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A numerical study of scalar dispersion downstream of a wall-mounted cube using direct simulations and algebraic flux models

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ABSTRACT

The dispersion of a passive scalar downstream of a wall-mounted cube is examined using direct numerical simulations and turbulence models applied to the Reynolds equations. The scalar is released from a circular source located on top of the obstacle, which is immersed in a developing boundary-layer flow. Direct simulations are performed to give insight into the mixing process and to provide a reference database for turbulence closures. Algebraic flux models are evaluated against the standard eddy-diffusivity representation. Coherent structures periodically released from the cube top are responsible for a counter-diffusion mechanism appearing in the streamwise scalar flux. Alternating vortex pairs form from the lateral edges of the cube, but the intensity profiles and probability density functions of scalar fluctuations suggest that they do not cause a significant flapping movement of the scalar plume. The gradient-transport scheme is consistent with the vertical and spanwise scalar flux components. From the comparative study with our direct simulations, we further stress that Reynolds stress predictions must be carefully evaluated along with scalar flux closures in order to establish the reliability of Reynolds-averaged computations. However, the analysis also shows that algebraic closures provide a significant improvement which cannot be achieved with the standard eddy-diffusivity model.

1. Introduction

The analysis and modeling of scalar dispersion around obstacles is an active area of research, mostly driven by the need to better understand and predict the transport of pollutants in urban areas (Britter and Hanna, 2003). With advances in numerical techniques and computer speed, numerical simulations have been employed over the years along with field and wind tunnel testing to address the topic. High-fidelity numerical models, such as Large-Eddy Simulations (LES), have recently been reported by several research groups to study the dispersion of transported scalars around single or multiple obstacles (e.g.,Sada and Sato, 2002; Tseng et al., 2006; Shi et al., 2008; Xie and Castro, 2009). However, the computational effort required by LES is such that numerical models based on the Reynolds equations (RANS) are frequently adopted to predict scalar dispersion in complex flows (Li et al., 2006). In this framework, turbulence models for the velocity field have been the focus of several studies, while only the standard gradient-diffusion hypothesis (SGDH) has been applied to modeling the turbulent scalar fluxes appearing in the averaged scalar transport equation. Although an isotropic eddy-diffusivity can be a questionable approximation even for simple shear flows (Quarmby, 1972; Quarmby and Quirk, 1974), examples of application of the standard flux model include fully-inhomogeneous flow conditions, such as the release from point sources located within obstacles arrays (Hsieh et al., 2007). This scenario is rather surprising since in such cases the modeling of turbulent transport is further complicated by the lateral spread of the scalar plume.

In a preliminary attempt toward the evaluation of refined models for the turbulent scalar flux (Rossi and Iaccarino, 2009a), we adopted algebraic flux models (AFMs) to predict the scalar dispersion from a line source downstream of a two-dimensional obstacle. Using an algebraic formulation, the isotropic eddy-diffusivity is replaced by a tensorial representation which potentially accounts for the anisotropic character of turbulent transport. Algebraic closures were found able to give much more reliable predictions of scalar flux components compared to the standard model, but the spanwise homogeneity of the flow and the scalar field limited the impact of the scalar flux anisotropy. Furthermore, although scalar flux components were available from experiments (Vinçont et al., 2000), the profiles were only measured at two streamwise locations downstream of the obstacle. Therefore, the dynamic of the scalar plume close to the source was difficult to examine. The improved reliability versus the isotropic eddy-diffusivity model has become clear when algebraic models have been applied to the

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scalar mixing from a point source over a wavy wall (Rossi, 2009b). A comparative study against a DNS database (Rossi and Iaccarino, 2009b), demonstrated that algebraic closures also represent a reasonable approximation for the spanwise scalar flux component when lateral transport comes into play.

In this work, we present a numerical study of scalar dispersion from a point source located on top of a wall-mounted cube. The objective of the analysis is twofold. First, we intend to provide further insight into turbulent mixing occurring in the presence of a three-dimensional obstacle. This is achieved by means of direct numerical simulations (DNS). Statistics of scalar fluctuations and fluxes, which are rarely reported from experimental studies, are computed and discussed. In addition, algebraic flux models are employed to close and solve the Reynolds-averaged scalar transport equation, and the results compared to those obtained using the standard eddy-diffusivity model. A comparative study against the established DNS database and available experimental measurements is performed in order to present a comprehensive evaluation of scalar flux models.

In the past, the scalar dispersion around wall-mounted cubes placed in a turbulent stream has been the subject of several studies. Robins and Castro (1977b) performed one of the first wind tunnel experiments and compared the measured data with simplified models for atmospheric dispersion. The effect of the source height was investigated, but measurements were limited to the mean concentration. Concentration fluctuations downstream of a cubical obstacle were later reported by Li and Meroney (1983a,b). In their study, several features affecting the plume dispersal were considered and discussed, such as the flow direction, the source position on top of the cube and the scalar emission rate. Numerical simulations have also been reported in the literature. One of the most recent analyses, performed by Tominaga and Stathopoulos (2009), evaluated several $k-\epsilon$ closures and the isotropic eddy-diffusivity model for scalar dispersion downstream of a cube. None of the previous studies, however, focused on direct computations including scalar dispersion or reported comparative studies between scalar flux models.

2. Flow and numerical setup

2.1. Overview

The numerical experiment consists of the continuous release of a passive scalar from a circular source located on top of a wall-mounted cube and centered on its surface. Numerical simulations based on the Reynolds equations have been performed with the cube immersed in both uniform and turbulent streams, while direct simulations are limited to the case of the uniform inflow.

The uniform inflow setup, given by a flat velocity profile at the inlet of the computational domain, is aimed at minimizing the uncertainty in the boundary conditions when the flow governing equations are solved directly (Rossi and Iaccarino, 2008). Available wake measurements from the experiment of Castro and Robins (1977) are employed to establish the reliability of our DNS database for the velocity field as well as the accuracy of flow field predictions from RANS models. Since concentration measurements were not available for the uniform inflow setup, the standard and the algebraic flux models are compared directly to the computed and partly validated DNS statistics. In order to limit the computational effort required by direct simulations, the bulk Reynolds number based on the free-stream velocity U_e and the cube height h for the uniform flow setup is 5000.

The turbulent inflow is considered next to match the experimental setup of Li and Meroney (1983a), which provides more realistic conditions for atmospheric dispersion around obstacles. In this case, only the standard and algebraic flux models have been employed and evaluated against experimental data. Nonetheless, since scalar flux profiles were not available from the experiments, the previous comparison with our DNS dataset provided useful guidelines toward the interpretation of numerical results. The bulk Reynolds number for the turbulent inflow setup is 11,000.

2.2. Flow and scalar governing equations

The flow is assumed incompressible and neutrally stable, and the scalar advection is approximated to a passive mechanism. The flow and scalar governing equations solved in the direct numerical simulations read as follows:

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{1}$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{1}{Re}\frac{\partial^2 u_i}{\partial x_j \partial x_j} \tag{2}$$

$$\frac{\partial c}{\partial t} + u_j \frac{\partial c}{\partial x_j} = \frac{1}{ReSc}\frac{\partial^2 c}{\partial x_j \partial x_j} \tag{3}$$

where the Schmidt number Sc gives the ratio between the kinematic viscosity and the scalar diffusivity. Note that a value of $Sc = 0.285$ is employed for both the uniform and turbulent inflow setup and that this value matches that of the experimental tracer fluid. The computational cost required by direct simulations increases exponentially with the Reynolds number as well as with the Schmidt number, quickly becoming unfeasible when applied to realistic conditions. The Reynolds-averaged flow and scalar equations are thus considered:

$$\frac{\partial U_i}{\partial x_i} = 0 \tag{4}$$

$$U_j \frac{\partial U_i}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{1}{Re}\frac{\partial^2 U_i}{\partial x_j \partial x_j} - \frac{\partial}{\partial x_j}(\overline{u_i u_j}) \tag{5}$$

$$U_j \frac{\partial C}{\partial x_j} = \frac{1}{ReSc}\frac{\partial^2 C}{\partial x_j \partial x_j} - \frac{\partial}{\partial x_j}(\overline{u_j c}) \tag{6}$$

where now the Reynolds stress tensor $\overline{u_i u_j}$ and the vector of scalar fluxes $\overline{u_j c}$ must be modeled in order to predict the mean flow U_j and the mean concentration field C. In this work, the Reynolds stress transport (RST) closure of Launder et al. (1975) is employed to close the averaged momentum equation away from the wall, while the one-equation model of Wolfstein (1969) is applied to the viscosity-dominated wall-region. Since the modeling of turbulence around a wall-mounted cube using RANS closures has been broadly covered in the literature (e.g.,Lakehal and Rodi, 1997; Rodi, 1997) and the present study focuses on the discussion of the scalar field prediction, the model equations for the Reynolds stresses are not reported here for the sake of brevity, whereas scalar flux models will be presented in detail in Section 3.

2.3. Numerical technique

In this work, both direct and Reynolds-averaged computations are carried out using unstructured finite-volume schemes. The computational grid is composed of blocks of hexahedral cells around the sides of the cube, while on top of the obstacle an hybrid mesh is adopted in order to fit the circular source. The grid is refined toward the cube surface and quadrilateral cells are employed around the source to capture the strong concentration gradients occurring along its boundary. Fig. 1 shows the grid adopted for RANS computations. In this case the grid is refined toward the edges of the cube, while uniform grid spacing, not shown for the sake of brevity, is employed for direct simulations in order to improve the numerical stability. The geometrical parameters, the