Scalar Dissipation Rate Characteristics in Steady and Unsteady Turbulent Round Jets

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ABSTRACT

The scalar dissipation rate (SDR) quantifies the mixing-rate between a turbulent jet and ambient fluids and is essential for modeling turbulent non-reacting/reacting flows. This study investigates SDR characteristics using Direct Numerical Simulation (DNS). For the steady-state jet, radial profiles of ensemble-averaged SDRs exhibit self-similar behaviours. The SDR is highest at the centreline, remains plateau at small radii, decreasing gradually at larger radii. The starting jet shows increased SDR values near the leading vortices, while recovering to steady-state jet values afterwards.

Key Words: Scalar dissipation rate, Direct Numerical Simulations, Turbulent jets

Characterisation of scalars mixing in turbulent jets remains a complex problem, yet fundamentally important for understanding the basic processes occurring in many applications such as combustion, pollutant emissions from industrial smokestacks or volcanic eruptions. In combustion applications, two streams of fluids, fuel and oxidizer, are introduced in a combustion chamber. Then, the two fluids need to be mixed at a right ratio for desired engine performances. Mixing processes in combustion are represented by two scalar variables, mixture fraction and scalar dissipation rates (SDR). Mixture fraction, denoted as ξ, is a conserved scalar defined as the fraction of the fluid mass originating from the fuel stream. Scalar dissipation rate, denoted by χ, represents the rate of mixing, related by the gradient of the mixture fraction. For a mixture with equal diffusivities D for all chemical species, SDR is defined as:

\[ \chi = 2D(\nabla \xi)^2 \]  

In non-premixed combustion systems, where the rate of chemical reaction is limited by the rate of mixing of fuel and oxidiser, the ensemble-average SDR is directly related to the mean reaction rate [1]. SDR also characterises how the turbulent straining of the fluid affects chemical processes within the flame [2–3] and thereby has a critical influence on extinction and ignition phenomena [4]. SDR-based turbulent combustion models typically require additional submodels such as conditionally-averaged SDR by mixture fraction and presumed probability density function of SDR.

Turbulence between different fluid streams acts to fold and stretch the diffusive interface, producing thin structures with relatively high scalar dissipation rate. Repeated folding and stretching of the scalar interface would act to increase scalar gradients exponentially, until the scalar length scale reduces to a viscous limit such as the Batchelor or Kolmogorov scale, resulting in a log-normal distribution of SDR [5–6]. The probability density function (PDF) of SDR for passive scalars has been found to be approximately log-normal in round turbulent jets, with deviations attributed to anisotropy [7]. Additional deviations from the log-normal distribution scalar dissipation rate arise in the case of chemically-reacting scalars for which reaction generate steep gradients at small scales [8].

Measuring SDR experimentally in turbulent flows are challenging because it requires three components of the scalar gradient within structures that are in the size of Kolmogorov or
Batchelor scales. Furthermore, such measurements are prone to experimental noise [9]. Notwithstanding these difficulties, numerous diagnostic developments have contributed to the measurements of passive and reactive scalar gradients in one [10], [11] or two dimensions [12]. However, for a complete description of scalar mixing, measurements in three dimensions are necessary, yet these remain a difficult task to carry out experimentally.

On the theoretical side, Peters & Williams [13] proposed a model for the ensemble-averaged SDR assuming that it can be related to the gradient of the ensemble-averaged mixture fraction. The key features of the model are: (i) employing a turbulent diffusivity \( \nu_t/Sc_t \) and (ii) assuming the derivatives in the streamwise and azimuthal directions are negligible, leading to

\[
\bar{\chi} = \left( \frac{2 \nu_t}{Sc_t} \right) \left( \frac{\partial \bar{\xi}}{\partial r} \right)^2,
\]

where \( Sc_t \) is the turbulent Schmidt number and \( \nu_t \) is the turbulent kinematic viscosity.

With ever increasing computational capabilities, nowadays, DNS has become able to resolve flows at higher Reynolds numbers. As such, it is possible to obtain the instantaneous scalar field in three-dimensions at a wide range of locations, allowing for experimental assumptions and theoretical models to be assessed.

The simulations are conducted using a compressible DNS code, HiPSTAR [14]. The flow domain uses a structured grid stretched in the downstream direction with a cylindrical configuration. A 4th order central finite difference scheme is used for the streamwise and radial directions, and a spectral decomposition is used in the azimuthal direction. The fluid is treated as a perfect gas, having the same temperature and density as the ambient fluid. The Reynolds number is 7 300 and the initial Mach number of the jet fluid is 0.304. Figure 1 shows a snapshot of SDR for the steady-state jet and three instances of the starting jet. The steady-state jet is established after 540 characteristic jet times (\( \tau \)) where \( \tau = D/U_0 \) with \( D \) as the jet inlet diameter and \( U_0 \) the inlet jet velocity. In addition to the steady-state jet, three realisations of a starting jet were simulated. For the latter, a step change in the inlet velocity occurs at time \( t/\tau = 0 \) from 0 to \( U_0 \). The jet is allowed to evolve for 66\( \tau \) when the leading vortices reach at around 26D downstream. Along with the fluid flow equations,

**Figure 1**: Non-dimensionalised scalar dissipation rate: (a) – (c) starting jet time instances, (d) steady state instantaneous snapshot, (e) steady state time-averaged.
the transport equation for mixture fraction is solved and used to evaluate SDR. A more detailed description about the code and setup can be found in Shin et al. [15].

As shown in Figure 1, SDR decreases with downstream distance. Near the inlet region, strong gradients are present, indicating intense mixing between the jet and ambient fluids. Further downstream, mixing becomes less intense, and SDR values are much decreased—note that SDR is coloured in log-scale. Moreover, the inlet region contains temporally and spatially coherent turbulent structures aligned at angles of 45° to 75° across where intense scalar mixing occurs. The angles are consistent with the observation by Feikema et al. [7] who explained that the counter-clockwise rotation of vortices at the interface between the jet and ambient fluids causes this. The rotation engulfs the ambient fluid radially inward in a location that is immediately upstream of each vortex and then convects the fluid downstream. As such, strong mixing occurs at the boundary of these regions, highlighted by dark red colour in Figure 1.

Radial profiles of SDRs for steady-state and starting jets are shown in Figure 2 a-b. In the Figures, the ensemble-averaged SDRs are scaled by their respective centreline values, denoted by $\chi_c$. The radius is scaled by the downstream distance $x$, where $x=X-X_0$, $X$ being the distance from the inlet and $X_0$ being the virtual origin with the value of 2.39D for this simulation. As such, the scaled radius is defined as $\eta=r/x$.

SDR profiles for the steady-state jet (Figure 2a) at different $x$-locations show a scatter among the dashed lines, however the scatter is narrow, indicating that self-similarity exists. There are two main possible reasons for the scatter: (i) noise in the centreline values which is used to normalise the radial profiles and (ii) the gradual development of self-similarity along the axial direction. Therefore, SDR profiles start to become self-similar at around $x/D=15$. Experimental investigations of Feikema et al. [7] on a gaseous propane jet, suitable for comparison with present simulation data, indicate the same general profiles behaviour with a decrease in dissipation in vicinity of the centreline, at small radii, followed by an increase and a peak in the shear layer region and a gradual decrease closer to the interface with ambient fluid. Figure 2b shows the short time-averaged SDR of the starting jet. The band of time average is chosen close toward the end of the simulation, in order to make sure SDR profiles upstream of the leading vortices region tend towards a quasi-steady-state. The averaged SDR is then normalised by their respective centreline values from the steady-state jet. As estimated in Figure 1c, the leading vortices are at around $x/D=16.5-17.5$ at 57.5τ. Increased SDR values for the
leading vortices region of the jet (at x/D=16 or 17.5) are followed by a slow decay towards steady-state jet SDR profiles (at x/D=14 or 15). The overall shape of profiles show a steeper decay with increasing radius compared to the steady-state jet. This is confirmed by observing the strong gradients in the starting jet at the leading vortices (Figure 1a–c).

For the self-similar region of the steady-state jet, an improved model for the ensemble-averaged SDR is developed. This extends from the analysis of Peters & Williams [13] for species production in turbulent diffusion flames and makes use of the available three-dimensional SDR data.

Analysis of the three SDR components indicates that axial and radial mixing occurs at similar intensity while the azimuthal mixing is twice as intense when compared to the first two. This allows Eq. (1) to be rewritten as:

\[ \chi = (8 \nu / Sc) \cdot \left( \frac{\partial \xi}{\partial x} \right)^2 \]  

The axial derivative in Eq. 3 can be expressed based on an existent analytical relation for the mean mixture fraction profile as:

\[ \frac{\partial \xi}{\partial x} = \left( \frac{\xi_c}{x} \right) \cdot f(\eta, \alpha, \beta) \]  

where \( \xi_c = c1 D/x \) and \( f(\eta, \alpha, \beta) \) is:

\[ f(\eta, \alpha, \beta) = \exp(-\gamma Sc \eta^2) \cdot \left[ -\alpha + \beta(\gamma Sc \eta^2) \right] \]

From the existing DNS data, \( \chi \) is 90, while the non-dimensionalised fluid kinematic viscosity and turbulent Schmidt number are given as \( \nu \approx 1.37 \times 10^{-4} \) and \( Sc = 0.72 \). Figure 2a, Eq. 3 agrees better with the mean SDR radial profile for the steady-state jet, especially in the vicinity of the centreline, while the model by Peters & Williams [13] approaches zero.

**Review**

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**References**


