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# Large eddy simulation of passive scalar transport in a high Schmidt number turbulent incompressible wake with experimental validation

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## HIGHLIGHTS

- LES is performed for passive scalar mixing in a high Schmidt number turbulent wake.
- The simulation is validated against PIV and PLIF data.
- Detailed comparisons of one-point statistics and spatial correlations were made.
- LES compared well with experiments, thus the transport mechanisms were well simulated.
- Two-point spatial correlations of passive scalar with velocity showed good agreement.

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## ABSTRACT

Large eddy simulation of the passive scalar transport in a high Schmidt number turbulent confined wake flow has been performed. The results are evaluated by comparison to particle image velocimetry (PIV) and planar laser-induced fluorescence (PLIF) data, including point-wise data as well as spatial correlations. In the LES simulations, the gradient diffusion hypothesis is used to close the transport equation for the passive scalar. Different discretization schemes are investigated in order to determine the best choice for ensuring boundedness of the passive scalar and to accurately predict the mixing rate. The simulation results compare well to experimental data, demonstrating that the transport mechanisms in this high Schmidt number turbulent flow are well predicted by the LES method. Two-point spatial correlations of passive scalar with velocity predicted by the simulation show good agreement with the experimental results, indicating that the turbulent coherent structures of the flow are reproduced by the simulation.



## 1. Introduction

The prediction of passive scalar transport in turbulent flows is of great importance in a wide range of applications. Turbulent mixing is relevant, for example, in the chemical process industry where reactants are mixed by turbulence, in dispersion of pollutants in the atmosphere or bodies of waters, and in combustion applications (Bo et al., 2003; Petersen et al., 2010). The accurate prediction of the transport of a passive scalar in computer simulations is beneficial in that it limits the need for costly experiments, both for design and research purposes. Thus this research topic has received much attention, and examples can be found throughout the literature (Burton and Dahm, 2005; Lubbers et al., 2001; Taveira et al., 2011).

However, accurate prediction of turbulent transport of a passive scalar is a challenging task. This difficulty arises from the wide range of scales present in turbulent flows. A direct numerical simulation (DNS) to the governing equations requires a high level of computer power. For cases where the Schmidt number is large (such as in a liquid), the smallest scale of the passive scalar will be much smaller than the smallest scale of turbulence. In such a case, the presence of a passive scalar widens the range of scales present in the flow field and increases the computational demand. Warhaft (2000) gives a review of passive scalars in turbulent flows and underlines the complexity of the topic.

Given the complexity and the high computational demand, it is clear that simulation of turbulent passive scalar transport in most cases is beyond the scope of DNS and calls for modeling. With modeling, the need to evaluate the assumptions implicit in the model and validate the accuracy of simulation results arises. Commonly, simulations are validated using relatively simple measurement data, such as point-wise velocity, pressure or concentration data. Examples

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of such validations can be found in Gousseau et al. (2012), Gromke et al. (2008), le Ribault (2008), and Rossi and Iaccarino (2009). Although such data can provide indications to whether the simulation is reliable or not, they may not provide insight into why or why not the model works. For that, more detailed information is needed. Particle image velocimetry (PIV) (Adrian, 1991) and planar laser-induced fluorescence (PLIF) are two non-intrusive full-field measurement techniques for measuring velocity and concentration, respectively. Simultaneous PIV/PLIF provides measurement data of velocity and concentration simultaneously and in a whole field (Boxx et al., 2009; Hu et al., 2002). Thus, both turbulent fluxes and spatial gradients can be obtained, key values in the prediction of turbulent transport. In addition, spatial information such as spatial correlations can be determined to provide valuable information about the turbulent coherent motion in the flow, which is a key feature in the transport of a passive scalar.

Two techniques for the modeling of turbulent flows are Reynolds-averaged Navier–Stokes (RANS) simulations and large-eddy simulation (LES). In RANS the governing equations are ensemble averaged, and the mean values are solved for while the effect of turbulence is modeled. In LES a filter is applied to the governing equations, and only the large scales of the flow are solved for while the effect of the smaller scales is modeled. The equation for the transport of a passive scalar in a turbulent flow is given as

$$\frac{\partial\tilde{\phi}}{\partial t}+\tilde{u}_i\frac{\partial\tilde{\phi}}{\partial x_i}=\Gamma\frac{\partial}{\partial x_i}\left(\frac{\partial\tilde{\phi}}{\partial x_i}\right)-\frac{\partial\lambda_i}{\partial x_i} \quad (1)$$

where $\phi$ is the concentration of the passive scalar, $u_i$ are the components of velocity, $x_i$ are spatial coordinates and $\Gamma$ is the molecular diffusivity. Tilde represents Reynolds averaging in the case of RANS and filtering in the case of LES. $\lambda_i$ is the turbulent flux, or in the LES framework the subgrid scalar flux, containing the unclosed terms and therefore requires modeling. The most common way of modeling the flux is to invoke the gradient diffusion hypothesis which states that the turbulent flux is aligned with and proportional to the gradient of the scalar concentration:

$$\lambda_i=-\Gamma_T\frac{\partial\tilde{\phi}}{\partial x_i} \quad (2)$$

where $\Gamma_T$ is the turbulent diffusivity or the eddy diffusivity, related to the turbulent viscosity or eddy viscosity, $\nu_T$, through

$$Sc_T=\nu_T/\Gamma_T \quad (3)$$

where $Sc_T$ is the turbulent Schmidt number which is often assumed to be constant.

The existing literature shows several examples of cases where the gradient diffusion hypothesis with a scalar turbulent diffusivity in the RANS framework does not hold. Tavoularis and Corrsin (1981) and Lemoine et al. (1999) studied a nearly homogeneous turbulent shear flow with a uniform mean temperature gradient and a circular heated jet with co-flow, respectively. In both cases it was found that the turbulent flux was not aligned with the mean temperature gradient.

Due to the different nature of the two simulation approaches, the gradient diffusion assumption may still be accurate in LES even in cases where the assumption is not valid for RANS. For example, Nilsen (2014) performed LES of a confined turbulent jet with co-flow with passive scalar transport and compared the results to simultaneous PIV/PLIF measurements. They modeled the subgrid scales with use of the gradient diffusion hypothesis in the LES framework and obtained satisfactory results. Also in the wake case presented here, experiments have shown that the turbulent fluxes from Reynolds averaging were not aligned with the mean concentration gradient (Feng et al., 2010). The question that arises is whether the success of the gradient diffusion hypothesis in the LES framework is universal.

Feng et al. (2010) performed simultaneous PIV/PLIF in a confined turbulent wake flow at Reynolds number 37,500. A RANS simulation by Liu et al. (2006) of the same flow showed some discrepancy in the mixing rate of the passive scalar. In the work presented here, the wake flow is simulated by LES with passive scalar transport at high Schmidt number and the results are compared in-depth to the PIV/PLIF data of

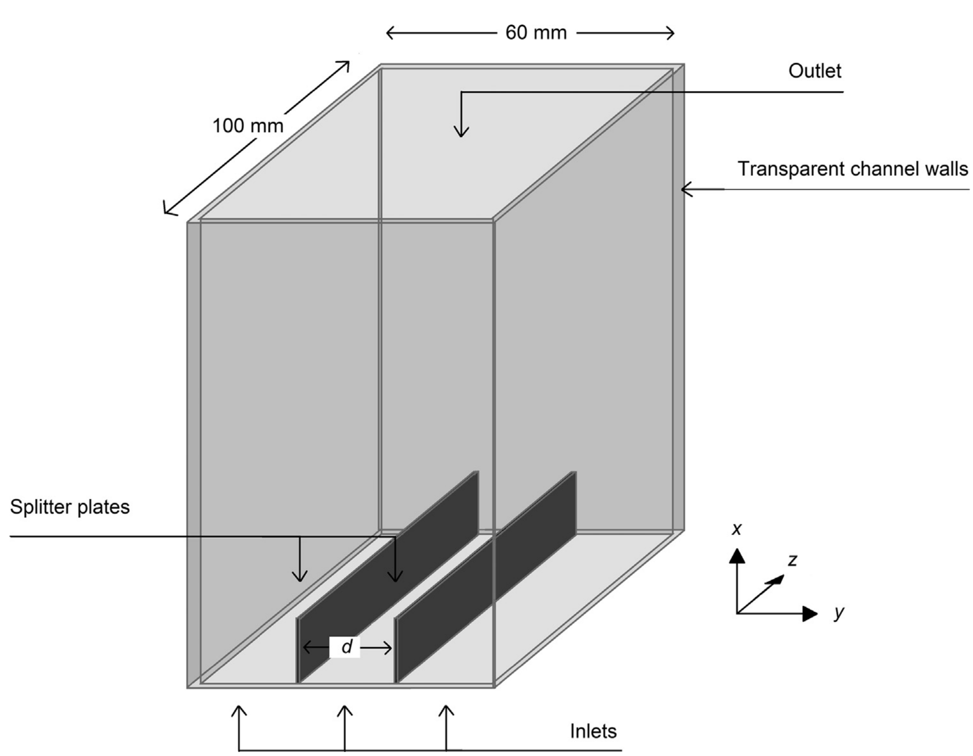


**Fig. 1.** Schematic of the experimental and simulation geometry.