Conditional statistics in a planar liquid jet with a second-order chemical reaction

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ABSTRACT

Conditional statistics, conditioned on mixture fraction, are experimentally investigated in a planar liquid jet with a second-order isothermal chemical reaction $A + B \rightarrow R$. Reactants A and B are contained in the jet and ambient flows, respectively, and are supplied into the test section under the non-premixed condition. Streamwise velocity, mixture fraction and concentrations of all reactive species are simultaneously measured by using an I-type hot-film probe and an optical fibre probe based on light absorption spectrometry. The cross-streamwise profiles of conditional mean concentrations and conditional mean reaction rate show that the conditional mean concentrations and the conditional mean reaction rate near the jet exit change with the cross-streamwise position, whereas they are independent of the cross-streamwise position in the downstream regions. On the jet centreline, the conditional mean reaction rate has a peak value on the condition that the conditional mean concentration of product R has a peak value. A comparison between the conditional mean reaction rate and the covariance of conditional concentration fluctuations shows that the covariance of conditional concentration fluctuations is so small that a first moment closure model for the conditional mean reaction rate is valid. The conditional mean streamwise velocity is almost linear to the mixture fraction for small mixture fraction fluctuations. The conditional scalar dissipation rate is calculated from the budget of the conditional moment closure equation. The results show that the conditional scalar dissipation rate has a single peak value in the upstream region, whereas in the downstream region, it has two peaks for the large and small mixture fraction values. The conventional mean scalar dissipation rate is calculated from the probability density function of the mixture fraction and the conditional scalar dissipation rate. The conventional mean scalar dissipation rate on the jet centreline decreases in the downstream direction as $(x^*)^{-2.9}$ (where x^* is the distance from the virtual origin), which is almost the same as that expected from scaling arguments.

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1. Introduction

Chemical reactions in the environment or in industrial equipment often occur in turbulent flows. In non-premixed systems, chemical reactions occur with turbulent mixing of reactants. Turbulent flows have a great influence on chemical reactions and mixing of chemical substances [1], and understanding turbulent flows with chemical reactions will help us develop numerical methods to predict them. Therefore, elucidating the mechanism of chemical reactions in turbulent flows is desired. Numerical methods for turbulent reactive flows [2] are important for predicting the efficiency of combustors or chemical reactors and for understanding pollutant formation in the atmosphere.

Direct numerical simulation (DNS), in which the governing equations (e.g., the continuity equation, the Navier–Stokes equations or the equations for energy and mass transfer) are numerically solved without any models, provides the most accurate and reliable solutions. However, because of the high computational cost of DNS, its application is limited to flows at low Reynolds numbers and in simple geometries. DNS has been employed for investigating chemical reactions in turbulent flows and developing models for turbulent reactive flows (e.g., [3–8]).

From a practical point of view, the Reynolds-averaged approach, in which the Reynolds-averaged governing equations are solved by using turbulent models, is useful for predicting turbulent flows because of its low computational cost. To apply the Reynolds-

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averaged approach to turbulent reactive flows, models for the turbulent mass flux and the mean chemical reaction rate are required to solve averaged equations for reactive scalar transfer. The gradient diffusion model [9] is often used to model the turbulent mass flux of reactive species [2,10], and various models have been proposed for the mean chemical reaction rate [10–13]. However, it has been pointed out that the gradient diffusion hypothesis is largely influenced by chemical reactions [14–17]. Additionally, models for the mean chemical reaction rate are valid only for particular flows. Therefore, the Reynolds-averaged approach is unsuited for reactive flows unless it is used with another numerical method to treat the effect of chemical reactions.

The conditional moment closure (CMC) method [18,19] was developed to simulate turbulent reactive flows. Because the CMC method is like the Reynolds-averaged approach, its computational cost is not high, and it can be applied to various flows and chemical reactions. Masri et al. [20] measured the temperature and concentrations of reactive species in a non-premixed jet flame of methanol, and showed that temperature and concentrations of reactive species strongly depend on the mixture fraction, which can be defined by the normalized concentration of nonreactive species. Thus, for the case in which reactants are mixed and react in a non-premixed system, the variables related to the chemical reactions depend on the mixture fraction. In the CMC method, turbulent reactive flows are simulated by solving the transport equations for conditional mean concentrations, conditioned on the mixture fraction. The conditional mean concentration of species α (Q_α), conditioned on the mixture fraction ξ, is defined as

$$Q_\alpha \equiv \langle \Gamma_\alpha | \xi = \eta \rangle \equiv \langle \Gamma_\alpha | \eta \rangle, \tag{1}$$

where Γ_α is the instantaneous concentration of species α, $\langle\rangle$ denotes an ensemble average, $\langle | * \rangle$ denotes an ensemble average conditioned on $*$ and η is the sample space variable for ξ. The transport equation for Q_α was derived by Klimenko [21] and Bilger [18] and can be written as

$$\frac{\partial Q_\alpha}{\partial t} + \langle U_i | \eta \rangle \frac{\partial Q_\alpha}{\partial x_i} - \langle N | \eta \rangle \frac{\partial^2 Q_\alpha}{\partial \eta^2} = \langle W_\alpha | \eta \rangle, \tag{2}$$

where U_i is the instantaneous i direction velocity, W_α is the production rate of species α by chemical reactions and N is the scalar dissipation rate, which is defined by

$$N \equiv D \frac{\partial \xi}{\partial x_i} \frac{\partial \xi}{\partial x_i}. \tag{3}$$

Here, D is the molecular diffusivity, which is often assumed to be independent of species. Solving Eq. (2) requires models for the conditional mean velocity $\langle U_i | \eta \rangle$, the conditional scalar dissipation rate $\langle N | \eta \rangle$ and the conditional mean reaction rate $\langle W_\alpha | \eta \rangle$. In the Reynolds-averaged approach, it is required to model the conventional mean reaction rate (where "conventional mean" denotes a time average or an ensemble average). Even for a simple second-order isothermal reaction, modelling the conventional mean reaction rate is not easy because concentration fluctuations arising from turbulence greatly contribute to the mean reaction rate and their contributions are not easy to predict [22,23]. Because concentration fluctuations from the conditional mean concentrations often have only a negligible contribution to the conditional mean reaction rate [18], the models for the conditional mean reaction rate $\langle W_\alpha | \eta \rangle$ are simpler than those for the conventional mean reaction rate. This is one of the advantages of using the CMC method.

To verify the numerical accuracy of the CMC method and the models for the unclosed terms used in the CMC method, it is important to investigate conditional statistics in turbulent reactive flows. Experimentally measuring conditional statistics in reactive flows requires simultaneous measurement of the mixture fraction

and other quantities. Conditional moments of the temperature and the mass fraction of reactive species have been measured in jet flames by Masri et al. [20], Barlow et al. [24,25] and others. In gas flows, many measurements of conditional statistics have been conducted. Bilger et al. [14] measured reactive concentrations in a scalar mixing layer with a second-order chemical reaction and investigated the conditional mean concentrations of reactive species [18]. Li and Bilger [26] measured the covariance of conditional concentration fluctuations in a reactive scalar mixing layer. Brown and Bilger [27] measured the conditional statistics in a reactive plume in grid turbulence. Most of conditional statistics measurements have been conducted in the gas phase, in which diffusion and mixing of reactive species are characterised by a lower Schmidt number (or Prandtl number) than those in the liquid phase. DNS has been used to investigate the conditional statistics and the models used for the CMC method (e.g., [6,28,29]). However, DNS can be applied only to flows at low Schmidt number ($Sc = v/D$, where v is the kinematic viscosity and D is the molecular diffusivity) because the smallest scale of scalar fluctuations, which is called the Batchelor scale, becomes small, being proportional to $Sc^{-1/2}$ [30]. Thus, there have been few investigations of conditional statistics in liquid flows. Most measurements of conditional statistics of reactive concentration have been conducted in flames, in which the Damköhler number, which is the ratio of flow to reaction time scales, is very large.

The scalar dissipation rate [31] is a key variable in turbulent reactive flows, especially for fast chemical reactions. When fast chemical reactions occur in a non-premixed system, the chemical reaction rate strongly depends on the scalar dissipation rate [32]. Models for the statistics of the scalar dissipation rate [33–35] are important for numerical simulations of reactive flows. However, measurement of the conditional scalar dissipation rate is a challenging problem, especially in liquid flows because a spatial resolution comparable to the Batchelor scale is required to accurately perform the measurement [36]. In jet flows in the gas phase, the scalar dissipation rate has been measured by Su and Clemens [37], Karpetis and Barlow [38] and Su et al. [39]. In a liquid jet, Kailasnath et al. [40] measured the scalar dissipation rate. However, the smallest scale of scalar fluctuations was not resolved in many of the previous scalar dissipation rate measurements.

The purpose of this study is to investigate the conditional statistics in a reactive jet at high Sc. Concentrations of reactive species and velocity are simultaneously measured in a planar liquid jet with a second-order isothermal reaction to investigate the conditional statistics. By using the measurement results of conditional statistics, the conditional scalar dissipation rate can be estimated from the budget of Eq. (2). This method to estimate the conditional scalar dissipation rate requires measurements of the conditional average of concentration, velocity and reaction rate. Because these conditional statistics are less sensitive to the spatial resolution of measurement than is the scalar dissipation rate [36], it is possible to estimate the conditional scalar dissipation rate from Eq. (2) even at high Sc. The conditional statistics have been investigated in turbulent reactive flows at low Sc, such as turbulent jet flames, and the models used in the CMC methods were verified based on those experimental and numerical results. Our experiments are conducted at high Sc and small Damköhler number compared with previous experiments on turbulent flames. Because of a difficulty of measuring concentrations of reactive species, data on the conditional statistics in reactive flows at high Sc are lacking. Therefore, it remains still unclear whether the models used in the CMC methods are applicable to turbulent reactive flows at high Sc. The present study will reveal the characteristics of the conditional statistics in the reactive jet at high Sc. Although previous studies showed that the conditional statistics are almost independent of positions across flows in a mixing layer [18] and a plume [27], we will show