



# Heat release effects on mixing scales of non-premixed turbulent wall-jets: A direct numerical simulation study

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## ABSTRACT

The present study concerns the role of heat release effects on characteristics mixing scales of turbulence in reacting wall-jet flows. Direct numerical simulations of exothermic reacting turbulent wall-jets are performed and compared to the isothermal reacting case. An evaluation of the heat-release effects on the structure of turbulence is given by examining the mixture fraction surface characteristics, diagnosing vortices and exploring the dissipation rate of the fuel and passive scalar concentrations, and moreover by illustration of probability density functions of reacting species and scatter plots of the local temperature against the mixture fraction. Primarily, heat release effects delay the transition, enlarge the fluctuation intensities of density and pressure and also enhance the fluctuation level of the species concentrations. However, it has a damping effect on all velocity fluctuation intensities and the Reynolds shear stress. A key result is that the fine-scale structures of turbulence are damped, the surface wrinkling is diminished and the vortices become larger due to heat-release effects. Taking into account the varying density by using semi-local scaling improves the collapse of the turbulence statistics in the inner region, but does not eliminate heat release induced differences in the outer region. Examining the two-dimensional premultiplied spanwise spectra of the streamwise velocity fluctuations indicates a shifting in the positions of the outer peaks, associated with large energetic structures, toward the inner region.

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## 1. Introduction

Flame–wall interaction is found in numerous combustion devices and it has been the subject of a number of studies (Vervisch and Poinso, 1998; Dabrieau et al., 2003; Wang and Trouvé, 2006). Among canonical problems for studying the interaction between a flame and a wall, the turbulent wall-jet configuration is a unique case, which includes interactions between turbulence scales of different sizes and the wall effects, as observed in many combustion systems. Small scales of turbulence are present close to the wall, whereas larger scales exist in the outer shear region. This makes the turbulent wall-jet a valuable test case for generic studies of reaction and mixing applications, see the review by Launder and Rodi (1981).

In the past three decades, direct numerical simulation (DNS) has become an essential tool to understand and model turbulent combustion. DNS numerically solves the set of equations describing turbulent flames by resolving all chemical and flow scales, Vervisch and Poinso (1998). Many industrial applications however, use Reynolds averaged Navier–Stokes (RANS) as the computational tool (Bilger, 2000; Peters, 2000) or are moving toward

using large eddy simulation (LES) for a more accurate design of turbulent combustion systems (Schumann, 1989; Veynante and Vervisch, 2002; Pitsch, 2006). In order to improve the current RANS and LES models for combustion applications, accurate knowledge of the averaged statistics and the subgrid-scale quantities is required. In particular, for reacting turbulent flows, the chemical source terms heavily depend on the choice of appropriate subgrid-scale models (Réveillon and Vervisch, 1996; Poinso and Veynante, 2001). It is now well established that the information needed to develop models may be provided by precise experimental data or by performing direct numerical simulations, Bilger et al. (2005).

Resolution requirements for DNS of wall-bounded flows scales largely with the Reynolds number ( $Re^{37/14}$ ), see Choi and Moin (2012), which makes it computationally expensive. Therefore, DNS data are in general limited and specifically the reports on the simulations of wall-jet flows, even on non-reacting cases, are still scarce. Ahlman et al. (2007) reported DNS of a turbulent plane wall-jet flow, which also includes the study of passive scalar mixing. This study was followed by Ahlman et al. (2009), in which the non-isothermal effects in the turbulent wall-jet were considered. Findings of that study concerning the density changes and the associated outcome for the appropriate scalings are used in the present work. However, the differences observed here result from

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the exothermic chemical reaction and are not always similar to those produced by density changes in non-isothermal non-reacting flows.

The first three-dimensional DNS of a reacting turbulent flow was performed by Riley et al. (1986) for a single irreversible non-premixed reaction in a turbulent mixing layer between an oxidizer and a fuel species disregarding heat release. Leonard and Hill (1988) used a similar approach to study mixing in homogeneous turbulence with two non-premixed reactants. Then, various flame problems have been explored with DNS using simple or complex chemistry (Mizobuchi et al., 2005; Yoo et al., 2011). Single-step global reaction is only a coarse approximation, but it still allows us to study the basis of the interaction between heat-release and turbulence in a three-dimensional flow. The single-step chemistry has been used extensively to analyze heat-release effects in turbulent flows and none of the major results were dismissed by multiple-step DNS analysis. Examples of using single-step chemistry for studying the fundamentals of turbulent combustion are the works by Boersma (1999) and Moureau et al. (2011). Other examples are in a planar mixing layer, (Givi et al., 1986; McMurtry et al., 1989), homogeneous reacting turbulence (Jaberi and Madnia, 1998), planar jet flows (Mehravaran and Jaberi, 2004) and three-dimensional DNS of mixing layers (Knaus and Pantano, 2009).

The heat release effects have been the subjects of a number of studies (Ruetsch et al., 1995; Diez and Dahm, 2007). McMurtry et al. (1989) investigated the heat-release effects on the large-scale structures in a turbulent mixing layer. Miller et al. (1994) also considered the reacting mixing layer, with low heat release, and carried out simulations for various Damköhler numbers. Heat release effects on the energy exchange between the kinetic and internal energies in a turbulent shear flow were studied by Livescu et al. (2002). The DNS of non-premixed jet by Pantano (2004) and the DNS of a hydrogen lifted flame by Mizobuchi et al. (2005) are two other works, where some of the heat release influences are visualized. The progress in research of the heat release effects in a turbulent shear layer was extended by the work of Knaus and Pantano (2009), where they addressed the heat release effects on the turbulence spectra. Neglecting the presence of the wall, for example in reacting turbulent shear layers, some of the previous studies suggested that, after appropriate scaling, the effect of heat release on the turbulence is rather small.

Up to now, numerical investigations of wall-bounded reacting flows have been restricted to the case of turbulent boundary layers and turbulent channel flows, see for example Ruetsch et al. (1995) or the work by Gruber et al. (2010), who investigated the turbulent flame-wall interaction in a channel flow. These studies have given some important insight, but much more remains to be studied in the area of wall-bounded turbulent combustion. Still, a number of DNS studies are devoted to the flame-wall interactions, including the works by Poinso et al. (1993), Bruneaux et al. (1996), Dabrieau et al. (2003) and Wang and Trouvé (2006).

In the present study, by performing a three-dimensional DNS, we concentrate on heat-release effects and turbulence-chemistry interactions. The main objective of this study is to address the influence of heat release on different turbulence and reactant statistics of turbulent wall-jet flows. The flow involves a simple reaction between an oxidizer and a fuel species. In our previous study of the isothermal reacting turbulent wall-jet, Pouransari et al. (2011), the flow was uncoupled from the reactions; thus, the influence of turbulent mixing on the reactions was studied in the absence of temperature effects. Here, a global exothermic reaction is considered, allowing for investigating the role of heat release in chemically reacting turbulent wall-jet flows. The heat release effects on fluctuation intensities of density and pressure, and also, the fluctuation level of the species concentrations, are examined. Taking into account the varying density by use of semi-local

scaling, the collapse of the turbulence statistics in the inner and the outer regions of turbulent wall-jet are studied. Detailed analysis of two-dimensional premultiplied spectra is performed to further explain the modifications of different scales, both in the inner and outer regions, due to heat release induced effects. The heat release influences for modeling aspects are briefly discussed. The flame wall interaction is analyzed by studying the reacting species probability density functions and the temperature scatter plots at various locations of the domain. The possibility of pre-mixed burning within the flame is investigated.

This paper is organized as follows. The governing equations are presented in Section 2 and the numerical method and different simulation cases are introduced in Section 3. Flow configurations and an overview of DNS results are provided in Section 4. Heat release effects on different turbulence and reactant statistics together with influences on time and length scales are discussed in Section 5. A discussion of probability density functions, scatter plots and the flame index is given in Section 6 and conclusions are drawn in Section 7.

## 2. Governing equations

The conservation equations of total mass, momentum and energy read

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0 \quad (1)$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \quad (2)$$

$$\frac{\partial \rho E}{\partial t} + \frac{\partial \rho E u_j}{\partial x_j} = \dot{\omega}_T - \frac{\partial q_i}{\partial x_i} + \frac{\partial (u_i (\tau_{ij} - p \delta_{ij}))}{\partial x_j} \quad (3)$$

Here  $\rho$  is the total mass density,  $u_i$  are the velocity components,  $p$  is the pressure,  $E = e + \frac{1}{2} u_i u_i$  is the total energy and  $\dot{\omega}_T$  is the heat release term due to the exothermic reaction. The summation convention over repeated indices is used. The heat fluxes  $q_i$  are approximated by Fourier's law  $q_i = -\lambda (\partial T / \partial x_i)$ , where  $\lambda$  is the constant coefficient of thermal conductivity and  $T$  is the temperature. The viscous stress tensor is defined as  $\tau_{ij} = \mu (\partial u_i / \partial x_j + \partial u_j / \partial x_i) - \mu (2/3) (\partial u_k / \partial x_k) \delta_{ij}$ , where  $\mu$  is the dynamic viscosity. The fluid is assumed to be calorically perfect and to obey the ideal gas law according to  $e = c_v T$ ,  $p = \rho R T$ , and a specific heat ratio of  $\gamma = c_p / c_v = 1.4$  is used. The viscosity is determined through the Sutherland's law

$$\frac{\mu}{\mu_j} = \left( \frac{T}{T_j} \right)^{3/2} \frac{T_j + S_0}{T + S_0}, \quad (4)$$

where  $T$  is the local temperature,  $T_j$  is the jet center temperature at the inlet and  $S_0 = 110.4K$  is a reference value.

Conservation of the species mass fractions is governed by

$$\frac{\partial \rho \theta_k}{\partial t} + \frac{\partial}{\partial x_j} (\rho \theta_k u_j) = \frac{\partial}{\partial x_j} \left( \rho \mathcal{D} \frac{\partial \theta_k}{\partial x_j} \right) + \dot{\omega}_k, \quad (5)$$

where  $\theta_k$  and  $\dot{\omega}_k$  are the mass fractions and the reaction rate of the oxidizer, fuel and passive scalar species. An equal diffusion coefficient  $\mathcal{D}$  for all scalars, is used to approximate the diffusive fluxes (constant Schmidt number approximation,  $Sc = 0.7$ , Lewis number is thus unity). The reaction is simplified as a single-step irreversible reaction between oxidizer species  $O$  and fuel species  $F$  that react to form a product  $P$ , whose rate is expressed with an Arrhenius law as,

$$\dot{\omega}_f = -k_f \rho^2 \theta_o \theta_f \exp(-Z_e/T), \quad (6)$$

where  $k_f$  is the pre-exponential constant. Because of this oversimplified chemistry, modification of the detail of the inner reaction zone by the presence of the wall cannot be studied thoroughly.

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