scale using the errorfunction model. (a) 5 mm filter size; (b) 40 mm filter size.

250, respectively. The scales inferred differ by less than 2%, sufficiently accurate for such dissipation rate measurements. We expect any filter size reasonably far away from the dissipation length scale (say $> 10 - 15\eta$) to give accurate estimations.

In the case that the resolution is insufficient, the relative resolution inferred from Fig. 6.8 can be used to estimate the amount of under-resolution and make corrections using Fig. 6.9. To examine the effectiveness of the error-function model for severely underestimated scalar fields, we perform the same analysis for a sample interval of $h = 0.614\text{mm}$, twice that used above (0.307 mm). Figure 6.11(a) shows that the method still is capable of selecting the well-resolved local scalar fields (resolved by the sixth- to tenth-order schemes) to determine accurately the measurement noise. For large SGS variance the local scalar fields are severely underresolved [Fig. 6.11(b)]. Using the
procedure for obtaining the scale in Fig. 6.8, we estimate the $h/w$ value for these scalar fields, which should be twice the value obtained for the single-spacing data ($2 \times 0.54 = 1.08$) shown in Fig. 6.8. The estimated value, however, is 0.92, approximately 15% smaller than expected (Fig. 6.12).

Figure 6.12: Estimation of the dissipation length scale for the double-spacing data. The SGS variance is 4.34.

To understand this discrepancy and to make corresponding corrections, we revisit the error-function model for the ramp-cliff structure. The model assumes that the errorfunction scalar profile ranges from -1 to 1. In reality, there are also background scalar fluctuations in addition to the ramp cliff in the local scalar fields. Thus, any dissipation value $\chi$ in the ramp-cliff structure no longer occurs at the $\phi$ value give by $\chi = \chi(\phi)$, but at values fluctuating around $\phi$ according to the distribution.
of the background scalar fluctuations. Figure 6.13 shows the conditional filtered density function (FDF), which is essentially the PDF for these conditional local scalar fields (see Refs. [45, 50] for details). The two peaks have Gaussian-like shapes, suggesting that the FDF can be modeled as a convolution of a double-delta function and a Gaussian PDF. We revise the model to allow the scalar values in the error function to fluctuate in the scalar space, with the fluctuations having a Gaussian distribution as suggested by the peaks in Fig. 6.13. These background fluctuations also result in additional dissipation rate whose conditional mean is largely independent of the scalar value as shown in Fig. 6.14 for $\phi''/\langle \phi'^2 \rangle^{1/2}_L < -1.5$ and $\phi''/\langle \phi'^2 \rangle^{1/2}_L > 1.5$. Thus, a constant dissipation rate due to the background fluctuations, approximately $10s^{-1}$, is added to the modeled dissipation rate of the error-function profile.

![Figure 6.13: The filtered density function of the SGS scalar (PDF of the conditional local scalar fields) for $\langle \phi \rangle_L = 0$ and $(\phi''^2)_{L}^{1/2} = 4.34$. The peaks have Gaussian-like shapes.](image)

The revised model is used to predict the ratios of the conditional dissipation rates obtained using schemes of different orders as a function of the SGS scalar value (Fig. 6.15). The predictions are compared with the experimental results. The h/w value is varied to find the best fit to the data. Detailed procedures for implementing the revised model are given in the following section. The resulting value for the doublespacing data is $h/w = 1.15$, which is then used as the corrected h/w value for the ramp-cliff structure. The revised length scale is approximately 25% larger than the original estimation, indicating strong effects of the revised model taking into account the background fluctuations. We repeat this procedure for the single-spacing data and obtained an h/w value of 0.60, only 10% larger than the original prediction, indicating that for reasonably well-resolved local fields the estimated length scale for the single-spacing data is affected to a much lesser degree by the
background fluctuations. The revised value for the double-spacing data is within 4% of twice the $h/w$ value for the revised single-spacing data, suggesting that the revised model provides a significant improvement over the original model.

Figure 6.14: Conditionally filtered dissipation rates after noise correction for the double-spacing data with $\langle \phi'' \rangle^{1/2}_L = 4.34$.

The fluctuations of the ramp-cliff structure in the scalar space and the background scalar fluctuations also affect the model prediction of the fully resolved conditionally filtered dissipation rate (see next section). Our calculations show that the dissipation rate at $\phi'' = 0$ is reduced by 20% compared to the original error-function model [Eq. 6.9]; therefore, the ratio of the revised model predictions using different schemes to the fully resolved dissipation rate are used and the results are shown in Fig. 6.16. Using the estimated $h/w$ values the amount of under-resolution of the conditionally filtered dissipation rate can be estimated. For the single- and doublespacing data the tenth-order scheme underestimates the peak conditionally filtered dissipation rate by 1% and 19.3%, respectively. The ratio of these estimated dissipation rates is 0.817, consistent with the peak dissipation rate values in Figs. 6.7(b) and 6.14, which have a ratio of 0.84, further validating the revised error-function model. Note that the amounts of under-estimation for the original error-function model are 1% and 13%, respectively. The corrected values differ by only 6.7% for the double-spacing data, further demonstrating the robustness of the present method.
Figure 6.15: The ratio of the conditionally filtered dissipation rate obtained using different finite difference schemes. Left ordinates: second- to tenth-order schemes. Right ordinates: fourth- to sixth-order schemes. The solid line, the thick solid line, and the dashed line represent experimental results, revised error-function model, and the original error-function model. (a) Single spacing; (b) double spacing. The SGS variance is 4.34.

6.4 Revised Model

The ramp-cliff model assumes an error-function scalar profile, therefore the dissipation rate has a Gaussian profile in physical space.

\[ \chi(x) = 2D \left( \frac{d\phi}{dx} \right)^2 = \frac{8D}{\pi w^2} e^{-2\left( \frac{x}{w} \right)^2} \]  

(6.20)

After substituting the physical-space variable with the scalar value \( x = w \cdot \text{erf}^{-1}(\phi) \), the dissipation rate profile in scalar space is

\[ \chi(\phi) = \frac{8D}{\pi w^2} \exp \left( -2 \left( \text{erf}^{-1}(\phi) \right)^2 \right) \], \quad \text{where} \quad -1 < \phi < 1 \]  

(6.21)

This dissipation rate is defined only for \(-1 < \phi < 1\). There are, however, background scalar fluctuations in addition to the ramp-cliff, which result in fluctuation of the dissipation \( \chi(\phi) \) in scalar space as well as background dissipation. These effects can be modeled by statistically shifting the error-function scalar profile in scalar space and a constant background dissipation. To do this, we
first extend $\chi(\phi)$ as following

$$
\chi_e(\phi) = \begin{cases} 
\frac{8D}{\pi w^2} \exp \left(-2 \left(\text{erf}^{-1}(\phi)\right)^2\right), & -1 < \phi < 1; \\
0, & \text{otherwise.}
\end{cases}
$$

The shifting in scalar space is accounted for by convolving $\chi_e(\phi)$ with a Gaussian kernel in scalar space,

$$
G(\psi; \sigma) = \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{\psi^2}{2\sigma^2}}
$$

which represents the distribution of the background fluctuations. The kernel bandwidth is determined by the Gaussian fit of two branches of the fdf except near $\phi'' = 0$. In this study, the bandwidth $\sigma$ is between 0.38 and 0.39, therefore 0.385 is chosen for the calculation. Therefore, the resulting dissipation rate model as a function of the scalar space variable is

$$
\langle \chi | \phi \rangle_m = \int \chi_e(\psi) G(\psi, \psi; \sigma) d\psi + \chi_b = \int_{-1}^{1} \frac{8D}{\pi w^2} e^{-2(\text{erf}^{-1}(\phi))} \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{(\phi-\psi)^2}{2\sigma^2}} d\psi + \chi_b
$$

where $\langle \chi | \phi \rangle_m$ and $\chi_b$ are the fully resolved conditional dissipation rate of the revised error-function model and the background dissipation rate, respectively. The background dissipation rate can be determined from the part of the noise corrected dissipation where independent of the scalar values. (See the following for the actual implementation.)

The dissipation rate of the revised error-function model calculated using a finite difference
scheme is obtained by first writing down an analytical expression for the dissipation rate of an error-function profile calculated using the scheme,

\[
\chi_N(x) = 2D \left( \frac{d\phi}{dx} \right)^2 = 2D \left( \frac{1}{h} \sum_{n=-N}^{N} a_n \phi(x + nh) \right)^2 = \frac{2D}{h^2} \left( \sum_{n=-N}^{N} a_n \text{erf} \left( \frac{x + nh}{w} \right) \right)^2
\]

(6.25)

Here \( \chi_N(x) \) is a continuous function in physical space. After substituting the physical space variable with the scalar value \( x = w \cdot \text{erf}^{-1}(\phi) \), the resulting expression, which is a function of the scalar variable, is convolved with the Gaussian kernel:

\[
\langle \chi| \phi \rangle_{m,N}(\phi) = \int_{-1}^{1} \frac{2D}{h^2} \left( \sum_{n=-N}^{N} a_n \text{erf} \left( \text{erf}^{-1}(\psi) + n \frac{h}{w} \right) \right)^2 \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{(\psi-x)^2}{2\sigma^2}} d\psi + \chi_b
\]

(6.26)

where \( \langle \chi| \phi \rangle_{m,N} \) is the dissipation rate calculated with a 2Nth order scheme. The integration here is performed numerically for a range of \( \phi \) values. In this case, the background dissipation rate is approximately \( 10s^{-1} \) for \( \left| \phi'' / \langle \phi'' \rangle_L \right| > 1.5 \). In the calculation, \( \chi_b \) is determined by equating \( \chi_b / \langle \chi| \phi \rangle_{m,N} \) to the measured ratio of the background to the peak dissipation at \( \phi'' = 0 \). The ratio of \( \langle \chi| \phi \rangle_{m,N} \) obtained from different schemes are then compared with experimental results in Fig. 6.15.
Chapter 7

Noise and Resolution Correction in Combustion

7.1 Introduction

The scalar dissipation rate is a key variable characterizing turbulent mixing. It is also an important variable in studying and modeling turbulent nonpremixed/partially premixed flames\[4, 33\]. The mean scalar dissipation rate, $\langle \chi \rangle = \langle 2D \nabla \xi \cdot \nabla \xi \rangle$, appears in the scalar variance equation as the rate of reduction of the variance of scalar fluctuations by mixing, where $D$, $\chi$, and $\xi$ are the molecular diffusivity, the scalar dissipation rate, and the scalar variable, respectively. The conditional mean scalar dissipation rate conditional on the scalar value, $\langle \chi | \xi \rangle$, is the mixing term evolving the scalar probability density function (PDF) in the PDF equation[36]. It is also a key quantity in the conditional moment closure and the laminar flamelet models[5, 32, 33]. Eswaran and Pope [15] were the first to obtain the conditional dissipation rate in a turbulent flow (using direct numerical simulation).

In a turbulent flow or a turbulent flame the scalar (mixture fraction) dissipation rate comes primarily from fluctuations at the smallest length scales. These fluctuations are much smaller than the integral-scale fluctuations. As a result, accurate measurements of the dissipation rate require both high spatial resolution and high signal-to-noise ratio, which are difficult to achieve even at moderate Reynolds numbers. It is, therefore, generally necessary to quantify the effects of measure-
ment resolution and noise on dissipation rate measurements. In a measurement system these effects, however, are usually present at the same time. For example, both the amount of dissipation resolved by the measurement system and the noise contribution increase with the resolution, making their effects difficult to separate and to quantify.

Because of its importance and the difficulties in its measurements, much effort has been devoted to quantifying and improving the accuracy of scalar dissipation rate measurements (e.g., Ref. [59, 6, 13, 31, 9]). One approach [56, 54] uses Pope's spectral model [38] and a noise model to fit the measurement data, allowing inference of the noise variance and the scalar dissipation length scale. Several recent studies used redundant signals to separate the noise contributions in thermal dissipation in flames [58, 25, 17].

A limitation of spectral approaches is that it cannot be applied to the conditional scalar dissipation rate. In addition, the so-called ramp-cliff scalar structure [46, 50, 52, 10] is usually present in turbulent passive scalar fields as well as in nonpremixed and partially premixed turbulent flames. The cliffs are a highly local structure and generate large local dissipation rate but do not necessarily contribute significantly to the spectrum. In addition, the spectrum calculated depends on ratio of the length of the signal record used to compute the spectrum to the thickness of the cliff. Spectral analysis, therefore, is generally not suited to characterize such highly local structures.

To overcome these difficulties, Cai and Tong [9] developed an analysis approach using conditional sampling to evaluate the noise contributions, enabling separation of the noise effects from resolution effects without a spectral model or redundant signals. Because this method does not rely on spectral analysis, it allows conditioning of the dissipation rate on the scalar value at the same location.

The most unique aspect of the present method is that rather than processing turbulent scalar fields as a general random process, the conditional-sampling procedure makes use of the unique properties of these fields. The method uses two conditioning variables, the filtered (locally averaged) scalar and the subfilter-scale (SFS) scalar variance (local scalar variance). When the SFS variance is small, the local scalar field is well mixed [45, 50]. The statistics of such a conditional scalar is well described by the Kolmogorov-Obukhov-Corrsin theory. The locally averaged scalar dissipation rate and the scalar variance spectral transfer rate are lower than the mean scalar dissipation rate. In the spirit of the Kolmogorov's refined similarity hypotheses, the local conditional Péclet number is expected to be lower than that based on the unconditioned statistics. The scalar dissipation
length scales for these fields, therefore, are larger than the mean scalar dissipation length scale [9]. By choosing sufficiently small SFS variance values, one can select local scalar fields with sufficiently large dissipation length scales so that they are well resolved by the measurement apparatus.

In implementing the method we first use conditional sampling to select fully resolved local scalar fields, which are then used to determine the measurement noise. Noise corrections are applied to the mean and conditional dissipation rate to examine the extent to which these statistics are resolved. Noise correction is applied further to potentially under-resolved local scalar fields, selected by using large SFS variance values. The noise-corrected dissipation rate along with a physical space model is then used to evaluate the extent of resolution of the scalar dissipation rate and the scalar dissipation length scales.

In present study, we employ the method to analyze the measured scalar dissipation rate in turbulent partially premixed (Sandia) flames [27, 2, 28]. The rest of the paper is organized as follows. Section 2 provides a brief description of the method, followed by a summary of the measurement system and experimental data in section 3. In section 4 we analyze the well-mixed and potentially under-resolved conditional local scalar fields to extract the noise variance, to perform noise correction, and to estimate the dissipation length scale of the potentially under-resolved fields and the extent they are resolved. We also quantify the extent of resolution of the mean scalar dissipation rate and the conditional dissipation rate. The conclusions are given in Section 5.

### 7.2 Brief description of the method

In this section we summarize the noise correction and length-scale estimation method developed by Cai and Tong [9]. For more details refer to that reference. The method uses conditional sampling to ensure selection of well-resolved and potentially under-resolved local scalar fields. In turbulent flames the Favre filtered (locally averaged) scalar,

$$\langle \xi \rangle_L \equiv \langle \rho \xi \rangle_{\ell} / \langle \rho \rangle_{\ell},$$  \hspace{1cm} (7.1)

and the Favre SFS scalar variance,

$$\langle \xi^2 \rangle_L \equiv \langle \rho \xi^2 \rangle_{\ell} / \langle \rho \rangle_{\ell} - \langle \xi \rangle_L^2$$  \hspace{1cm} (7.2)
are used as conditioning variables. Here \( \langle \cdot \rangle_L \) and \( \langle \cdot \rangle_{L} \) represent a conventional local average, \( \int (\cdot) G(x - x') dx' \), and a Favre local average respectively, and \( G \) is the top-hat filter function.

The conditional sampling procedure selects well-mixed local scalar fields when the SFS variance is small compared to the mean SFS variance [45, 50, 52, 10]. These fields have larger dissipation length scales because the mixing process is not intense. For SFS variance much larger than the mean SFS variance, the local scalar is highly segregated and contains the ramp-cliff structure [46, 50]. The scalar dissipation rate is very large inside the cliffs. At the same time, the cliffs in the local scalar are likely to have smaller length scales. Using conditional sampling with different SFS variance values, we can select local scalar fields that can be well resolved and those that are potentially under-resolved to evaluate their dissipation length scales. The well-resolved local fields are used to evaluate the measurement noise variance, which is then used to remove the noise contributions from the potentially under-resolved scalar fields, effectively separating the noise effects from the resolution effects.

For many measurement systems, including the one used to obtain the one-dimensional images in the the Sandia flames[27, 2], the noises at different measurement locations (pixels) are uncorrelated random variables and are additive to the scalar values:

\[
\xi = \xi^* + n.
\]  

where \( \xi^* \), \( \xi \), and \( n \) are the true scalar value, the measured value, and the noise, respectively. To make noise corrections the noise variance is needed. For the Sandia system, noise in the measured mixture fraction is dominated by shot noise in the measurement of major species, and the noise variance in the cold fuel-air mixture may be modeled as proportional to mixture fraction. To account for the dependence of the noise variance on the temperature we consider only the dependencies of the Raman scattering signal levels on the mixture density but not on the the mixture compositions. Because the species number densities are proportional to the mixture density, so is the total scattering signal and is the noise variance. Consequently, the model noise variance for the normalized signal (\( \xi \)) is inversely proportional to the density, hence is proportional to the temperature because pressure variations are small in low-speed flows. The variance of noise is then modeled as proportional to

\[
104
\]
both the mixture fraction and the temperature,

\[
\langle n^2|\xi, T \rangle = \sigma_n^2(\xi, T) = B \cdot \xi \cdot T \tag{7.4}
\]

To obtain the scalar dissipation rate numerical (usually finite difference) schemes are usually needed to calculate the derivatives as experimental data are generally discrete samples. Different schemes involve different numbers of samples and different weights to the samples. Consequently, the calculated scalar dissipation rate and the noise are scheme dependent. A generalized form of an explicit central finite difference scheme for the derivative is

\[
h \cdot \frac{\tilde{d}\xi}{dx} = a_1(\xi_1 - \xi_{-1}) + a_2(\xi_2 - \xi_{-2}) + a_3(\xi_3 - \xi_{-3}) + a_4(\xi_4 - \xi_{-4}) + \ldots \tag{7.5}
\]

where \( h \) and \( \frac{\tilde{d}\xi}{dx} \) are the distance between adjacent samples (sample spacing) and the estimated derivative, respectively. The schemes used in the present study and their coefficients are given in table 7.1.

Table 7.1: Coefficients for central finite difference schemes

<table>
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<th>order</th>
<th>( a_1 )</th>
<th>( a_2 )</th>
<th>( a_3 )</th>
<th>( a_4 )</th>
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<tbody>
<tr>
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<td>1/2</td>
<td>0</td>
<td>0</td>
<td>0</td>
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</tr>
<tr>
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<td>-1/12</td>
<td>0</td>
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<tr>
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<tr>
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<tr>
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<td>2100/2520</td>
<td>-600/2520</td>
<td>150/2520</td>
<td>-25/2520</td>
<td>2/2520</td>
</tr>
</tbody>
</table>

By including this noise model in the finite difference scheme in Equation (7.5), the measured derivative is

\[
h \cdot \frac{d\xi}{dx} = a_1(\xi_1 - \xi_{-1}) + a_2(\xi_2 - \xi_{-2}) + a_3(\xi_3 - \xi_{-3}) + a_4(\xi_4 - \xi_{-4}) + \ldots
\]

\[
= a_1(\xi_1^* - \xi_{-1}^*) + a_2(\xi_2^* - \xi_{-2}^*) + a_3(\xi_3^* - \xi_{-3}^*) + a_4(\xi_4^* - \xi_{-4}^*) + \ldots
\]

\[
+ a_1(n_1 - n_{-1}) + a_2(n_2 - n_{-2}) + a_3(n_3 - n_{-3}) + a_4(n_4 - n_{-4}) + \ldots
\]

\[
= h \cdot \frac{d\xi^*}{dx} + a_1(n_1 - n_{-1}) + a_2(n_2 - n_{-2}) + a_3(n_3 - n_{-3}) + a_4(n_4 - n_{-4}) + \ldots, \tag{7.6}
\]
where \( \frac{\partial c^*}{\partial x} \) is the estimated derivative without noise. The measured Favre mean dissipation rate is

\[
\langle \chi \rangle_F = \langle \rho \chi \rangle / \langle \rho \rangle = \left( 2 \rho D \left( \frac{\partial c^*}{\partial x} \right)^2 \right) / \langle \rho \rangle
\]

\[
= \left( 2 \rho D \left( \frac{\partial c^*}{\partial x} \right)^2 \right) / \langle \rho \rangle + \frac{2}{h^2} B \sum_{i=-N}^{N} \rho D a_i^2 n_i^2 / \langle \rho \rangle
\]

\[
\approx \left( 2 \rho D \left( \frac{\partial c^*}{\partial x} \right)^2 \right) / \langle \rho \rangle + \frac{2}{h^2} B \sum_{i=-N}^{N} a_i^2 \langle \rho D \xi_i T_i^* \rangle / \langle \rho \rangle
\]

\[
\approx \left( 2 \rho D \left( \frac{\partial c^*}{\partial x} \right)^2 \right) / \langle \rho \rangle + \frac{2}{h^2} BC_N
\]

(7.7)

where \( C_N = \sum_{i=-N}^{N} a_i^2 \langle \rho D \xi_i T_i \rangle / \langle \rho \rangle \) and \( \left( 2 \rho D \left( \frac{\partial c^*}{\partial x} \right)^2 \right) / \langle \rho \rangle \) are a scheme dependent factor and the estimated noise corrected dissipation rate, respectively.

When all the schemes can resolve the turbulence scalar field, the noise-corrected Favre mean dissipation rate does not depend on the scheme. The Favre mean dissipation rate before noise correction, when plotted against \( C_N \), is a straight line with a slope of \( \frac{2}{h^2} B \) with the intercept as the noise-corrected dissipation rate. This linear relationship can be used to determine the noise variance (\( B \) in Eq. 4). If the scalar field is not fully resolved by some lower-order schemes, then the higher-order schemes that can fully resolve it form a straight line on the \( \langle \chi \rangle_F - C_N \) plot. This relationship also can be applied to the Favre conditional dissipation rate and the Favre conditionally filtered dissipation rate. In the present work all the dissipation rate statistics are Favre statistics; therefore, for convenience we omit the term “Favre” for the rest of the paper.

Employing the conditional sampling method we can select fully resolved local scalar fields and determine the noise variance according to Eq. 7. The noise variance is then used to correct the dissipation rate from the potentially under-resolved local scalar fields. The noise-corrected dissipation rates from the different schemes are then analyzed to evaluate the scalar dissipation length scales and the extent of resolution.

For the potentially under-resolved local scalar fields, the \( \langle \chi \rangle_F - C_N \) relationship might not be linear. A model is needed to evaluate the extent of under-resolution. When the SFS variance is large, the local scalar field contains the ramp-cliff structure, which has a large dissipation rate and a small length scale; therefore, it is the cause for the under-resolution. To evaluate the extent
of under-resolution of the ramp-cliff structure, the error function is used as a model for the scalar profile \[9\].

An error-function scalar profile with a width \(w\) is

\[
\xi(x) = \frac{1}{2} + \frac{1}{2} \text{erf}\left(\frac{x}{w}\right) = \frac{1}{2} + \frac{1}{\sqrt{\pi}} \int_0^\frac{x}{w} e^{-x'^2} \, dx'.
\] (7.8)

The dissipation rate is calculated at \(\xi = 0.5\) where the dissipation is at its maximum. Here \(w\) corresponds to the \(1/e\) point of the maximum scalar derivative. A comparison between selected schemes is shown in Figure 10 of Ref. \[9\]. For a given scheme, as the distance between adjacent samples, \(h\), increases, the calculated dissipation rate decreases. For a fixed \(h\), higher-order schemes resolve more dissipation rate. By comparing the measured dissipation rate to that calculated from error-function profile using different schemes, the width of the profile, \(w\), can be inferred. The percentage of the dissipation resolved can also be estimated using the model.

### 7.3 Experimental data

The experimental data used in this study were obtained in piloted turbulent partially pre-mixed methane flames (Sandia flames D and E, see Ref.\([27, 2, 28]\) for more details). The fuel stream is premixed \(\text{CH}_4\) and air with a ratio of 1:3 by volume. The fuel jet with a diameter \(d = 7.2\) mm was mounted approximately 17 cm above the 25 cm\(^2\) exit of a wind tunnel contraction, which supplied a laminar co-flow of air at 0.9 m/s. The jet exit Reynolds numbers for flames D and E are 22,400 and 33,600 respectively.

The measurement system employed combined line-imaging of Raman scattering, Rayleigh scattering, and laser-induced CO fluorescence. Simultaneous measurements of major species (\(\text{CO}_2\), \(\text{O}_2\), \(\text{CO}\), \(\text{N}_2\), \(\text{CH}_4\), \(\text{H}_2\text{O}\), and \(\text{H}_2\)), mixture fraction (obtained from all major species), temperature, and the radial component of scalar dissipation rate were made. The mixture fraction is calculated using a variation of Bilger’s definition, which has been modified by excluding the oxygen terms\([2]\).

The issue of measurement uncertainty was addressed in Ref.\([2]\), which concluded that the accuracies of the measured species mass fractions, temperature, and mixture fraction are sufficient. For example, the measured values of the scalar (mixture fraction) variance in uniform calibration flows were \(10^{-6}\) in air and \(10^{-5}\) in flat stoichiometric flame products and in jet fluid, respectively.
The length of the imaging line is 6.13 mm with a imaging pixel spacing of 0.2044 mm. The
SFS scalar variance is calculated using a segment (3.065 mm or 15 pixels) of each line image. Our
recent work [9] showed that the noise and the length scale inferred do not depend on the size of
the segment. In the analyses 6000 line images are used at each measurement location. Due to the
limited data size, we employ kernel methods for computing the conditional dissipation rate and the
conditionally filtered dissipation rates. We use a bin width of $\Delta \ln \langle \xi''^2 \rangle = 1.3$ to achieve reasonable
statistical convergence.

7.4 Results

In this section the noise correction and length scale estimation method for mixture fraction
dissipation is applied to turbulent partially premixed jet flames (Sandia Flames).

We first analyze the well-resolved local scalar fields selected using the conditional sampling
procedure to obtain the noise variance, which is then used to correct for the dissipation rate of these
and the potentially under-resolved scalar fields as well as the mean and conditional dissipation rate.
The extent of the resolution of these statistics are examined. The potentially under-resolved fields
are analyzed using the error-function model.

7.4.1 Well-resolved local scalar field

The mean dissipation rate conditional on the scalar value obtained from the conditional
local scalar fields is the conditionally filtered dissipation rate (See Ref. [50]). At each measurement
location it is calculated using five central difference schemes. As the scheme order increases, the
conditionally filtered dissipation rates increases. Figure 7.1a shows the results in Flame D at $x/D = 15$ for
$\langle \xi \rangle_L = 0.35$ and $\langle \xi''^2 \rangle_L = 5.2 \times 10^{-4}$, the latter much smaller than the mean SFS variance
($2.36 \times 10^{-2}$). The dissipation-$C_N$ relationship essentially is linear, indicating that the increases in
the dissipation rate values using the higher-order schemes come from increased noise contributions;
therefore, the local scalar fields for small SFS variance are well resolved by all the schemes. Note
that the noise-corrected conditionally filtered dissipation (the intercept) is of the same order as the
noise contributions.

For a somewhat larger SFS variance, $\langle \xi''^2 \rangle_L = 2.6 \times 10^{-3}$ (Fig. 7.1b), the conditionally
filtered dissipation rates obtained using the fourth- and higher-order schemes form a straight line
while the dissipation rate using the second-order scheme is below this line, indicating that the higher-order schemes are capable of resolving the smallest scalar length scales in this case but second-order scheme is not. The intercept of the straight line (\( \sim 9.58 \text{s}^{-1} \)) is lower than the dissipation rate calculated using the second-order scheme (\( \sim 10.22 \text{s}^{-1} \)), indicating that when using second-order scheme the effect of the noise is greater than that of the insufficient resolution. The constant \( B \) in the noise variance model is determined as \( 1.2 \times 10^{-7} \). This value is consistent with the noise variance obtained in a laminar flame at Sandia (unpublished data).

For large SFS variance, \( \langle \xi''^2 \rangle_L = 6.7 \times 10^{-2} \) (Fig. 7.1c), the dissipation-C\(_N\) plot is curved. The results using the eighth- and lower-order schemes are below the straight line going through the tenth-order scheme point and having the same slope as in Figs. 1a & b, indicating that the eighth- and lower-order schemes are resolving less dissipation rate than the tenth-order scheme. Note that the dissipation rate using the second- and fourth-order schemes is less than the intercept of straight line (\( \sim 166.0 \text{s}^{-1} \)), indicating that even without correcting for noise these schemes are underestimating the dissipation rate. There is, however, no evidence to show that whether the tenth-order scheme is capable of fully resolving the scalar scales. Thus, the true dissipation is equal or higher than the intercept of the straight line. This case will be analyzed using the error-function model in subsection 4.3.

7.4.2 Noise corrections

The conditionally filtered dissipation rates conditioning on mixture fraction using schemes of different orders at three different SFS scalar variances \( \langle \xi''^2 \rangle_L = 5.2 \times 10^{-4}, 2.6 \times 10^{-3} \) and \( 6.7 \times 10^{-2} \) are given in Figure 7.2a, 7.3a and 7.8a respectively. All the figures show that the calculated dissipation rate increase as the order of schemes increases. We subtract the noise contributions and show the results in Fig. 7.2b, 7.3b and 7.8b.

For small SFS scalar variance (\( \langle \xi''^2 \rangle_L = 5.2 \times 10^{-4} \), Figure 7.2), the corrected dissipation rate calculated using second-to tenth-order schemes largely overlap, indicating that all the schemes are sufficient to resolve the smallest scalar dissipation length scale in these scalar fields and that the noise contributions have been removed. Increasing the SFS scalar variance to \( \langle \xi''^2 \rangle_L = 2.6 \times 10^{-3} \) (Fig. 7.3), the conditionally filtered dissipation rate using fourth- or higher-order schemes overlap, indicating that these schemes are sufficient to resolve all the scalar length scales and noise contributions have been removed. Note that for \( 0.2 < \xi < 0.45 \), the second-order scheme only
slightly under-resolves the scalar but for $\xi > 0.45$, the deviations from the other schemes are larger. We find that these deviations are a result of the noise variance for these mixture fraction values slightly differing from the model given by Eq. 4.

The noise correction procedure also can be applied to the mean scalar dissipation rate, $\langle \chi \rangle_F$, and the conditional dissipation, $\langle \chi | \xi \rangle_F$. The mean dissipation rate profiles at the three downstream locations ($x/d = 7.5$, 15, and 30) in both flames D and E are shown in Fig. 7.4. The noise-corrected profiles using the tenth-order scheme at $x/d = 30$ are close to the uncorrected ones using the second-order scheme whereas at $x/d = 7.5$ they are close to those using the fourth- or sixth-order schemes because for the former the resolution is expected to be better due to larger dissipation length scales. These profiles are in general agreement to those obtained using filtering and extrapolation in Fig. 5 of Ref. [3]. The peak measured mean dissipation rate is plotted against $C_N$ in Fig. 7.5. The dashed lines start from the data points for the tenth-order scheme with the same slope (noise variance) as that Fig. 1a, representing the measured dissipation rate by the lower-order schemes if these schemes could fully resolve the dissipation rate, i.e., the measurements were only affected by the noise. Perhaps with the exception of flame E at $x/d = 7.5$, the dissipation rate values obtained by the eighth-order scheme are well within a fraction of 1% of the tenth-order results, indicating that the mean dissipation rate is well resolved by the eighth- and tenth-order schemes.

The results for the measured conditional dissipation rate are shown in Fig. 7.6. Except at $x/d = 7.5$, the conditional dissipation rate is double-peaked with a minimum slightly to the rich side of the stoichiometric mixture fraction. The rich-side peaks are higher than the lean-side ones. The lean-side peak conditional dissipation rate vs. $C_N$ are shown in Fig. 7.7. The $\xi$ values (see the captions) corresponding to the lowest ratio between dissipation rate obtained using the second- and tenth-order schemes. Again, perhaps except for flame E at $x/d = 7.5$, the conditional dissipation is well resolved. The difference between the eight-and tenth-order results near the rich-side peak is due to the noise variance slightly deviating from the noise model.
Figure 7.1: Conditionally filtered scalar dissipation rate (near the stoichiometric mixture fraction) vs. $C_N$ at $x/d = 15$ in flame D. The data points (increasing $C_N$) represent the measured dissipation rate using the second- to tenth-order finite differencing schemes, respectively. The intercept of the straight lines represent the noise-corrected dissipation rate. (a) Well-resolved local fields, $\langle \xi''^2 \rangle_L = 5.2 \times 10^{-4}$; (b) Under-resolved by the second-order scheme, $\langle \xi''^2 \rangle_L = 2.6 \times 10^{-3}$; (c) Potentially under-resolved local fields, $\langle \xi''^2 \rangle_L = 6.7 \times 10^{-2}$. 
Figure 7.2: Conditionally filtered dissipation rate before and after noise correction at $x/d = 15$ in flame D. Small SFS variance $(\langle \xi'^2 \rangle_L = 5.2 \times 10^{-4})$.

Figure 7.3: Conditionally filtered dissipation rate before and after noise correction at $x/d = 15$ in flame D. Medium SFS variance $(\langle \xi'^2 \rangle_L = 2.6 \times 10^{-3})$. 
Figure 7.4: Measured mean dissipation rate profiles. The curves with circles are noise-corrected profiles obtained using the tenth-order scheme. (a, c & e) flame D at x/d=7.5, 15, and 30 respectively; (b, d, & f) flame E at the same locations.
Figure 7.5: Measured mean dissipation rate (1/s) vs. $C_N$ at $x/d=7.5$, 15, and 30 in flames D and E. The intercept of each dashed straight line is the noise-corrected mean dissipation rate.
Figure 7.6: Measured conditional dissipation rate (1/s) after noise correction: (a, c & e) flame D at x/d=7.5, 15, and 30 respectively; (b, d, & f) flame E at the same locations.
Figure 7.7: Measured conditional dissipation rate (1/s) vs. $C_N$: (a, c, & e) flame D at $x/d=7.5, 15,$ and 30 with the mixture fraction values at 0.397, 0.367, and 0.317, respectively; (b, d, & f) flame E at the same locations with with the mixture fraction values at 0.387, 0.336, and 0.302, respectively.
7.4.3 Estimation of length scales and the extent of resolution for under-resolved scalar field

As shown in the previous subsection, for large SFS variance the local scalar fields are potentially under-resolved. In this part we address the issue of resolution and length scale associated with these fields and the extent to which they are under-resolved.

For large SFS scalar variance \( \langle \xi''^2 \rangle_L = 6.7 \times 10^{-2} \), although Fig. 7.8 shows that the conditionally filtered dissipation rate values using different schemes are closer after the noise correction, lower-order schemes still give lower dissipation rates. The conditionally filtered dissipation rate at other locations and in flame E is shown in Fig. 7.9.

After correcting for the noise, the measured dissipation rate is only affected by the resolution, which is expected to be worst when the SFS scalar variance is largest, due to the sharp cliffs in the local scalar. Because the scalar dissipation length scales are not known a priori, we need to use experimental data to infer them. Comparing the measured scalar spectrum to a model spectrum can provide an estimate of the average dissipation length scale, but not that of the cliffs, which dominate the scalar dissipation rate for large SFS variance. To estimate the length scales of the cliffs we use the error function as a model for the ramp-cliff structure in the SFS scalar fields and calculate the dissipation rate using different schemes with a range of sample spacings (spatial resolution) \[9\].

Figure 7.8: Conditionally filtered dissipation rates before and after noise correction at \( x/d = 15 \) in flame D. Large SFS variance \( \langle \xi''^2 \rangle_L = 6.7 \times 10^{-2} \).
Figure 7.9: Conditionally filtered dissipation rates after noise correction. (a, c & e) flame D at $x/d=7.5, 15,$ and 30 respectively. The SFS variance values are $6.6 \times 10^{-2}, 6.7 \times 10^{-2},$ and $6.3 \times 10^{-2},$ respectively; (b, d, & f) flame E at the same locations. The SFS variance values are $8.4 \times 10^{-2}, 5.0 \times 10^{-2},$ and $4.5 \times 10^{-2},$ respectively.
In the discussion on using finite difference schemes to compute derivatives (Eq. 5), the effects of finite sample spacing, \( h \), is considered, while the effects of the probe volume is not. In Cai and Tong (2009), the measurements were made using probes with a size (cold wires of 0.625 \( \mu \)m in diameter) much smaller than the sample spacing (equivalent to 0.307mm); therefore, the probe sampling volume has negligible effects on the measured dissipation rate. In laser diagnostics, however, the sampling volume (the pixel size) is often comparable to the sample spacing, which also affects the derivative measurements. In the present study the pixel size of the imaging system is approximately the same as the sample spacing (no gap between pixels) and is effectively a top-hat filter in physical space. Thus, the samples can be considered to have been taken from the pixel-averaged scalar fields at the center of each pixel. In the following we consider the effects of the pixel filtering on the evaluations of the length scales and the dissipation rate.

We use the ratios of the dissipation rate calculated with different schemes to infer the scalar dissipation scale [9]. By equating the ratios from the measured dissipation rates and from the error-function model, a scalar dissipation scale can be inferred. To include the effects of pixel averaging, the error function is first pixel-averaged with a pixel size equal to the sample spacing. It then is used to calculate the dissipation rate.

The ratios of the dissipation rate obtained at \( x/d = 15 \) in flame D are shown in Fig. 7.10. Here the lowest ratios (at \( \xi \approx 0.384 \)) are compared with the error-function model because these ratios correspond to the smallest scalar length scale. The horizontal axis is the ratio of sample spacing to the scalar profile width, \( h/w \). The ratio of the second- to the tenth-order estimations is approximately 0.883, giving a \( h/w \) of 0.454 (\( w = 0.45 \) mm). The scales inferred from all the other schemes also agree very well, indicating the overall success of the noise correction and resolution/length scale estimation.

The inferred length scale and the error-function model can be used to estimate the extent of under-resolution of the ramp-cliff structure. Figure 7.11 gives the ratio of the dissipation rate of error-function profile obtained using pixel averaging and finite differencing to the true dissipation rate (obtained analytically) as a function of \( h/w \). At the sample interval of \( h/w = 0.454 \), the second-through the tenth-order schemes underestimating the dissipation rate by 15.1\%, 5.8\%, 4.2\%, 3.7\%, and 3.5\%, respectively.

It is interesting to compare these amounts of underestimation to those without considering pixel averaging. Using a figure similar to Fig. 7.10 (see Fig. 8 in Ref. [9]), the same second- to
tenth-order ratio of 0.883 gives an \( h/w \) value of 0.445, very close to the value of 0.454 obtained above. Figure 9 in Ref. [9] shows that with this \( h/w \) value the schemes underestimate the dissipation rate by 12.1\%, 2.5\%, 0.8\%, 0.3\%, and 0.2\%, respectively. Consequently, when the finite difference schemes can resolve well the scalar derivative, other effects such as pixel averaging, can have a non-negligible influence on the resolution of the scalar dissipation rate.

The 3.3\% difference in the resolved dissipation rate for the tenth-order scheme due to pixel averaging is for local scalar fields with large SFS variance. For the well-resolved local scalar fields, the scalar dissipation length scale is much larger than the pixel size; therefore, the pixel averaging has a negligible effect on the corrected dissipation rate. Consequently, the analysis in section 4.1 is not affected by the finite pixel size.

The noise-corrected conditionally filtered dissipation rate vs. \( C_N \) obtained in both flames D and E are shown in Fig. 7.12. The mixture fraction values correspond to the peak dissipation rate in Fig. 7.9. Similar to flame D at \( x/d = 15 \), in all the other cases the eighth-order scheme resolve slightly less than the tenth-order scheme. Analyses using the error-function model gives a \( h/w \) value of 0.40 (\( w = 0.511 \text{ mm} \)) at \( x/d = 7.5 \) and 30 in flame D respectively, corresponding to 97.3\% resolution of the dissipation rate. The \( h/w \) values for flame E at \( x/d = 7.5 \), 15, and 30 are 0.594, 0.576, and 0.530 (\( w = 0.344 \), 0.355, and 0.386 mm) respectively, corresponding to 93.4\%, 93.8\%, and 95.0\% resolution of dissipation rate. These results also show that the conditional dissipation rate in Fig. 7.7 is well resolved because it contains dissipation rate from both the well-resolved and the potentially under-resolved local fields. The length scales obtained in flame D are approximately 30\% larger than those in flame E for all the downstream locations considered. It is interesting to note that the Batchelor scales given in Ref. [54] also show an approximately constant ratio for the two flames, although the difference is approximately 20\%.
Figure 7.10: Estimation of the length scale by comparing the ratio of dissipation rate obtained from data (solid squares) to that from the model (curves). The ratios obtained using different schemes are shown.

Figure 7.11: Estimation of the resolved dissipation rate obtained using the estimated length scale and the error-function model.
Figure 7.12: Conditionally filtered dissipation rate vs. $C_N$. (a), (c), and (e): flame D at $x/d=7.5$, 15, and 30, respectively. The mixture fraction values are 0.515, 0.384, 0.364 respectively; (b), (d), and (f): flame E at the same locations. The mixture fraction values are 0.465, 0.394, 0.424 respectively.
7.4.4 Conditionally filtered dissipation rate conditional on both mixture fraction and temperature

In the transport equation of the filtered joint density function of mixture fraction and temperature, one of the mixing terms is the conditionally filtered scalar dissipation rate conditional on both mixture fraction and temperature. In this part we examine the dissipation length scale associated with this quantity and the extent to which they are resolved. We focus on the cases with large SFS variance when the smallest length scale and potential under-resolution occur.

When the SFS variance is large, the local SFS scalar fields contain burning or extinguished flamelets. When the scalar dissipation rate increases, the temperature decreases; therefore, the scalar dissipation length scale is likely to decrease with temperature. The decrease can occur for two reasons: an increased strain rate that results in a higher dissipation rate, and a reduced scalar diffusivity at a lower temperature. As a result, when both the mixture fraction and temperature are used as conditioning variables, evaluations of the resolution and length scale need to be performed for a range of temperatures. Here we evaluate the resolution for each error-function profile at the mixture value where the dissipation rate is least resolved. The length scale, therefore, represents the smallest length scale for the dissipation rate.

We compute the ratio of the measured scalar dissipation rate obtained using the second-order scheme to that using the tenth-order scheme at each temperature for the entire range of mixture fraction (Fig. 7.13). The lowest point at each temperature represents the location (in the scalar space) of the least resolved portion of the scalar profile. This ratio is compared with the error-function model to obtain an $h/w$ value and to determine the fraction of the dissipation resolved. The results for Sandia flames D and E at three downstream locations are shown in Fig 7.14. In general, $h/w$ decreases ($w$ increases) when the temperature increases, consistent with the properties of laminar flamelets. In some cases we limit the temperature to approximately 1800K because very close to the equilibrium temperatures, the scalar field is well-resolved by both schemes, with the ratio close to unity and less sensitive to the $h/w$ value (Fig. 7.11). As a result, at these temperatures the statistical uncertainties in calculating the ratio can have a large impact on the inferred $h/w$ values (e.g., the ratio can exceed unity slightly, for which $h/w$ is not defined). In these cases, however, the scalar is well-resolved; therefore, the $h/w$ value is not important for interpreting the dissipation rate results.

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For flame D at $x/d = 7.5$ the $h/w$ value is approximately 0.30 at 1850K (Fig. 7.14), i.e., the width of the error-function profile is three times the sample spacing. The dissipation rate is more than 98% resolved by the tenth-order scheme (Fig. 7.15). The $h/w$ value increases to approximately 0.68 at 1300K, corresponding to approximately 91% resolution of the dissipation rate and indicating that the measurement resolution is adequate, even for the highest dissipation rate at this location. Moving to $x/d = 15$, $h/w$ is also $\approx 0.3$ at 1800K, indicating well-resolved dissipation. The temperature at this location, however, can drop much lower due to local extinction. At 700K, $h/w$ increases to nearly 1.0, corresponding to a narrower error-function profile due to both high strain rate and reduced diffusivity at low temperatures. Only 72% of the largest dissipation rate is resolved. At this location, the measurement resolution is capable of adequately resolving the dissipation rate down to 1300K. Further downstream at $x/d = 30$, where the dissipation rate has reduced, the maximum $h/w$, which occurs at 1000K, is less than 0.75, smaller than those at the upstream locations. Approximately 90% of the dissipation at this temperature is resolved.

The $h/w$ values for flame E are generally higher than those for flame D at the same downstream locations, reflecting the higher Reynolds number for flame E. At $x/d = 7.5$ there is already a significant amount of local extinction. The $h/w$ value reaches 1.4 at 750K, the highest of all cases. Only 72% of the dissipation at this temperature is resolved, the least resolved case. Nonetheless, at 1800K, 98% of the dissipation is resolved because the flamelets are expected to be only mildly strained. At $x/d = 15$ and 30, the results are qualitatively similar to those for flame D, with the resolved dissipation rate a few percentages lower.

Overall the smallest length scale in flame E are smaller than that in flame D, consistent with the expected Reynolds number dependence. The results show that to fully resolve the smallest length scale associated with the conditionally filtered dissipation rate in these flames, the pixel size needs to be reduced by one half.

In this paper we have discussed two types of scalar dissipation length scales, one associated with the conditionally filtered dissipation rate conditional on the mixture fraction, the other with the conditionally filtered dissipation rate conditional on both the mixture fraction and temperature. The former represents the average dissipation length scale for all the ramp-cliffs in the conditional SGS fields with large SGS variance, which are regions of high dissipation rate. The latter separates the ramp-cliffs according to their peak temperatures, providing more detailed length scale information. These length scales are complementary to the dissipation length scales given in Ref. [54], which
represents the length scales associated with the mean dissipation rate. In general, for a given random field the length scales for different statistics are different, and may require different spatial resolution to resolve them fully. It would also be interesting to quantify the distribution of the instantaneous length scales of the scalar fields in a way similar to those of temperature fields [17].

Figure 7.13: Ratio of the measured dissipation rate using the second-order scheme to that using the tenth-order scheme in flame D at \( x/d = 15 \). The lowest value at each temperature (near the dashed line) represents the least resolved part of the mixture fraction profile.
Figure 7.14: Length scale of the scalar (ramp-cliff) structure as a function of temperature. The SFS variance values are given in Fig. 8.
Figure 7.15: Estimation of the resolved dissipation rate as a function of temperature. (a), (c), and (e) flame D at $x/d=7.5$, 15, and 30, respectively; (b), (d), and (f): flame E at the same locations.
Chapter 8

Data Reduction of Simultaneous Rayleigh and PLIF measurements

8.1 Rayleigh scattering

8.1.1 Signal model

We model the Rayleigh signal as following\cite{43}:

\[ S_{\text{Ray}}^* (i, j, t) = \text{Res}_{\text{Ray}}(i, j) \cdot I(i, t) \cdot \sigma_{\text{eff}}(i, j, t) + \text{BG}_{\text{Ray}}(i, j) + n(i, j, t) \]  \hspace{1cm} (8.1)

\( S_{\text{Ray}}^* \) is the Rayleigh signal, \( I \) is the intensity, \( \sigma_{\text{eff}} \) is the effective Rayleigh cross section. \( \text{Res}_{\text{Ray}} \) is the response. This model equation holds for all Rayleigh scattering images (e.g. main field images and reference images). \( i, j \) are the image coordinate which is the same as in matrix notation, \( t \) is the time. The effective Rayleigh cross section is modeled as mole weighted average of species Rayleigh cross sections.

\[ \sigma_{\text{eff}} = \sum_{s=1}^{N_s} X_s \sigma_s \quad \text{with} \quad \sum_{s=1}^{N_s} X_s = 1 \] \hspace{1cm} (8.2)

where \( N_s \) is the number of species, \( X_s \) and \( \sigma_s \) is the mole fraction and the Rayleigh cross section of the \( s \)th species respectively. Technically, the \( \text{BG}_{\text{Ray}} \) term is not limited to the backgrounds in the
experiments. It is a result of all effects to the signal that is not affected by laser intensity. Similarly, the response term contains all the contributions to the final signal that is proportional to the laser intensity. We can also interpret the above model as linear approximation of general model \( S = f(I) \) in which signal is a generic function of incident intensity (not local intensity). Therefore, secondary effects like absorption, beam steering and multiple scattering are not considered. The secondary effects will be discussed in a separate section.

In most cases, the background BG can be measured easily. In our studies, the backgrounds are measured by fulfilling the imaging field with helium which has very small Rayleigh cross section.

Depending on how incident laser intensity is determined, the experimental reduction procedure is divided into two cases, which are discussed in following two sections.

### 8.1.2 Measurements with reference images

In year 2008 data, the laser intensity is determined from the reference images. The advantage is reference stream can be far form the main jet, which enables the main camera to be used for further downstream locations. The reference images use the same model equation:

\[
S^r_{\text{Ray}}(i,j,t) = \text{Res}^r_{\text{Ray}}(i,j) \cdot I^r(i,t) \cdot \sigma^r_{\text{eff}}(i,j,t) + \text{BG}^r_{\text{Ray}}(i,j) + n^r(i,j,t) (8.3)
\]

Notation is same as Eqn (8.1) except the superscript \( r \) indicates the reference images.

Ideally, the background and response for both main and reference camera should be determined during the calibration process. However, this is not done in year 2008 data. Also knowing both responses is redundant for the current experiment.

The 08 data reduction for Rayleigh was done in following way:

After matching images (see section image matching), we assume that the laser profile didn’t change along propagating from reference camera focal point to main camera focal point. This assumption is equivalent to that the Rayleigh absorption is negligible.

Then we compare the main and reference image models:

\[
S_{\text{Ray}}(i,j,t) = \text{Res}_{\text{Ray}}(i,j) \cdot I(i,t) \cdot \sigma_{\text{eff}}(i,j,t) + \text{BG}_{\text{Ray}}(i,j) + n(i,j,t) \quad (8.4)
\]

\[
S^r_{\text{Ray}}(i,j,t) = \text{Res}^r_{\text{Ray}}(i,j) \cdot I^r(i,t) \cdot \sigma^r_{\text{eff}}(i,j,t) + \text{BG}^r_{\text{Ray}}(i,j) + n^r(i,j,t) \quad (8.5)
\]
where \( I' \) has been replaced by \( I \)

Backgrounds should be done from imaging helium flat field and subtracted from the raw signal, which has little concern. Therefore, let

\[
S_{\text{Ray}}(i, j, t) = S_{\text{Ray}}^r(i, j, t) - \text{BG}_{\text{Ray}}(i, j) = \text{Res}_{\text{Ray}}^r(i, j) \cdot I(i, t) \cdot \sigma_{\text{eff}}(i, j, t) + n(i, j, t) \quad (8.6)
\]

\[
S_{\text{Ray}}(i, j, t) = S_{\text{Ray}}^r(i, j, t) - \text{BG}_{\text{Ray}}^r(i, j) = \text{Res}_{\text{Ray}}^r(i, j) \cdot I(i, t) \cdot \sigma_{\text{eff}}^r(i, j, t) + n^r(i, j, t) \quad (8.7)
\]

The noise terms can be dropped. But for further explanation on noise control, they are kept for now.

To determine the laser profile, one stripe of the reference image is used. In principle, any \( j \) position (along laser propagation) can be used and one pixel is enough. But if we average over more pixels, the noise is reduced because

\[
\text{var} \left[ \frac{1}{N} \sum_{j=1}^{N} n^r(i, j_0 + j, t) \right] = \frac{1}{N} \text{var} \left[ n^r(i, \cdot, t) \right] \quad (8.8)
\]

as long as \( n^r(i, \cdot, t) \) can be considered as iid random variables. However when involving spatial average of signal, the spatial variation of responses is not negligible,

\[
\frac{1}{N} \sum_{j=1}^{N} S_{\text{Ray}}^r(i, j_0 + j, t) = \frac{1}{N} \sum_{j=1}^{N} \left\{ \text{Res}_{\text{Ray}}^r(i, j_0 + j) \cdot I(i, t) \cdot \sigma_{\text{eff}}^r(i, j_0 + j, t) + n^r(i, j_0 + j, t) \right\} \quad (8.9)
\]

\[
= \frac{I(i)}{N} \sum_{j=1}^{N} \text{Res}_{\text{Ray}}^r(i, j_0 + j) \sigma_{\text{eff}}^r(i, j_0 + j, t) + \frac{1}{N} \sum_{j=1}^{N} n^r(i, j_0 + j, t) \quad (8.10)
\]

In most cases we average over a stripe with constant known Rayleigh cross section, say within ambient air.

\[
\frac{1}{N} \sum_{j=1}^{N} S_{\text{Ray}}^r(i, j_0 + j, t) = \frac{I(i, t) \sigma_{\text{air}}}{N} \sum_{j=1}^{N} \text{Res}_{\text{Ray}}^r(i, j_0 + j) + \frac{1}{N} \sum_{j=1}^{N} n^r(i, j_0 + j, t) \quad (8.11)
\]

Of course the response related term \( \sum_{j=1}^{N} \text{Res}_{\text{Ray}}^r(i, j_0 + j) \) still depends on \( i \) and \( j_0 \). Therefore, for practical use, \( j_0 \) should be at least fixed for each \( i \) to make the response term only \( i \) dependent. For
matlab coding convenience, $j_0$ is fixed for all $i$. Then the laser intensity is determined,

$$I(i,t)\sigma_{air} = \frac{\sum_{j=1}^{N} S_{Ray}(i, j_0 + j,t)}{\sum_{j=1}^{N} \text{Res}_{Ray}(i, j_0 + j)} - \frac{\sum_{j=1}^{N} n^r(i, j_0 + j,t)}{\sum_{j=1}^{N} \text{Res}_{Ray}(i, j_0 + j)}$$  \hspace{1cm} (8.12)

The laser intensity is substituted into main camera equation with noise term dropped:

$$S_{Ray}(i,j,t) = \text{Res}_{Ray}(i,j) \cdot \frac{\sum_{j=1}^{N} S_{Ray}(i, j_0 + j,t)}{\sum_{j=1}^{N} \text{Res}_{Ray}(i, j_0 + j)} \cdot \frac{\sigma_{eff}(i,j,t)}{\sigma_{air}}$$ \hspace{1cm} (8.13)

$$\frac{S_{Ray}(i,j,t)}{(1/N) \sum_{k=1}^{N} S_{Ray}(i,j_0 + k,t)} \cdot \frac{(1/N) \sum_{k=1}^{N} \text{Res}_{Ray}(i,j_0 + k)}{\text{Res}_{Ray}(i,j)} = \frac{\sigma_{eff}(i,j,t)}{\sigma_{air}} = \sum_s X_s \cdot \frac{\sigma_s}{\sigma_{air}}$$ \hspace{1cm} (8.14)

As a result, to determine the mole fraction, knowing the relative response

$$\frac{(1/N) \sum_{k=1}^{N} \text{Res}_{Ray}(i,j_0 + k)}{\text{Res}_{Ray}(i,j)}$$ \hspace{1cm} (8.15)

and relative Rayleigh cross section $\sigma_s/\sigma_{air}$ is sufficient.

### 8.1.2.1 Calibration

By principle, the calibration procedure should be fulfilling the main camera imaging area with species of known cross section while keeping all other setup the same as experiments. Also, if possible, span the cross section values over the full measurement range. However, this was never done for all of the experiments. So an alternative approach (which is used) is given here.

The given data have “flatfield” images without corresponding “reference” images. So a detour is made to determine the relative response. We first determine the response ratio of main camera and a fix stripe, using “flatfield” images. Then determine the response of “reference” camera and the fix stripe, using actual images.

**Step 1**: find a stripe on the upstream of laser beams without backgrounds and within which area only air appears during experiments, say

$$S_{Ray}(i,j,t) = \text{Res}_{Ray}(i,j) \cdot I(i,t) \cdot \sigma_s(i,j,t)$$

where $j$ takes from $j_c$ to $j_c + N_c$.  

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Step 2: take the average along laser propagating direction. The reason for this is the noise control.

\[
\overline{S}_{\text{Ray}}(i,t) = \frac{1}{N_c + 1} \sum_{j=j_c}^{j_c+N_c} \text{Res}_{\text{Ray}}(i,j) \cdot I(i,t) \cdot \sigma_s(i,t)
\]

\[
= \frac{I(i,t) \cdot \sigma_s(i,t)}{N_c + 1} \sum_{j=j_c}^{j_c+N_c} \text{Res}_{\text{Ray}}(i,j)
\]

\[
= I(i,t) \cdot \sigma_s(i,t) \text{Res}_{\text{Ray}}(i)
\]

Step 3: divide each image column by this stripe. In this way, effects of laser profile are deducted, so is the absolute imaging response.

\[
\frac{S_{\text{Ray}}(i,j,t)}{S_{\text{Ray}}(i,t)} = \frac{\text{Res}_{\text{Ray}}(i,j) \cdot I(i,t) \cdot \sigma_s(i,t)}{I(i,t) \cdot \sigma_s(i,t) \text{Res}_{\text{Ray}}(i)} = \frac{\text{Res}_{\text{Ray}}(i,j)}{\text{Res}_{\text{Ray}}(i)}
\] (8.16)

Step 4: find the ratio of responses of the above stripe and reference image using images taken during experiments.

\[
\overline{S}_{\text{Ray}}(i,t) = \frac{1}{N} \sum_{j=1}^{N} S_{\text{Ray}}(i,j_0 + j,t) = \frac{I(i,t) \sigma_{\text{air}}}{N} \sum_{j=1}^{N} \text{Res}_{\text{Ray}}(i,j_0 + j)
\] (8.17)

and

\[
\overline{S}_{\text{Ray}}(i,t) = I(i,t) \cdot \sigma_{\text{air}}(i,t) \overline{\text{Res}}_{\text{Ray}}(i)
\] (8.18)

Note that the ratio of the two above gives a response ratio:

\[
\frac{\overline{S}_{\text{Ray}}(i,t)}{\overline{S}_{\text{Ray}}(i,t)} = \frac{(1/N) \sum_{j=1}^{N} \text{Res}_{\text{Ray}}(i,j_0 + j)}{\text{Res}_{\text{Ray}}(i)}
\] (8.19)

Step 5: (8.19)/(8.16) gives the relative response in (8.15).

As it can be seen from step 3, effect of Rayleigh cross section is eliminated as long as it is uniform along the laser beam direction. This property was used to double check the secondary effects like absorption. The result response ratios in (8.16) from different “flatfield” images (i.e. from different cross section values) were compared. The results are similar with less than 2% deviations and no trend was found. Since higher cross section induces higher absorption. This results confirms that absorption being a secondary effect is negligible.
8.1.3 Secondary effects

The word “absorption” here stands for the effect of light intensity decline due to the scattering. As mentioned in previous section, effects of absorption in current experiments are negligible for Rayleigh scattering due to its low cross section.

When the effect of absorption may not be negligible, it can be modeled by varying laser intensity along beam direction (i.e. using local intensity instead of incident intensity).

Effects of beam steering can be corrected by ray tracing algorithm [26].

Helium cross section is assumed to be zero, helium “flatfield” is treated as background. Since helium cross section is about 2% of air, and less than 0.5% of ethylene [43], this assumption introduces at most 2% of systematic error.

8.2 PLIF

8.2.1 Signal model

We model the PLIF signal as following [43]:

\[ S^*_{\text{PLIF}}(i,j,t) = \text{Res}_{\text{PLIF}}(i,j) \cdot E(i,j,t) + \text{BG}_{\text{PLIF}}(i,j) + n(i,j,t) \]  (8.20)

where \( S^*_{\text{PLIF}} \), \( \text{Res}_{\text{PLIF}} \), \( E \), \( \text{BG}_{\text{PLIF}} \) and \( n \) are the PLIF signal on detector, detector responses, PLIF emission, background and noise respectively. This model is essentially the generalization of the Rayleigh signal model. The treatments of background and response are similar to Rayleigh scattering. Any of helium, air or ethylene flatfields can be treated as background for PLIF.

By assuming linear fluorescence, the PLIF photon emission is modeled as linear function of local light intensity with proportional constant being the effective fluorescence cross section.

\[ E = \kappa_{\text{eff}} \cdot I \]  (8.21)

where \( I \) is the laser intensity, \( \kappa_{\text{eff}} \) is the effective PLIF cross section. The effective PLIF cross section is linear to acetone concentration of acetone seeded air flow and the acetone PLIF cross section of
pure stream. To count on the quenching effects[14], a quenching correction factor is also considered.

\[
\kappa_{\text{eff}} = R_Q \cdot X_1 \cdot C \cdot \kappa_0 \tag{8.22}
\]

where \(X_1\) is the mole fraction of acetone seeded air flow, \(C\) is the mole fraction of acetone vapor in acetone seed flow and \(\kappa_0\) is the acetone fluorescence cross section, \(R_Q\) is a quenching correction.

This model equation holds for acetone seeded PLIF images (e.g. main field images and reference images). Note that due to strong absorption of acetone, laser intensity decline cannot be neglected. Therefore, the laser intensity considered here is local intensity. It is connected to incident intensity \(I_0\) by an absorption correction factor.

\[
I(i, j, t) = R_{ab}(i, j, t) \cdot I_0(i, t) \tag{8.23}
\]

### 8.2.2 Quenching model

![Two-level scheme for modeling quenching](image)

Figure 8.1: A two-level scheme for modeling quenching. \(W_{12}, W_{21}, A_{21}, Q_{12}\) and \(Q_{21}\) are the absorption rate, induced emission rate, spontaneous emission rate, collisional excitation rate and collisional de-excitation rate respectively.

Thurber et al[44] have shown that the acetone fluorescence can be modeled through a detail calculation over 24 vibrational modes in order to determine the temperature and pressure dependency. However in current experiment, since the pressure and temperature in unchanged, the relative portions of contributions from different vibrational levels are unchanged. Therefore, we can combine the overall effect of various vibrational levels as an apparent single level which energy level is an average of different vibrational levels weighted by their number densities. As a result, a two
level system is used for PLIF signal model (figure 8.1). By assuming constant irradiance, thermal equilibrium and steady state, it has been shown that the fluorescence yield is \[ Y = \frac{A_{21}}{Q_{21} + A_{21}} \quad (8.24) \]

In this equation, \( A_{21} = 8 \times 10^7 \text{s}^{-1} \) from Hanson and Lee’s experiments[22]. An estimate of quenching rate of air can be performed similar to Thurber thesis. Using an estimated collisional radius of Lennard-Jones potential[40], \( \sigma_{\text{ace}} = 4.6\text{Å} \) and \( \sigma_{\text{air}} = 3.711\text{Å} \) and estimated excitation energy \( \epsilon_{\text{ace}}/k_B = 560.2\text{K} \) and \( \epsilon_{\text{air}}/k_B = 78.6\text{K} \). This gives a collisional radius \( \sigma_{\text{ace-air}} = (\sigma_{\text{ace}} + \sigma_{\text{air}})/2 = 4.16\text{Å} \) and collisional excitation energy \( \epsilon_{\text{ace-air}} = \sqrt{\epsilon_{\text{ace}}\epsilon_{\text{air}}} = 2.90 \times 10^{-21}\text{J} \). The total number of collisions is \( Q_{21} = \frac{P}{k_B T} \pi \cdot \frac{\sigma_{\text{ace-air}}^2}{\mu} \cdot \Omega \simeq 1.04 \times 10^{10} \text{s}^{-1} \gg A_{21} \quad (8.25) \)

where \( \Omega = \frac{1}{0.636 + 0.567 \log_{10} \left( \frac{k_B T}{\epsilon_{\text{ace-air}}} \right)} \quad (8.26) \)

and \( \mu = m_{\text{ace}}m_{\text{air}}/(m_{\text{ace}} + m_{\text{air}}) \) is the reduced mass.

To count on the species dependency of collisional quenching, we note that the collisional rate is proportional to the quencher number density for constant temperature and pressure. Therefore, the overall quenching effect is modeled as a single quenching rate which is number-density-weighted average of quenching rate from each species.

\[ Q_{21} = X_1 \cdot C \cdot q_{\text{ace}} + X_2 q_{\text{eth}} + [X_1(1 - C) + X_3]q_{\text{air}} \quad (8.27) \]
\[ = X_1 \cdot C \cdot q_{\text{ace}} + X_2 q_{\text{eth}} + [1 - X_1C - X_2]q_{\text{air}} \quad (8.28) \]

Since we only know the effective quenching coefficients for a fixed composition, they are,

\[ q_1 = r q_{\text{ace}} + (1 - r)q_{\text{air}} \quad (8.29) \]
\[ q_2 = r q_{\text{ace}} + (1 - r)q_{\text{eth}} \quad (8.30) \]
\( Q_{\text{eff}} = (1 - r) X_1 C_{\text{ace}} + X_2 (q_2 - r q_{\text{ace}}) + [1 - X_1 C - X_2] (q_1 - r q_{\text{ace}}) \)  
\( = q_1 (1 - X_1 C) + X_2 (q_2 - q_1) + q_{\text{ace}} (X_1 C - r) \)

8.2.3 Measurements with reference images

8.2.3.1 Calibration

The PLIF response was determined with the help of Rayleigh response. For “flatfield” images, the

**Step 1**: find the same stripe as Rayleigh reduction on the upstream of laser beams without backgrounds

\[ S_{PLIF}(i, j, t) = R_{PLIF}(i, j) \cdot I(i, j, t) \cdot \kappa(i, t) \]

where \( j \) takes from \( j_c \) to \( j_c + N_c \)

**Step 2**: take the average along laser propagating direction same as Rayleigh reduction, so that PLIF and Rayleigh responses can be compared.

\[ \overline{S}_{PLIF}(i, t) = \frac{1}{N_c + 1} \sum_{j=j_c}^{j_c+N_c} R_{PLIF}(i, j) \cdot I(i, j, t) \cdot \kappa(i, t) \]
\[ = \frac{I(i, t) \cdot \kappa(i, t)}{N_c + 1} \sum_{j=j_c}^{j_c+N_c} R_{PLIF}(i, j) \]
\[ = \overline{T}(i, t) \cdot \kappa(i, t) \overline{R}_{PLIF}(i) \]

where \( I(i, j, t) \) was approximated by \( \overline{T}(i, t) \) by assuming that laser absorption is negligible within the stripe.

**Step 3**: divide each image column by this stripe. In this way, effects of laser profile are deducted, so is the absolute imaging response.

\[ \frac{S_{PLIF}(i, j, t)}{S_{PLIF}(i, t)} = \frac{R_{PLIF}(i, j) \cdot I(i, j, t) \cdot \kappa(i, t)}{I(i, t) \cdot \kappa(i, t) \overline{R}_{PLIF}(i)} = \frac{R_{PLIF}(i, j) \overline{I}(i, j, t)}{\overline{R}_{PLIF}(i) \overline{T}(i, t)} \]  
(8.33)

**Step 4**: By assuming

\[ \frac{R_{PLIF}(i, j)}{R_{PLIF}(i)} \approx \frac{R_{Ray}(i, j)}{R_{Ray}(i)} \]  
(8.34)

The intensity decrease with beam propagation is modeled as exponential function according to Beer’s
\[
\frac{I(i,j,t)}{I(i,t)} = C e^{\alpha_j} \tag{8.35}
\]

Using curve fitting \( C \) and \( \alpha \) can be determined. Then this absorption matrix was substitute back into (8.33) so that \( \text{Res}_{\text{PLIF}}(i,j) / \text{Res}_{\text{PLIF}}(i) \) is determined.

**Step 4**: Unlike Rayleigh scattering images, there is no way to determine the ratio of responses of the above stripe and reference image. However, according to Rayleigh images responses, this response ratio is very close to be constant. Therefore, a constant stripe and reference response ratio is assumed here. As a result the PLIF response is determined. This is the most problematic part, according to the result, spatial statistics show a strong fixed pattern.

**Step 5**: To deduct the effects of acetone concentration variation, acetone cross section variation in reference images is used. They are modeled to be linear dependent with coefficients determined by comparing pure acetone signal in main camera with corresponding acetone signal in reference image.

### 8.3 Image matching

The reference and main cameras focus on different locations, therefore, it is necessary to match locations of two images so that the laser profile calculated from reference images can be correctly substituted into main field images. Though the profiles from reference and main field images are different by a factor of response, it is possible to compare the patterns of two profiles and determine the laser intensity and laser profile simultaneously, but it involves intensive computation. It happened that, the response changes slower from different pixels than the laser profiles. As a result, laser profile peaks in reference images correspond peaks in main field images. As laser intensity varies, the locations for peak pairs are collected and plotted, the result shows a perfect linear relation to match image pairs.
Chapter 9

Conclusions

In the first part of this work, the filtered mass density function and the conditionally filtered dissipation rates which evolve the FMDF are studied experimentally. Data obtained in turbulent partially premixed flames (Sandia flames D and E) are used to compute SGS statistics conditional on Favre filtered mixture fraction and the Favre SGS scalar variance.

The results show that the FMDF has qualitatively different shapes for small and large SGS variance. For small SGS variance the FMDF is unimodal but for large SGS variance it is bimodal with the two peaks outside of the reaction zone. These FMDF shapes correspond to quasi-equilibrium distributed reaction zones and laminar flamelets (including extinguished flamelets), respectively. Changing the filter scale from 3.07 to 4.91 mm does not alter the shapes of the FMDF.

The conditionally filtered mixture fraction dissipation for small SGS variances is generally consistent with quasi-equilibrium distributed reaction zones with a relatively weak dependence on the mixture fraction. For the extinguished samples it is not very large and is not sensitive to the temperature, suggesting that these may be samples extinguished at some upstream locations. For large SGS variance, the dissipation is large near $\xi = 0.4$, where the maximum gradient in a cliff is located. The dissipation is higher for lower temperatures, consistent with strained laminar flamelets. For the extinguished samples, the measured dissipation rate component exceeds the extinction dissipation rate. The results are consistent with extinguished flamelets.

The conditionally filtered temperature dissipation for small SGS variances has a minimum (close to zero) near the peak temperature at approximately $\xi = 0.45$. Away from this mixture fraction value the dissipation increases. For the extinguished samples with very low temperatures
(T < 1300K), the dissipation is lower compared to those with intermediate temperatures (1300 – 1600K). The latter is due to the mixing between burning and very low temperature samples. Therefore, the mixture fraction is well mixed but temperature is not.

For large SGS variance, the dissipation indicates strained or extinguished laminar flamelets. However, the pilot flame plays an important role. For samples not far from equilibrium, the dissipation is consistent with strained laminar flamelets with the maximum dissipation occurring near \( \xi = 0.55 \). Further away from equilibrium at moderate temperatures (as high as 1700 K) there are dissipation peaks which are probably a result of the rapid mixing between the pilot gas and the lean or rich mixtures, corresponding to extinguished flamelets. There is also evidence that each of these flamelets is split by the pilot gas. At much lower temperature the dissipation is lower because the temperatures of the extinguished flamelets are lower, corresponding to lower dissipation.

We note that there have previous efforts to infer \( \chi \) from \( \chi_T \) experimentally. The present work shows that although there are some similarities between the two dissipation rates, in the reaction zone they are qualitatively different with the latter being dependent on both the turbulence and turbulence-chemistry interaction. Therefore, the mixture fraction structure near the stoichiometric mixture fraction, arguably the most important part of the structure, cannot be inferred from the temperature dissipation. The implications are that the two variables are related to different processes and that they cannot be modeled the same way.

The results in the present study show that the different mixture fraction structures for small and large SGS variances as reflected by the unimodal and bimodal FMDF have a strong impact on the small-scale mixing as reflected by the results for conditionally filtered mixture fraction dissipation and turbulence-chemistry interaction as reflected by the results for the conditionally filtered temperature dissipation. The results have implications for understanding multiple reactive scalar SGS mixing and for modeling SGS mixing.

Then we used the same data to study the influence of the SGS mixture fraction structure on the diffusion of the mixture fraction and temperature. The Favre filtered mixture fraction and the Favre SGS scalar variance were used as conditioning variables for analyzing the scalar filtered mass density function and other SGS variables.

For SGS scalar variance small compared to its mean, there are generally two mixing states, one involving the fully burning samples at high temperatures and one involving the burning and extinguished samples at lower temperatures. For the burning samples, the conditionally filtered dif-
fusion of the mixture fraction and temperature, represented by streamlines, generally move towards the ridgeline of the FMDF and then diffuse along it. There are, therefore, two mixing processes, one fast and one slow. Mixing between burning and extinguished samples generally causes the streamlines to converge to an intermediate temperature of approximately 1600K.

For large SGS scalar variance, the mixing processes are more complex. Part of the streamline pattern is consistent with flamelets. The streamlines for very rich and lean mixtures generally converge towards the ridgeline of the FMDF and move upward along it, again indicating two mixing processes, one fast and one slow. Low temperature samples are largely extinguished flamelets, which cause the streamlines to move in straight lines predominately in the direction of the mixture fraction towards $\xi = 0.4$, approximately the center of the ramp-cliff structure. At $x/D = 15$ the mixing of the pilot flame and the fuel stream also appear have a strong impact on the streamline pattern, resulting in nearly straight streamlines connecting the fuel and the pilot in the scalar space, indicating that the dissipation rate is large and that there is essentially no reaction in this region.

The results show that the mixing regimes and the resulting streamline patterns for the conditionally filtered diffusion are important SGS mixing characteristics of the flames. These patterns are challenging tests for mixing models.

We further investigated the filtered mass density function and conditionally filtered dissipation rate condition on mixture fraction, temperature and reactive species. The results show that different mixing regimes result in different FMDF and dissipation rates. The results for CO show that within the reaction zone, the chemistry results in sharp interface of CO mass fraction which induces strong mixing within reaction zone. Its mixing behavior shows a mixing between four scalars in scalar space, which provides a challenge for mixing models.

In the second part of this work, a conditional sampling-based method for noise and resolution corrections for scalar dissipation rate measurements is developed and demonstrated using experimental data obtained in a turbulent jet. The method employs a conditional-sampling procedure to separate the noise from resolution effects, both strongly influencing the accuracy of dissipation rate measurements.

The conditional-sampling method makes use of the properties of local turbulent scalar fields based on Kolmogorov’s refined hypotheses. These properties are demonstrated by the experimental results. The filtered scalar value and the SGS scalar variance are used as conditioning variables. The procedure ensures the selection of well-resolved local scalar fields by using sufficiently small
SGS variance values, allowing determination of the contribution from measurement noise to the measured scalar dissipation rate without redundant measurements. The experimentally determined noise variance is used to correct potentially under-resolved local scalar fields, effectively separating the effect of noise from that of resolution. The noise-corrected dissipation rate then is used to estimate the scalar dissipation length scale (the relative measurement resolution) and to make corrections for insufficient resolution.

Explicit finite difference schemes of different orders are used to calculate the scalar derivative. For the well-resolved local scalar fields, all the schemes should give the same dissipation rate, and any differences are due to the measurement noise. The spectral responses and the noise contributions of the schemes are exploited to determine the measurement noise. The results confirm that these fields are indeed well resolved. The noise variance then is determined from the data.

For potentially under-resolved local scalar fields selected using large SGS variance values, the data are used first to examine the extent of under-resolution. For local scalar fields that cannot be resolved by the eighth-order scheme, the error-function model is used to estimate the scalar dissipation length scale (FWHM of the scalar dissipation rate profiles). The model then is revised to allow fluctuations of the error-function scalar profile in the scalar space due to the background scalar fluctuations, and to include the background dissipation rate. The ratios of the measured dissipation rates obtained using different schemes are compared to the model calculations to infer the dissipation length scale. The results demonstrate the validity of the error function as a model for the ramp-cliff scalar profile when the SGS variance is large.

The present method can provide the dissipation length scale, guide selection of a measurement system resolution using a preliminary run, and be used to make corrections for noise and under-resolution. The conditional dissipation rate (without filtering) can be evaluated first by plotting its values obtained using different schemes without conditioning on the SGS variance. If the resolution is sufficient, the noise-corrected conditional dissipation rate is obtained. If the resolution is insufficient, it can be obtained by summing the conditionally filtered dissipation rate for all the bins weighed by the probability for each bin. The correction procedure for under-resolution is applicable for all SGS fields having bimodal FDFs, including some having intermediate values of the SGS variance. In practice, for a measurement system with a reasonable resolution, only the bins with the highest SGS variance values should need significant corrections for under-resolution. The lower bins most likely only need noise correction and can be combined as one large bin. In the case that
bins with unimodal FDFs are also under-resolved, the measurement system is probably not suitable for the intended flow.

The present study shows that the local analysis method based on the conditional-sampling procedure is capable of correcting noise and resolution effects accurately for a sample spacing twice (or even larger) of the spacing required to fully resolve the scalar field. The choice of filter size is not critical. Generally, filter sizes ranging from 10 to 15 Kolmogorov scales to one-fourth of the integral length scale can be used. The parameters in the revised model are deduced from the experimental data; therefore, the procedure is very robust.

The method has several advantages over previous methods: (1) The use of conditional sampling allows separation of noise from the resolution effects to evaluate the noise contribution and dissipation length scales, and to make accurate corrections. The conditional sampling and the use of the varying spectral response of the finite difference schemes of different orders allow accurate determination of the noise variance, even when the noise contribution is greater than the dissipation rate. We emphasize that the conditional-sampling procedure for selecting local scalar fields is based on the physics of turbulence. The basis for selecting the fully resolved local scalar fields is Kolmogorov's refined similarity hypotheses. To our best knowledge, this is the first time that the concept of K62 is being used for such a purpose. The basis for selecting the local scalar fields containing the ramp-cliff structure is based on the authors recent work on the filtered density function and dissipation of subgrid-scalar fields. The conditional-sampling procedure, therefore, makes use of the physics of the turbulence to extract information for analyzing the measurement noise and resolution. This method is in contrast to previous techniques in that for noise correction no external input such as redundant measurements or spectral models beside the data is needed. (2) It is applicable to the conditional dissipation rate, which is essential for many applications. (3) It can capture the effects of the ramp-cliff structure on the conditional dissipation rate. The ramp-cliff structure is local in space and is not well represented in spectral correction methods.

The method can be extended to more complex situations such as turbulent flames where noise is dependent on species mass fractions and temperature, and dissipation length scale is not uniform (larger in the reaction zone). When laser diagnostic techniques are used in flames the noise often is shot-noise limited and the noise variance is dependent on the scalar. For example, in mixture fraction measurements the noise variance is often proportional to mixture fraction. For such data, the mean dissipation rate is replaced by the conditional mean of the measured dissipation rate. The
conditional noise variance then can be obtained from the procedure described above. Note that because the noise depends on the scalar, spectral analysis is not capable of obtaining the conditional noise variance.

The conditional sampling-based method for noise correction and resolution estimation for scalar dissipation rate measurement was used to study turbulent partially premixed flames (Sandia flames D and E). The results show that the noise variance determined is accurate and the noise correction procedure is capable of removing the noise contributions from the measured dissipation rate, as indicated by the collapse of the well-resolved dissipation rate calculated using finite difference schemes of various orders. The mean dissipation rate is well resolved at all measurement locations except perhaps at $x/d = 7.5$ in flame E, where the resolution is slightly worse. The conditional dissipation rate is also well resolved at all locations in both flames D and E.

The potentially under-resolved fields were selected using large SFS variance. We used the error-function model to estimate the length scale and the extent of resolution of these fields after their dissipation rate is corrected for noise. The effect of the finite sampling volume (pixel size) on the resolution was included in the model calculation in addition to that of the finite sampling interval. The ratios of the measured dissipation rate using finite difference schemes of second- to tenth-orders were compared to model calculations to infer the width of the scalar (ramp-cliff) structure. The results for the conditionally filtered dissipation rate conditional on the mixture fraction show that the ratio of the sample interval to the width ranges from 0.4 to 0.454 in flame D and 0.53 to 0.59 in flame E. The percentage of the conditionally filtered dissipation rate using the tenth-order scheme ranges from 96.5% to 97.3% in flame D and 93.4% to 95% in flame E. Thus, the conditionally filtered dissipation rate conditional on the mixture fraction is quite well resolved for these local fields. Note that these fields have dissipation rate much larger than the mean dissipation rate; therefore, the latter is better resolved.

We further analyzed the conditionally filtered dissipation rate conditional on the both the mixture fraction and temperature, again focusing on the local fields with large SFS variance values. The dissipation length scale was found to increase with downstream distance and is larger in flame D. Detailed analyses show that at each location, the length scale decreases with temperature, probably due to the higher strain rate and lower diffusivity. The ramp-cliff structure is generally quite well resolved (>90%) for temperatures higher than 1300K. At lower temperatures the length scale of the ramp-cliff structure is smaller, with the value at 700K approximately one half of those at 1800K.
As a result, the percentage of the dissipation rate resolved is lower. The results show that to fully resolve these fields with low temperatures, which are extinguished flamelets, the pixel size needs to be reduced by approximately one half. We note that these are events with low probability, consequently the majority of the scalar fields are well resolved.

In Cai and Tong[9] a revised error-function model was developed to take into account the fluctuations of the ramp-cliff structure in the mixture fraction space and the dissipation rate due to the background scalar fluctuations. In that study the measurements were made at 80 jet diameters downstream of the nozzle, where the background scalar fluctuations were significant compared to those of the ramp-cliff structure. The data for the present study were obtained within 30 jet diameters from the nozzle, where significant turbulence-chemistry interaction occurs, the magnitudes of the background scalar fluctuations are much smaller, thereby having negligible effects on the estimated resolution. Consequently, the revised model was not used here.

In the present study the effect of the finite pixel size were considered along with the finite sample spacing to address the issue of measurement resolution. The effect was considered as a pre-sampling (top-hat) filter due to pixels of a finite size; therefore, such a treatment is not limited to pixel filtering. It can be generalized, without much difficulty, to include other factors that can be considered pre-sample filtering, such as optical blurring, etc. In the error-function model, a pre-sampling filter can be applied to the error-function profile before the other processing procedures; therefore, is simple to implement. It is also straightforward to use different filters.
Bibliography


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