Chemical Engineering Science 90 (2013) 221–241

Contents lists available at SciVerse ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

Statistics of the scalar dissipation rate using direct numerical simulations and planar laser-induced fluorescence data

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HIGHLIGHTS

- ► Scalar mixing was studied in similar turbulent flows with 3D DNS and 2D acetone PLIF.
- ► The DNS and experiment agree on the observed scalar statistics and their evolutions.
- ► The unconditional and conditional scalar dissipation rate PDFs are nearly lognormal.
- ► The ratio std. deviation/mean scalar dissipation grows from 0 initially to $2.3 \pm 20\%$.
- ► Similarly the conditional dissipation ratio grows to ~ 1.4; both increasing with *Re*.

ARTICLE INFO

Article history:
Received 28 August 2012
Received in revised form
6 December 2012
Accepted 17 December 2012
Available online 26 December 2012

Keywords:
Fluid mechanics
Mixing
Turbulence
Scalar dissipations rate
Direct numerical simulation
Laser-induced fluorescence

ABSTRACT

The statistics of the scalar dissipation rate (SDR) in gaseous flows with Schmidt numbers close to unity were examined in a joint numerical and experimental effort, in a shearless mixing layer in the presence of decaying turbulence using three-dimensional Direct Numerical Simulations (DNS), and in an axisymmetric plume formed by the continuous low-momentum release of an acetone-laden stream (used as a tracer to measure the passive scalar) along the centreline of a turbulent pipe flow of air downstream of a turbulence generating grid using Planar Laser-Induced Fluorescence (PLIF). For the flows examined good agreement was found between the DNS and the experiment, both of which indicate that: (i) the probability density functions of the unconditional and conditional SDR show small departures from lognormality; (ii) the ratio of the standard deviation of the unconditional SDR to its respective Reynolds-averaged mean, as well as the ratio of the standard deviation of the conditional SDR to its conditional mean (these ratios do not vary strongly with the value of the mixture fraction at which it is evaluated), both increase over a few Kolmogorov time scales from zero (at the injector nozzle in the experiment and initially in the DNS) to some value downstream and at later times; (iii) the long-time values of the ratios of the standard deviation to the mean of the conditional and unconditional SDR increase with the turbulent Reynolds number; (iv) for the same turbulent Reynolds number, the DNS and the experiment showed that the ratio related to the unconditional SDR increases to a long-time value of approximately 2.3 ($\pm 20\%$), while the ratio related to the conditional SDR increases quickly to a value that stays within the range 1.0–1.4 (or, 1.2 ± 0.2) and reaches a maximum value of 1.3–1.4 by the end of the DNS run and at the downstream edge of the experimental domain. The development of the conditional SDR fluctuations is discussed by comparing the early and late stages of mixing. The agreement between the PLIF measurements, which can only resolve two-dimensional fields, and the DNS, which provides access to the fully resolved three-dimensional field, suggests that the present conclusions are not limited by resolution or the lack of measurement in the third dimension. The results are useful for the development and validation of turbulent reacting flow models such as advanced flamelet, Conditional Moment Closure (CMC), and transported Probability Density Function (PDF) closures.

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http://dx.doi.org/10.1016/j.ces.2012.12.026

1. Introduction

1.1. Motivation

The mixing of two (or more) miscible fluids of different composition and/or temperature is a phenomenon with ubiquitous industrial application, from certain types of evaporators, condensers and thermal management (e.g., "forced-air") systems, to mixers for the production of chemical components or the dilution and removal of unwanted by-products, to inhomogeneous-mixture combustors and other chemical reactors. Typically, the aim in these settings is to enhance the rate at which the two (or more) fluids come together to form a uniform well-mixed fluid, which decreases the required size of the associated components and increases the rates of heat and mass transfer, and/or reaction (i.e., heat exchange, production, reaction or heat release). In other situations enhanced mixing has a positive effect on a related overall process or system. For example, in the non-premixed (inhomogeneous) autoignition and combustion of a gaseous fuel in a turbulent high-temperature air stream, it has been observed that the propensity for dangerous "flashback" reduces as the turbulence levels in the flow are increased and the mixing processes is made more vigorous (Markides and Mastorakos, 2005, 2011; Markides, 2008).

The present paper focuses on the mixing of *conserved* scalars from initially separated regions in a gaseous flow, which includes the mixing of fluid streams with different composition but without reaction or phase change, and of fluid streams at different temperatures but without external heat loss/gain or internal energy generation. Although the present study investigates non-reacting flows, an extension can be made readily to the mixing of scalars that remain conserved in *reacting* flows (e.g., Bilger et al., 1990).

1.2. Theoretical background

Often, turbulence is used to promote mixing. The governing equation for the mean transport of the normalised passive scalar concentration (local scalar mass fraction, or mixture fraction ξ), in a turbulent flow with constant density ρ and molecular diffusion coefficient D is,

$$\frac{\partial\langle\xi\rangle}{\partial t}+\langle u_j\rangle\frac{\partial\langle\xi\rangle}{\partial x_j}=\frac{\partial}{\partial x_j}\left[D\frac{\partial\langle\xi\rangle}{\partial x_j}-\left\langle u_j'\xi'\right\rangle\right], \quad (1)$$

where the angled brackets $\langle\cdot\rangle$ denote Reynolds ensemble averaging. The two terms on the left-hand side (LHS) of Eq. (1) describe the unsteadiness and advection of the mean scalar concentration (or, mixture fraction) $\langle\xi\rangle$ by the mean flow field, and the two terms inside the bracket on the right-hand side (RHS) are transport terms associated with molecular and turbulent diffusion. In high Reynolds number (*Re*) flows the molecular diffusion term $\partial(D\partial\langle\xi\rangle/\partial x_j)/\partial x_j$ is negligible compared to the turbulent term $\partial\left\langle u_j'\xi'\right\rangle/\partial x_j=\left\langle u_j'\partial\xi'/\partial x_j\right\rangle$, which involves the turbulent scalar fluxes $\left\langle u_j'\xi'\right\rangle$. These fluxes arise directly from the nonlinearity of the instantaneous advection of the scalar ξ in the turbulent flow described by the term $\partial(u_j\xi)/\partial x_j=u_j\partial\xi/\partial x_j$, and require some form of approximate *closure* relationship before Eq. (1) can be solved for the flow in question.

Now, the governing equation for the variance of the turbulent scalar fluctuations ξ' that appear in the turbulent scalar flux terms $\left\langle u_j'\xi'\right\rangle$ in Eq. (1) is

$$\frac{\partial\left\langle\xi'^2\right\rangle}{\partial t}+\langle u_j\rangle\frac{\partial\left\langle\xi'^2\right\rangle}{\partial x_j}=\frac{\partial}{\partial x_j}\left[D\frac{\partial\left\langle\xi'^2\right\rangle}{\partial x_j}-\left\langle u_j'\xi'^2\right\rangle\right]+P_\xi-\varepsilon_\xi. \quad (2)$$

The terms on the LHS describe the unsteadiness and mean advection of the scalar variance, while the first term on the RHS describes the transport of the scalar variance by molecular and turbulent diffusion. At high *Re*, as before, the molecular diffusion term $\partial\left(D\partial\left\langle\xi'^2\right\rangle/\partial x_j\right)/\partial x_j$ is negligible compared to the turbulent transport described by $\partial\left\langle u_j'\xi'^2\right\rangle/\partial x_j=\left\langle u_j'\partial\xi'^2/\partial x_j\right\rangle$, which contains the *unclosed* turbulent scalar variance fluxes $\left\langle u_j'\xi'^2\right\rangle$.

Two important terms make their appearance on the RHS of Eq. (2); the mean scalar gradient term P_ξ and mean dissipation rate ε_ξ, which are given by

$$P_\xi=-2\left\langle u_j'\xi'\right\rangle\frac{\partial\langle\xi\rangle}{\partial x_j}; \quad (3a)$$

$$\varepsilon_\xi=2D\left\langle\frac{\partial\xi'}{\partial x_j}\frac{\partial\xi'}{\partial x_j}\right\rangle=\langle\chi\rangle-2D\frac{\partial\langle\xi\rangle}{\partial x_j}\frac{\partial\langle\xi\rangle}{\partial x_j} \quad (3b)$$

The term P_ξ describes the process by which large-scale mixing due to the *mean* scalar gradients in the flow $\partial\langle\xi\rangle/\partial x_j$ can generate turbulent scalar fluctuations ξ', whereas the mean dissipation rate ε_ξ is always positive and represents the molecular destruction of the turbulent scalar fluctuations ξ' at the smallest scales in the flow. Eq. (3a) indicates that the term P_ξ is related to the aforementioned turbulent scalar fluxes $\left\langle u_j'\xi'\right\rangle$ and so it does not introduce the need for an additional closure hypothesis (see Eq. (1) and the discussion immediately below this). This leaves the *unclosed* mean dissipation rate ε_ξ, or equivalently the *fluctuating, instantaneous* scalar dissipation rate (SDR) defined as $\chi\equiv 2D(\partial\xi/\partial x_j)\cdot(\partial\xi/\partial x_j)$, as an additional *unclosed* variable in turbulent mixing flows (Sreenivasan, 2004; Warhaft, 2000) with a primary role in governing the dissipation of the scalar variance that determines the *micromixing* described by Eq. (3b).

1.3. Relevance and importance

Beyond the central importance of the SDR χ in turbulent mixing, it is also an essential element in the understanding of turbulent reacting flows (Peters, 2000; Veynante and Vervisch, 2002; Bilger, 2004). In particular, the SDR χ (and its fluctuations χ') can affect practically important phenomena, such as pollutant emission, flame extinction and autoignition, as mentioned previously. For example, localised flame extinction in non-premixed combustion is typically associated with high values of local, instantaneous SDR χ (Peters, 2000), whereas autoignition occurs where χ is low (Mastorakos et al., 1997a).

Consequently, a detailed knowledge of the statistical properties of the mixture fraction ξ (i.e., normalised scalar concentration), SDR χ, and of the *conditional* SDR $\chi|\xi=\eta$[2] at a particular mixture composition $\xi=\eta$, is required in advanced theoretical and modelling approaches for the prediction of turbulent reacting flows and, specifically, the Probability Density Functions (PDFs) of the unconditional and conditional SDR χ are often needed. Such approaches include the conventional flamelet method (Peters, 2000), advanced flamelet and transported PDF methods that include the fluctuations of the SDR χ' (Pitsch and Fedotov, 2000; Blanquart and Pitsch, 2005; Soulard et al., 2004), stochastic well-stirred reactor models (Oberlack et al., 2000), and the Conditional Moment Closure (CMC) (Klimenko and Bilger, 1999). The CMC method relates the reacting scalars (i.e., the species concentrations and temperature) to a conserved scalar (i.e., the mixture fraction ξ), whose dissipation rate χ is a crucial parameter. In CMC

[2] Notation signifies the scalar dissipation rate χ conditional on a value of ξ, with η the sample space variable corresponding to ξ.