

# Direct Numerical Simulation of Eddy Diffusivity in a Plane Jet with a second-order reaction

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## 1 Introduction

Turbulent flows with chemical reactions can be seen in various fields. Therefore, it is important to establish numerical methods to predict turbulent reactive flows.

Reynolds-averaged approach is often used for predictions of reactive flows. In this approach, Reynolds-averaged scalar transport equations are solved by using models for a turbulent mass flux  $\langle u_i \gamma_\alpha \rangle$  and an averaged production rate by chemical reactions. Here,  $u_i$  and  $\gamma_\alpha$  are fluctuation components of  $i$  direction velocity ( $U_i$ ) and concentration of species  $\alpha$  ( $\Gamma_\alpha$ ), respectively, and  $\langle * \rangle$  denotes an ensemble average of variable  $*$ . One of the simplest models for  $\langle u_i \gamma_\alpha \rangle$  is a gradient diffusion model [1], in which  $\langle u_i \gamma_\alpha \rangle$  is given by

$$\langle u_i \gamma_\alpha \rangle = -D_{\alpha,i} \frac{\partial \langle \Gamma_\alpha \rangle}{\partial x_i}. \quad (1)$$

Here,  $D_{\alpha,i}$  is the eddy diffusivity of species  $\alpha$  corresponding to the  $i$  direction.  $D_{\alpha,i}$  has a significant effect on the prediction of  $\langle u_i \gamma_\alpha \rangle$ . Bilger et al. [2] and Komori et al. [3] have experimentally shown that the eddy diffusivity of reactive species is affected by chemical reactions. However, the effects of chemical reactions on the eddy diffusivity have not been investigated sufficiently.

In this study, a planar jet with a second-order chemical reaction is simulated by DNS, and the eddy diffusivity  $D_{tA,x}$  of reactant species A corresponding to the  $x$  direction and the Damkhöler number effects on  $D_{tA,x}$  are investigated in detail.

## 2 Direct Numerical Simulation

Figure 1 shows a sketch of the flow. A planar jet containing reactant A is ejected into a main flow containing the other reactant B through a slit with width of  $d$ . Product R is formed by a second-order chemical reaction which can be written as  $A+B \rightarrow R$ . We assume that this second-order reaction is isothermal and concentrations of reactive species behave as passive scalars. The computational domain is resolved by  $475 \times 425 \times 65$  grid points. The grid is equidistant in the  $x$  and  $z$  directions. In the  $y$  direction, the grid is stretched near the lateral boundaries. The spatial resolution is the same order as the Kolmogorov scale.

The governing equations for this problem are the incompressible Navier – Stokes equations, the continuity equation, and the passive scalar transport equations in their instantaneous, local form:

$$\frac{\partial U_i}{\partial x_i} = 0, \quad (2)$$

$$\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 U_i}{\partial x_j \partial x_j}, \quad (3)$$

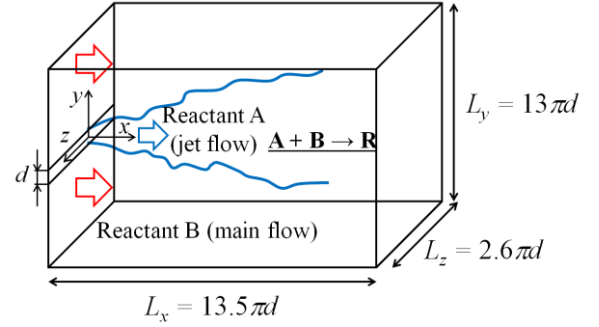


Fig. 1 Sketch of the flow

$$\frac{\partial \Gamma_\alpha}{\partial t} + U_j \frac{\partial \Gamma_\alpha}{\partial x_j} = D_\alpha \frac{\partial^2 \Gamma_\alpha}{\partial x_j \partial x_j} + S_\alpha. \quad (4)$$

Here,  $\nu$  is the kinetic viscosity,  $D_\alpha$  is the molecular diffusivity of species  $\alpha$ , which is assumed to be constant for species A, B, and R, and  $S_\alpha$  is the production rate of  $\Gamma_\alpha$  by the chemical reaction and given by  $S_R = -S_A = -S_B = k\Gamma_A\Gamma_B$ , where  $k$  is the reaction rate constant. Equation (4) is solved for concentration of product R and mixture fraction  $\xi$  which is defined by  $\xi \equiv (\Gamma_A - \Gamma_B + \Gamma_{B0})/(\Gamma_{A0} + \Gamma_{B0})$ , where  $\Gamma_{\alpha 0}$  is the initial concentration of species  $\alpha$ . Because  $S_A = S_B$ , the production rate of  $\xi$  by the chemical reaction is zero. The concentrations of reactants A and B are calculated from  $\Gamma_R$  and  $\xi$  by using mass conservation law written as follows:

$$\Gamma_A = \Gamma_{A0}\xi - \Gamma_R, \quad \Gamma_B = \Gamma_{B0}(1-\xi) - \Gamma_R. \quad (5)$$

The fractional step method is used to solve the governing equations which are spatially discretized by using central differences, and the Poisson equation is solved by conjugate gradient method. The variables are stored on a staggered grid arrangement. The third-order Runge – Kutta method and the Crank – Nicolson method are used for temporal discretization.

The traction-free condition and the convection outflow condition are applied at the lateral boundaries and the outlet boundary, respectively. Periodic boundary conditions are applied in the  $z$  direction. Velocity data at the inflow boundary is generated by superimposing random fluctuations on the mean velocity profile. The velocity profile at the jet exit is a top-hat profile with smooth edges which is measured at the exit of the planar jet in our experimental apparatus [4]. The mean streamwise velocity  $U_M$  of the main flow at the inflow boundary is  $0.056U_J$ , where  $U_J$  is the streamwise velocity averaged in the jet exit. The Reynolds number defined by  $Re = U_J d / \nu$  is set to

2,000. The concentrations of reactive species are imposed at the inflow and lateral boundaries to satisfy that  $\Gamma_A = \Gamma_{A0}$  and  $\Gamma_B = \Gamma_R = 0$  in the jet exit, and  $\Gamma_B = \Gamma_{B0}$  and  $\Gamma_A = \Gamma_R = 0$  in the main flow. Therefore,  $\xi = 1$  in the jet exit and  $\xi = 0$  in the main flow. Schmidt number ( $Sc = \nu/D_\omega$ ) is set to 1

The initial concentrations are set to  $\Gamma_{A0} = 0.4$  [mol/m<sup>3</sup>] and  $\Gamma_{B0} = 0.2$  [mol/m<sup>3</sup>]. The Damkhöler number  $Da$  is the ratio of a time scale of the flow and a time scale of the chemical reaction, and in this study, is defined by  $Da = k(\Gamma_{A0} + \Gamma_{A0})d/U_J$ . Simulations are carried out at the different Damkhöler numbers  $Da = 0.1, 1, \text{ and } 10$ .

### 3 Results and discussion

Figure 2 shows the axial profile of mean concentration  $\langle \Gamma_A \rangle$  of species A on the jet centreline for  $Da = 0.1, 1, \text{ and } 10$  and for the non reactive case. In Fig. 2,  $\langle \Gamma_A \rangle$  is normalized by initial concentration  $\Gamma_{A0}$ .  $\langle \Gamma_A \rangle$  monotonically decreases in  $x$  direction. In Fig. 2, it is also shown that as  $Da$  increases,  $\langle \Gamma_A \rangle$  becomes small and the chemical reaction rapidly proceeds.

Figure 3 shows the axial profiles of streamwise turbulent mass flux  $\langle u\gamma_A \rangle$  of species A on the jet centreline for  $Da = 0.1, 1, \text{ and } 10$  and for the non reactive case.  $\langle u\gamma_A \rangle$  is normalized by  $U_J$  and  $\Gamma_{A0}$ . Figure 3 shows that the chemical reaction makes  $\langle u\gamma_A \rangle$  large in the upstream region ( $x \leq 22 \sim 30$ ), but makes small in the downstream region.  $\langle u\gamma_A \rangle$  shows the dependency on the Damkhöler number.

Figure 4 shows the eddy diffusivity  $D_{tA,x}$  of species A corresponding to the  $x$  direction. In Fig. 4,  $D_{tA,x}$  is normalized by  $U_J$  and  $d$ .  $D_{tA,x}$  is calculated from Eq. (1). Figure 4 shows that  $D_{tA,x}$  becomes small due to the chemical reaction, and the effect of the chemical reaction on  $D_{tA,x}$  for  $Da = 10$  is smaller than that for  $Da = 0.1$  and 1. Thus, it is found that  $D_{tA,x}$  is largely affected by the chemical reaction, and the change of  $D_{tA,x}$  by the chemical reaction depends on the Damkhöler number.

### 4 Conclusion

A planar jet with a second-order reaction ( $A + B \rightarrow R$ ) is investigated for the different Damkhöler numbers ( $Da = 0.1, 1, \text{ and } 10$ ) by DNS. The eddy diffusivity  $D_{tA,x}$  for reactant A corresponding to the streamwise direction is calculated on the jet centreline from the mean concentration  $\langle \Gamma_A \rangle$  and the streamwise turbulent mass flux  $\langle u\gamma_A \rangle$ . The results show that eddy diffusivity is largely affected by the chemical reaction. For reactant A, the chemical reaction makes  $D_{tA,x}$  small, and the effect of the chemical reaction on  $D_{tA,x}$  for  $Da = 10$  is smaller than that for  $Da = 0.1$  and 1. The effect of the chemical reaction on  $D_{tA,x}$  depends on the Damkhöler number. These results imply that the gradient diffusion models may cause a significant error of the turbulent mass flux estimation when they are applied to reactive flows without considerations of the effect of reactions on the eddy diffusivity.

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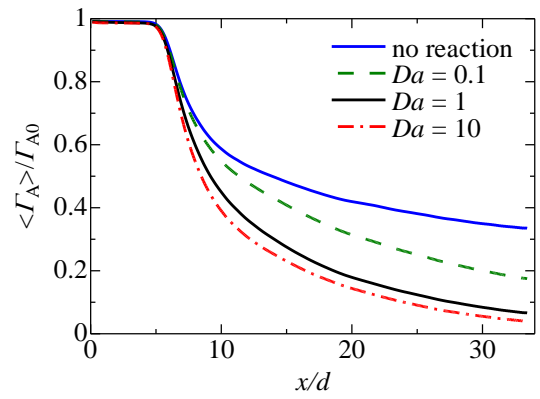


Fig. 2 Axial profiles of mean concentration of reactant A

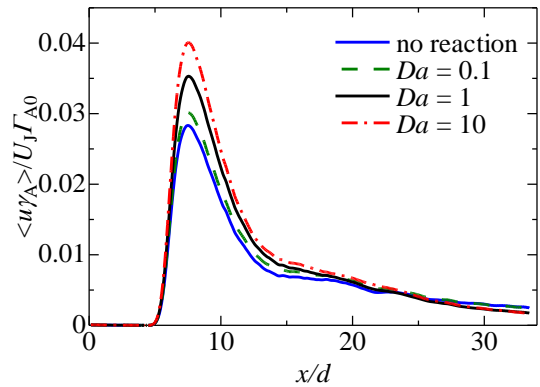


Fig. 3 Axial profiles of streamwise turbulent mass flux of reactant A

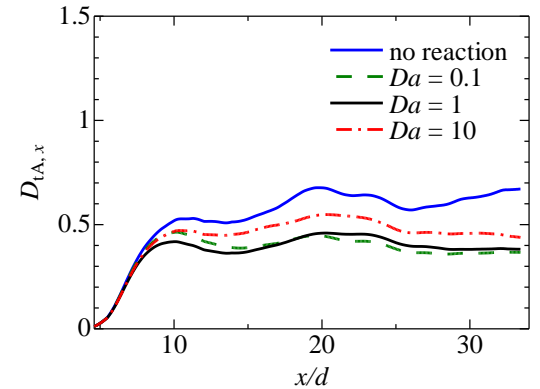


Fig. 4 Axial profiles of eddy diffusivity of reactant A corresponding to the streamwise direction

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