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CFD simulation of pollutant dispersion around isolated buildings: On the role of convective and turbulent mass fluxes in the prediction accuracy

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ABSTRACT

Computational Fluid Dynamics (CFD) is increasingly used to predict wind flow and pollutant dispersion around buildings. The two most frequently used approaches are solving the Reynolds-averaged Navier–Stokes (RANS) equations and Large-Eddy Simulation (LES). In the present study, we compare the convective and turbulent mass fluxes predicted by these two approaches for two configurations of isolated buildings with distinctive features. We use this analysis to clarify the role of these two components of mass transport on the prediction accuracy of RANS and LES in terms of mean concentration. It is shown that the proper simulation of the convective fluxes is essential to predict an accurate concentration field. In addition, appropriate parameterization of the turbulent fluxes is needed with RANS models, while only the subgrid-scale effects are modeled with LES. Therefore, when the source is located outside of recirculation regions (case 1), both RANS and LES can provide accurate results. When the influence of the building is higher (case 2), RANS models predict erroneous convective fluxes and are largely outperformed by LES in terms of prediction accuracy of mean concentration. These conclusions suggest that the choice of the appropriate turbulence model depends on the configuration of the dispersion problem under study. It is also shown that for both cases LES predicts a counter-gradient mechanism of the streamwise turbulent mass transport, which is not reproduced by the gradient-diffusion hypothesis that is generally used with RANS models.

1. Introduction

Computational Fluid Dynamics (CFD) is increasingly explored and used to predict wind flow and pollutant dispersion around buildings. Accurate numerical simulation of this complex coupled process requires careful simulation of each of its constituents: (1) the incoming Atmospheric Boundary Layer (ABL) flow; (2) the turbulent wind flow around the buildings submerged in the ABL; and (3) the transport process of the pollutant by convection and diffusion in the turbulent wind-flow pattern. Because of the turbulent and inherently transient nature of the flow around buildings, the accuracy of pollutant dispersion simulations is strongly influenced by the turbulence modeling approach used, which is generally either steady Reynolds-averaged Navier–Stokes (RANS) or Large-Eddy Simulation (LES).

In turbulent flows, dispersion can be seen as the combination of the molecular, convective and turbulent mass transport, where the first is often negligibly small compared with the two others. Several earlier research efforts have compared the performance of RANS and LES approaches for pollutant dispersion in idealized urban geometries like street canyons (e.g. [1–4]) and arrays of buildings (e.g. [5,6]). Other efforts have compared RANS and LES for isolated buildings (e.g. [7,8]), or in real urban environments (e.g. [9,10]). Overall, LES appears to be more accurate than RANS in predicting the mean concentration field because it captures the unsteady concentration fluctuations. Moreover, this approach provides the statistics of the concentration field which can be of prime importance for practical applications.

Most of the aforementioned studies have analyzed the prediction accuracy of CFD by comparing the resulting mean concentrations on and around building surfaces. Only few of them have analyzed the performance of RANS and LES by focusing on the mass transport process itself. Tominaga and Stathopoulos [3] compared the lateral and vertical turbulent fluxes inside a street canyon computed with RANS and LES. Yoshie et al. [8] employed these two approaches to illustrate the horizontal distribution of the lateral turbulent mass flux around an isolated building with non-isothermal ABL flow. Rossi et al. [11] compared the performance of different turbulent flux models for RANS for dispersion around a cube. Direct Numerical Simulation was also performed for a uniform inflow profile and a Reynolds number equal to 5000. To the

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best of our knowledge, only Tominaga and Stathopoulos [7] provided some information about convective and diffusive fluxes for the case of dispersion around a building in an ABL flow, but their study focused at only a few locations on the roof.

In this paper, we present a detailed analysis of the transport process of a pollutant in the turbulent wind-flow pattern around isolated buildings. The relative influence of convective and turbulent fluxes in the transport process is analyzed and the role of these fluxes in the prediction accuracy of RANS and LES simulations is clarified. For this purpose, two cases with distinctive features in terms of the transport process are selected, for which also detailed wind tunnel experiments are available:

1. Dispersion from a stack located immediately downstream of an isolated rectangular building [12].
2. Dispersion from a rooftop vent on an isolated cubical building [13].

In case 1, the stack is relatively high and discharges the pollutants outside the building wake, which decreases the influence of the building on the dispersion of the plume. In case 2, the source is located directly on the roof of the building and the pollutant gas is released with low momentum ratio into the rooftop separation bubble. Validation of the CFD simulations is performed by comparing the numerical results with the wind-tunnel concentration measurements presented in [12,13]. For case 1, concentration profiles along three lines located five building heights downstream of the building are used whereas for case 2, concentration contours on the roof and in the wake of the building are used.

Some details about the numerical procedure are given in the next section. Then, for each case, the experiment is outlined, the numerical model is described and the results are presented and analyzed.

2. Governing equations

2.1. RANS and turbulence models

With the RANS approach, the Reynolds-averaging operator is applied to the flow equations. Only the averaged quantities are computed and the effect of turbulence on the average flow field – symbolized by the Reynolds stresses – is modeled with turbulence models. In this study, four turbulence models will be used and compared: the standard k–ε model (SKE) [14], the realizable k–ε model (RLZ) [15], the renormalization-group (RNG) k–ε model [16], and the Reynolds-stress model (RSM) with a linear pressure–strain model and wall-reflection effects [17,18]. The relevant equations can be found in the references. For brevity, only the model constants are given here. They are the default values in Fluent 6.3. For SKE: $C_\mu = 0.09$; $C_{1\varepsilon} = 1.44$; $C_{2\varepsilon} = 1.92$; $\sigma_k = 1.0$; $\sigma_\varepsilon = 1.3$. For RLZ: $C_{1\varepsilon} = 1.44$; $C_2 = 1.9$; $\sigma_k = 1.0$; $\sigma_\varepsilon = 1.2$. For RNG: $C_\mu = 0.0845$; $C_{1\varepsilon} = 1.42$; $C_{2\varepsilon} = 1.68$. For RSM: $C_\mu = 0.09$; $C_{1\varepsilon} = 1.44$; $C_{2\varepsilon} = 1.92$; $C_1 = 1.8$; $C_2 = 0.6$; $C'_1 = 0.5$; $C'_2 = 0.3$; $\sigma_k = 1.0$; $\sigma_\varepsilon = 1.3$.

2.2. LES and subgrid-scale models

With LES, a spatial-filtering operator is applied to the Navier–Stokes equations to separate the smallest scales of motion, which have a more universal behavior and can therefore be modeled, and the large scales, which are explicitly resolved. The effect of the smallest scales on the resolved flow field is modeled with a subgrid-scale (SGS) model. In this study, the dynamic Smagorinsky SGS model [19–21] is used. LES is particularly interesting when dealing with mass transport phenomena since this process is mainly governed by the largest scales of motion.

2.3. Numerical procedure

For the RANS simulations presented here, all the transport equations (momentum, energy, k, ε and concentration) are discretized using a second-order upwind scheme. Pressure interpolation is second order. The SIMPLE algorithm is used for pressure–velocity coupling. Convergence is assumed to be obtained when the scaled residuals [22] reach 10^{-5}.

For LES, the filtered momentum equation is discretized with a bounded central-differencing scheme. A second-order upwind scheme is used for the energy and concentration equations. Pressure interpolation is second order. Time integration is second-order implicit. The non-iterative fractional step method [23] is used for time advancement.

2.4. Wall treatment

In order to properly simulate the approaching ABL flow in the computational domain, horizontal homogeneity must be achieved, i.e. the vertical flow profiles that are prescribed at the inlet must be preserved along the domain before reaching the buildings [24,25].

For RANS simulations with the Fluent 6.3 CFD code, the standard wall functions [26] are applied to the wall boundaries (ground, building and stack surfaces). For the ground, the wall functions are modified for roughness [27], which is specified by an equivalent sand-grain roughness height k_s and a roughness constant C_r. Horizontal inhomogeneity of the ABL can be limited by adapting k_s and C_r to the inlet ABL profiles, following the equation by Blocken et al. [24]: $k_s = 9.793 z_0/C_r$, where z_0 is the aerodynamic roughness length of the terrain.

To the authors' best knowledge, such a relation does not exist for LES with Fluent. In this case, the centroids of the wall-adjacent cells are assumed to fall in the logarithmic-law region of the boundary layer [22] and the wall roughness is not taken into account. The same boundary condition is used for the smooth walls, i.e. the building and stack surfaces.

In both RANS and LES simulations, the upstream domain length is kept as short as possible (5H) to limit horizontal inhomogeneity [24]. A posteriori verification showed that the maximum wall-normal distance of the first centroid at the wall boundaries was approximately 100 wall units ($z^+ = zu^*/\nu$, where z is the wall-normal distance, u^* is the friction velocity and ν is the kinematic viscosity of the fluid) for case 1 and 40 for case 2.

2.5. Dispersion modeling

The instantaneous pollutant concentration (c, kg m^{-3}) is treated as a scalar transported by an advection–diffusion equation (Eulerian approach):

$$\frac{\partial c}{\partial t} + \vec{u} \cdot \nabla c = -\nabla \cdot \overrightarrow{q_m} + s_c \qquad (6)$$

where $\vec{u}$ is the velocity vector; s_c is a source term; and $\overrightarrow{q_m}$ is the mass flux due to molecular diffusion.

Applying the Reynolds decomposition to the variables ($x = X + x'$ where $X = \langle x \rangle$ and x' are the mean and fluctuating components of x, respectively) and averaging Eq. (6) yields:

$$\nabla \cdot (\overrightarrow{Q_m} + \overrightarrow{Q_c} + \overrightarrow{Q_t}) = S_c \qquad (7)$$

In this equation, $\overrightarrow{Q_m}$ is the mean molecular mass flux (kg m^{-2} s^{-1}), proportional to the gradient of mean concentration:

$$Q_{m,i} = -D_m \frac{\partial C}{\partial x_i} \qquad (8)$$

where D_m is the molecular mass diffusivity (m^2 s^{-1}). In general, the molecular mass flux is negligible in comparison with the mean