LARGE EDDY SIMULATIONS OF TURBULENT LIQUID FLOWS WITH CHEMICAL REACTIONS

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ABSTRACT

A subgrid-scale (SGS) model for the filtered reaction term is presented to develope large eddy simulations (LES) of nonpremixed, turbulent reacting liquid flows. The SGS model is based on the SGS probability density function (PDF) and SGS conditional expectation. The SGS PDF is assumed to have the beta distribution and the SGS conditional expectation was modeled using the filtered data obtained from direct numerical simulations (DNS) of liquid flows with second-order chemical reactions.

To confirm the accuracy of the SGS model, the LES was applied to a liquid mixing layer flow downstream of a turbulence-generating grid with a chemical reaction. The large eddy probability density function (LEPDF) model and the present model were used as the SGS models for a rapid reaction and for a moderately fast reaction, respectively. The predictions of the LES were compared with the measurements by Komori et al. (1993, 1994) to examine the proposed SGS models. The results show that the predictions of the LES are in good areement with the mesurements.

Furthermore, to investigate the applicability of the present LES to other reacting liquid flows, both experiment and LES were performed in a turbulent mixing layer with a rapid reaction. The predictions were also in good agreement with the measurements. These results show that the present LES taking account into the SGS distributions can accurately estimate the concentration statistics in various types of reacting liquid flows.

INTRODUCTION

Large eddy simulation (LES) is a very attractive tool to numerically simulate a turbulent reacting flow. Large scales (grid-scales : GS) are computed in the LES directly from the solutions of the filtered Navier-Stokes and mass conservation equations, and small scales (SGS) are modeled to close the SGS stress, SGS mass fluxes and filtered chemical reaction source term. One of the major issues toward the development of the LES is to employ an adequate SGS model for the filtered chemical reaction source term. Gao and O'Brien (1993) proposed a SGS model based on the LEPDF of concentration fluctuations of chemical species and derived a transport equation of the LEPDF. However, the equation needed a lot of closure hypotheses, so that it took a high computational cost. On the other hand, Cook and Riley (1994) proposed a beta assumed-p.d.f approximation, in which the GS concentrations were directly solved using a conserved scalar approach. The conserved scalar approach assumes that the scale of chemical reaction is so fast compared to that of turbulent mixing, which is limited to a rapid reaction. Thus, simple and adequate SGS modeling for the filtered reaction source term in a turbulent reacting flow is still crucial especially for a moderately fast reaction. In addition, the previous models have been proposed only for turbulent reacting air flows, and therefore it is not clear whether the previous SGS models can be applied to turbulent reacting liquid flows.

The purpose of this study is, therefore, to develop the LES which is applicable to turbulent reacting liquid flows.

LARGE EDDY SIMULATION

By applying a filter operation indicated by an overbar, the continuity, momentum, and mass conservation equations can be written as

$$\frac{\partial \overline{U_i}}{\partial x_i} = 0 \quad , \tag{1}$$

$$\frac{\partial \overline{U_i}}{\partial t}+\frac{\partial \overline{U_j}\,\overline{U_i}}{\partial x_j}=-\frac{\partial \overline{P}}{\partial x_i}+\frac{1}{Re}\frac{\partial^2 \overline{U_i}}{\partial x_j \partial x_j}-\frac{\partial \tau_{ij}}{\partial x_j}, \quad (2)$$

$$\frac{\partial \overline{\Gamma_i}}{\partial t}+\frac{\partial \overline{U_j}\,\overline{\Gamma_i}}{\partial x_j}=\frac{1}{ReSc}\frac{\partial^2 \overline{\Gamma_i}}{\partial x_j \partial x_j}-\frac{\partial q_{ij}}{\partial x_j}\pm\overline{\omega}, \quad (3)$$

where U_i are the velocity components, Γ_i are the concentration of the species i and P is the pressure. The dimensionless parameters appearing in the governing equations are the Reynolds number Re and Schmidt number Sc. When a second-order, irreversible and isothermal reaction ($A+B\rightarrow P$) is considered, the filtered chemical reaction source term is expressed as

$$\overline{\omega}=Da\,\overline{\Gamma_A\Gamma_B}, \quad (4)$$

where Da is the Damkohöler number.

The effects of the unresolved SGS in the above filtered equations ((1) ~ (3)) appear in the SGS stress term τ_{ij}, SGS mass flux term q_{ij}, and filtered chemical reaction source term $\overline{\omega}$. These terms need to be modeled to represent the effects of the SGS by the filtered quantities at the resolved scales (GS).

SUBGRID-SCALE MODEL

Rapid reaction case

For a rapid reaction, the timescale of chemical reaction is smaller than that of turbulent diffusion so that the time step Δt must be sufficiently smaller than the time scale of chemical reaction. However, the extremely small time step can not be set in the supercomputer. Therefore, the SGS model of Cook & Rilly (1994) was applied for a turbulent liquid flow with a rapid reaction.

Moderately fast reaction case

The filtered reaction source term can be decomposed into two terms,

$$\overline{\omega}=Da\,\overline{\Gamma_A\Gamma_B}=Da\left(\overline{\Gamma_A}\,\overline{\Gamma_B}+\overline{\gamma'_A\gamma'_B}\right), \quad (5)$$

where γ'_i are the concentration fluctuations of chemical species i at SGS.

A primitive model which neglects the mixing of two species at SGS gives

$$\overline{\omega}=Da\overline{\Gamma_A}\,\overline{\Gamma_B}. \quad (6)$$

The primitive model can not accurately calculate the filtered reaction source term when the species are not completely mixed at SGS.

In this study, the model which has considered the mixing of the chemical species at SGS, is derived using the probability density function of species A ($P(\Gamma_A)$) and conditional expectation of the product of species A and B for a given Γ_A ($<\Gamma_A\Gamma_B|\Gamma_A>$) as

$$Da\,\overline{\Gamma_A\Gamma_B}=Da\int_0^1 <\Gamma_A\Gamma_B\,|\Gamma_A>P(\Gamma_A)\,d\Gamma_A. \quad (7)$$

In the above equation, the filtered chemical reaction source term can be calculated by giving appropriate models for $P(\Gamma_A)$ and $<\Gamma_A\Gamma_B|\Gamma_A>$. Usually $P(\Gamma_A)$ is assumed to follow beta-assumed PDF model, whereas any model for $<\Gamma_A\Gamma_B|\Gamma_A>$ has not been proposed. Therefore, it is an important subject to propose an appropriate model for $<\Gamma_A\Gamma_B|\Gamma_A>$. Here, we attempted to propose a model for $<\Gamma_A\Gamma_B|\Gamma_A>$ by using the filtered data obtained from the DNS for stationary isotropic liquid turbulence. The proposed model is shown as

$$<\Gamma_A\Gamma_B\,|\Gamma_A> = \alpha\left\{-\beta\left(\Gamma_A-\frac{1-\overline{\Gamma_P}}{2}\right)^2+\frac{1}{4}(1-\overline{\Gamma_P})^2\right\}, \quad (8)$$

$$\alpha=\alpha_1\,\alpha_2,$$

$$\alpha_1=\begin{cases}-(\overline{\Gamma_A}-1)^{16}+1 & (\overline{\Gamma_A}\le\overline{\Gamma_B})\\ -(\overline{\Gamma_B}-1)^{16}+1 & (\overline{\Gamma_A}\ge\overline{\Gamma_B}),\end{cases}$$

$$\alpha_2=\frac{0.25(1-\overline{\Gamma_P})^2-C_\alpha\sqrt{\overline{\gamma'^2_P}}}{0.25(1-\overline{\Gamma_P})^2} \qquad C_\alpha=0.2,$$

$$\beta=\left\{1-\overline{\Gamma_P}\left[\overline{\Gamma_A}+\frac{1-\Gamma_P}{2}\right]\right\}^2.$$

The accuracy of the model was confirmed by the DNS data.

LARGE EDDY SIMULATIONS OF TURBULENT LIQUID FLOWS

To assess whether the present SGS models for a rapid reaction and a moderately fast reaction are applicable for turbulent reacting flows, the LES was carried out for a reacting mixing-layer liquid flow downstream of a turbulence-generating grid. Figure 1 shows the schematic diagram of the computational domain. The computational domain was $520\times80\times80$ mm in the streamwise, vertical and spanwise directions. A turbulence-generating grid was located at 2.0×10^{-2} m downstream from the entrance. The mesh size M and thickness of the square rod were 2.0×10^{-2} m and 2.0×10^{-3} m, respectively. The numbers of grid points used here were $260\times80\times80$ in the streamwise, vertical and spanwise directions.

The governing equations for the LES are given by (1) ~ (3). These equations were discretized on a staggard mesh arrangement to construct a finite-difference formation. The spatial derivatives in the filtered N-S equations and mass conservation equations were approximated by a second-order central difference. The HSMAC method was used to solve the N-S equation. The time integration of the N-S and mass conservation equations was carried out by a second-order Runge-Kutta method.

Figure 2 shows that streamwise distributions of the time-averaged concentration of chemical product P in a reacting mixing layer flow downstream of a turbulence-generating grid. The predictions by the LES are in good agreement with the measurements

for both a rapid reaction and a moderately fast reaction. Figure 3 shows the streamwise distributions of the mean squared concentration fluctuation of chemical species A for a rapid reaction. The original LES can not take account into the SGS fluctuation of chemical species, so that the predictions shown by a dotted line become smaller than the measurements. To include the effect of the SGS fluctuation on the time-averaged mean squared concentration fluctuations, a correction method, which is given by

$$\langle \gamma_A'^2 \rangle = \langle \overline{\Gamma_A}^2 \rangle - \langle \overline{\Gamma_A} \rangle^2 + c_f' \langle \widetilde{\overline{\Gamma_A}}^2 - \widetilde{\overline{\Gamma_A}}^2 \rangle, \quad (9)$$

was proposed. Here, ~ indicates the value by applying a test-filter with the twice filter width. The correlation coefficient $c_f' = 5.0$ was determined by the DNS data for stationary isotoropic liquid turbulence. The corrected predictions shown by a solid line in Fig. 3 are in good agreement with the measurements.

Furthermore, to examine the applicability of the present LES to other reacting liquid flows, both experiment and LES were performed in a turbulent reacting mixing layer with a rapid reaction. The details of the measurement system are given by Komori et al. (1993, 1994). Figure 4 shows the schematic diagram of the computational domain. The computational domain was 280×80×80 mm in the streamwise, vertical and spanwise directions. The numbers of grid points used here were 280×80×40, respectively. The governing equations and the computational method are the same as in the LES of a reacting mixing layer flow downstream of a turbulence-generating grid.

Figure 5 shows the vertical distributions of the time-averaged concentration of chemical product P at two stations of x = 0.15 and x = 0.25 m. The η' is the non-dimensional vertical distance. The predictions by the LES are very close to the measurements. Figure 6 shows the vertical distributions of the mean squared concentration fluctuation of chemical species A for a rapid reaction. The predictions by (9) are also in good agreement with the measurements.

CONCLUSIONS

A new SGS model for the filtered chemical reaction source term was proposed using the filtered data obtained by the DNS of a turbulent liquid flow. Furthermore, the SGS model was examined by applying the LES to turbulent liquid flows with a rapid reaction and a moderately fast reaction. The main results from this study can be summarized as follows.

(a) The present SGS model, which consists of the PDF and conditional expectation, can well predict the chemical reaction source term.

(b) The present LES is applicable to turbulent reacting liquid flows. The LES can well predict not only the time-averaged concentration but also the time-averaged concentration fluctuations.

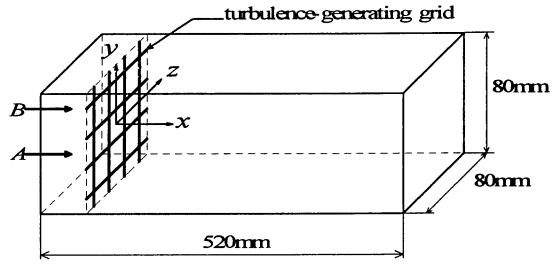

Figure 1 : The computational region in a mixing layer flow downstream of a turbulence-generating grid.

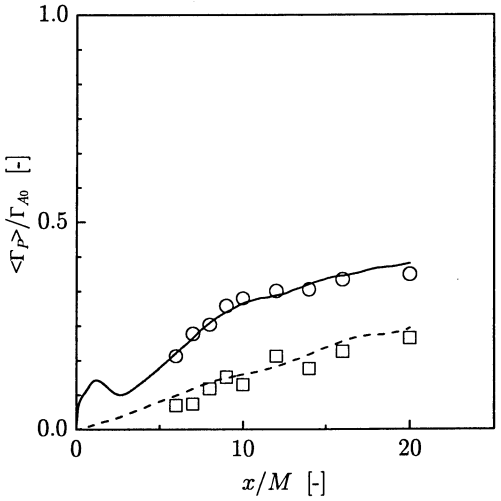

Figure 2 : Streamwise distributions of the mean concentration of chemical product P. Symbols denote the measurements and the lines are the predictions by the LES: ○, —, a rapid reaction; □, - -, a moderately fast reaction.

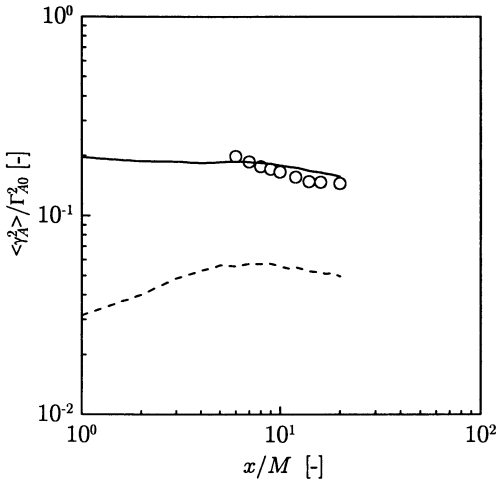

Figure 3 : Streamwise distributions of the mean squared concentration fluctuation of species A for a rapid reaction: ○, measurements; —, predictions by the conventional LES method; - -, predictions by the corrected LES method with SGS variance.

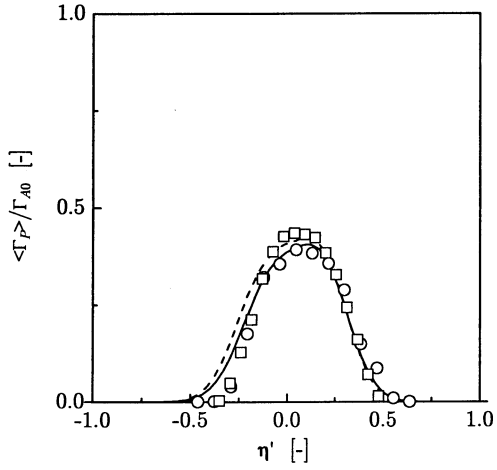

Figure 5 : Vertical distributions of the mean concentration of chemical product P: ○, —, at x = 0.15m; □, - -,at x = 0.25m.

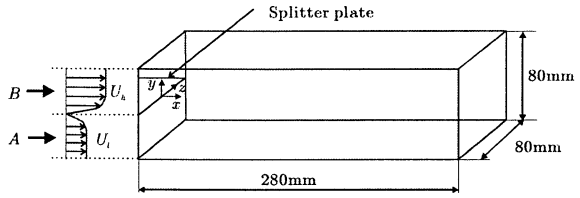

Figure 4 : The computational region of a mixing layer.

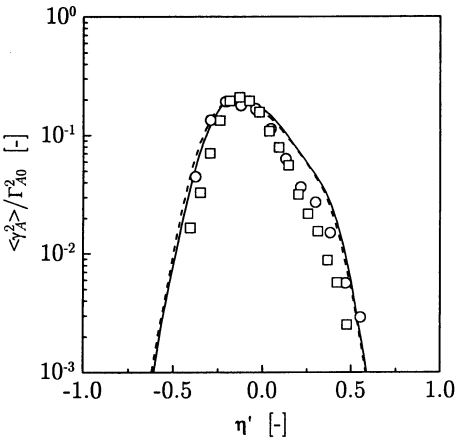

Figure 6 : Vertical distributions of the mean squared concentration fluctuation of species A: ○, —, at x = 0.15m; □, - -, at x = 0.25m.

Acknowledgments

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