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Numerical analysis of pollutant dispersion around elongated buildings: an embedded large eddy simulation approach

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Abstract

High fidelity, scale-resolving numerical simulations of flow and pollutant dispersion around several elongated isolated buildings are presented in this paper. The embedded large eddy simulation (ELES) is used to model flow and concentration fields for six test cases with various source-building geometries. Specifically, the influence of building aspect ratio, wind direction, and source location is examined with these cases. Results obtained from the present ELES model are evaluated using available wind tunnel measurements, including those of streamwise and spanwise velocities, turbulent kinetic energy, and streamwise, lateral, and spanwise pollutant concentrations. Comparisons indicate that the ELES provides realistic representations of the flow and concentration fields observed in wind tunnel experiments, and captures several complex phenomena including the lateral shift and enhanced descent of the plume for rotated/elongated buildings. Furthermore, the ELES provides a means to study the advective and turbulent concentration fluxes, plume shapes, and geometry of vortical structures that is used to examine turbulent transport of pollutants around buildings. We investigate the enhancement of vertical and lateral plume spread as the building aspect ratio is increased. In addition, through the study of advective and turbulent concentration fluxes, we shed light on the physics behind higher ground-level concentrations observed for rotated buildings.

Keywords

Pollutant dispersion; Elongated building; Downwash; CFD; LES

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1. Introduction

The flow around a building in a turbulent atmospheric boundary layer includes several complex phenomena such as separation and reattachment, wake and recirculation, and horseshoe and arch vortices. The interaction of pollutants released near a building with these complex features often results in ground-level concentrations that are significantly larger than those occurring in the absence of the building. Elevated plumes brought quickly to the ground by these complex flows is referred to as building downwash. Many studies (e.g., Castro and Robins, 1977; Fackrell, 1984; Huber, 1989; Thompson, 1993; Snyder, 2005, Olesen et al., 2009) have shown that the magnitude and extent of the downwash effects depend on parameters including the building aspect ratio, the source height and location with respect to the building, and the meteorological conditions.

Wind tunnel and water channel measurements are common research methods to study the flow and dispersion around buildings. Smoke visualizations, velocity and turbulence measurements, and tracer concentration measurements have all demonstrated the complexity of the building-induced flow and the influence on nearby plume concentrations. For example, while examining simple rectangular buildings for a wide range of plume heights and locations, Thompson (1993) demonstrated that buildings with a wider dimension perpendicular to the incident flow have a down-washing effect that extends to higher plumes than that for buildings with otherwise similar dimensions. Snyder (2005) examined flow fields and Huber (1989) examined tracer concentration fields for releases near buildings at varying angles to the incident flow. They found a stronger downwash effect, higher ground-level concentrations, and strong lateral shifts in the plume when the building was at an oblique angle to the wind.

Dispersion models such as AERMOD (Cimorelli et al., 2005), OML (Olesen et al., 2007), and ADMS (Carruthers et al., 1994; Robins et al., 1997) have been developed on the basis of wind tunnel measurements such as those mentioned above. These operational models use a steady-state, Gaussian dispersion approach and serve as important tools for both air quality research and management. However, these models do not currently account for the asymmetry in the wake and the associated lateral and vertical shifts in the plume. Continuing to improve our understanding of the characteristics of the flow and pollutant dispersion near sources influenced by building wakes is crucial for the development of improved parametrizations in these models.

Recently, a wind tunnel study (Perry et al., 2016) was conducted at the United States Environmental Protection Agency (U.S. EPA) to specifically examine the influence of elongated rectangular buildings on the near-field dispersion of pollutants downwind of neutrally-buoyant pollutant releases. Four parameters were examined: building aspect ratio, source stack height, source location with respect to the building, and building angle with respect to the incident wind. These experimental scenarios both complement and enhance historical wind tunnel data related to building downwash. The results of Perry et al. (2016) suggest that wind direction has a strong influence on both the location and magnitude of maximum ground-level concentrations (GLCs). Specifically, the asymmetry of the building-induced wake for obtuse angles skews the lateral plume distribution and enhances the

descent of plume material to the surface. Wind angle effects were particularly significant for sources located on the corner of a building. For the range of buildings studied, they also found that building wake influences on GLCs diminishes rapidly for stack heights above twice the building height. Finally, the wind tunnel results were used to demonstrate some inadequacies of the AERMOD model in simulating some of these wind-angle and stack location effects.

Despite being a critical basis for developing near-field pollutant dispersion algorithms, wind-tunnel studies can be somewhat constrained by the required time and expense, resulting in limited scenarios studied as well as limited spatial coverage of flow and concentration data. It is important to note that in these extremely complex flow situations, understanding the complete velocity, turbulence, and concentration fields around a building is important for adequate dispersion model development. The relative low cost and availability of a detailed and continuous set of data, make computational fluid dynamics (CFD) an important complementary tool for investigating near-field pollutant dispersion. This is evident from the increasing number of CFD simulation studies in this field in recent years (see Tominaga and Stathopoulos (2013) for a review). Most of these previous CFD studies have been carried out employing the steady Reynolds-averaged Navier-Stokes (RANS) equations with two-equation turbulence models (Li et al., 1997; Tominaga and Stathopoulos, 2009; Tominaga and Stathopoulos, 2017). Although the RANS simulations were generally able to predict the gross flow and concentration behavior, they fail to correctly describe the anisotropic and unsteady nature of the problem, which is manifested in the significant underestimation of the lateral plume spread (Tominaga and Stathopoulos, 2009). Therefore, scale-resolving methods including large eddy simulation (LES) and hybrid RANS/LES, which directly resolve (to some extent) the more influential, energy carrying eddies and models only the small (subgrid) scales, have been used and promising results were obtained (Tominaga and Stathopoulos, 2010; Gousseau et al., 2011; Jadidi et al., 2016a). Nevertheless, these studies are generally limited to cubical buildings perpendicular to the wind direction (Tominaga and Stathopoulos, 2010; Jadidi et al., 2016a), thus not addressing the complexities arising in the case of an elongated/rotated building.

The objective of the present paper is to employ a scale-resolving turbulence model, namely the embedded LES (ELES), to study near-field pollutant dispersion around elongated/rotated buildings. It includes the evaluation of the ELES performance against wind tunnel measurements, as well as the analysis of the computational results for various source-building geometries while emphasizing the aspects important for dispersion modeling.

2. Description of Test Cases

The CFD simulations are designed to match six cases examined in the wind tunnel study of Perry et al. (2016). While Perry et al. (2016) examined a range of building aspect ratios, source heights and locations, and wind angles, a smaller subset of the cases available are the focus of the present study (Table 1). Four of the cases selected employed two building aspect ratios, $L:W:H = 1:2:1$ and $1:8:1$ (where L = streamwise length, W = cross-stream width, and H = height = 150 mm), each oriented perpendicular (0°) and 45° to the approach flow. For these four cases, the source is located at the middle of the downwind face (DM0) of the

building with a stack height of $1.5H$ (see Fig. 1). Two additional cases include a 1:2:1 building oriented perpendicular to the wind with a source located at the downwind corner of the building (DC+) with stack height of $1.5H$, and at the downwind middle (DM0) with stack height of $1.2H$. Table 1 summarizes the configurations of these six cases. Each case is defined by four variables: building aspect ratio, wind direction, stack height, and stack location. For example, case D (8-45-1.5-DM0) includes a 1:8:1 building rotated 45° with a stack height of $1.5H$ located at downwind middle (DM0).

A 1:150 scale was used for the wind tunnel study (Perry et al., 2016) which makes the full scale equivalent building height equal to 22.5 m. A tracer source consisting of a 7-mm diameter porous plastic ball was at the edge of the building at elevations of $1.5H$ and $1.2H$. The approach boundary layer developed for this study was designed to simulate flow in a typical suburban area with the use of Irwin spires (Irwin, 1981) and a series of roughness tabs arrayed on the floor of the wind tunnel. The tabs (38 mm high, 76 mm wide, and 1 mm thick) were spaced 305 mm both laterally and longitudinally, with each row offset laterally by half the tab spacing to provide a staggered pattern to condition and maintain the boundary layer throughout the test section. The resulting boundary layer had a full-scale equivalent roughness length of 0.36 m, displacement height of 0 m, and a friction velocity of 0.25 m s^{-1} . The wind speed at building height (U_0) was maintained at 2.77 m s^{-1} in the tunnel. This wind speed along with a building height of 150 mm provides a sufficiently high Reynolds number (27,700) for Reynolds number independence. The wind tunnel results represent all wind speeds that result in neutral atmospheric conditions.

Velocity and turbulence profiles were measured in the study using Laser Doppler Velocimetry. Rosemount Model 400A hydrocarbon analyzers (flame ionization detectors) were used to process samples of tracer gas released from the source and measured throughout the tunnel. To compute the velocity and concentration results, signals were sampled at 20 Hz over 120 s intervals. Results of the wind tunnel data, as well as the CFD model, are presented in normalized concentration units $\chi = C/C_0$ with $C_0 = \frac{Q}{H^2 U_0}$, where C

is the background-adjusted concentration (g m^{-3}), U_0 is the reference wind (m s^{-1}), and Q is the tracer gas emissions rate (g s^{-1}). To account for residual tracer concentrations in the wind tunnel lab, at the beginning and end of each measured profile the background was sampled and the measurements adjusted. In addition, at the beginning of each measurement day, the hydrocarbon analyzers were calibrated against a range of standardized gases. The uncertainty of the measurements of mean concentration field were estimated to be 5% (Perry et al., 2016). A full description of the wind tunnel study and associated findings can be found in Perry et al. (2016).

3. Computational Methodology

The CFD simulation consists of numerically solving the transport equations of mass (concentration) and momentum in a computational domain with predefined initial/boundary conditions. The fluctuating turbulent motions in the flow contribute significantly to the transport of mass and momentum, and hence, need to be addressed in the simulation.

3.1. The embedded LES (ELES)

The principal difficulty in computing turbulent flows resides in the dominance of non-linear effects and the continuous and wide spectrum of observed scales. In the direct numerical simulation (DNS) approach, no extra model is applied so that motions of all sizes have to be resolved numerically by a grid which is sufficiently fine (Pope, 2000). Hence, the computational requirements increase rapidly with the Reynolds number. The storage capacity and speed of present-day computers are still not sufficient to allow a DNS solution for practically relevant turbulent flows such as those around buildings. An alternative approach is to average or filter (for RANS or LES, respectively) the governing equations and to solve for the averaged/filtered velocity, pressure, and concentration fields. By averaging or filtering the governing equations, flow characteristics of some of the length scales of the flow need not be computed (instead they are modeled, depending on which type of modeling is used), and in general a much coarser grid spacing can be used.

Applying a low-pass filter to and ensemble averaging of the governing equations result in the LES and the RANS equations, respectively. Using a combined notation, these equations can be written as:

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0 \quad (1)$$

$$\frac{\partial \bar{u}_i}{\partial t} + \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left[\nu \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \tau_{ij}^{\text{model}} \right] \quad (2)$$

$$\frac{\partial \bar{c}}{\partial t} + \bar{u}_j \frac{\partial \bar{c}}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\alpha \frac{\partial \bar{c}}{\partial x_j} - q_j^{\text{model}} \right] \quad (3)$$

where $\bar{u}_i$, $\bar{p}$, and $\bar{c}$ are filtered (averaged) velocity, pressure, and concentration for the LES (RANS) set of equations, respectively. Last terms in Eq. (2) and (3) are known as the Reynolds stress tensor and the turbulent scalar flux vector for RANS, and the subgrid scale (SGS) stress tensor and the SGS scalar flux vector for LES, respectively. These terms that appear as a result of filtering or averaging need to be modeled.

From a mathematical point of view, the LES and RANS equation are identical with the exception of the form of these terms. This gives rise to the interest to develop a new generation of turbulence models called hybrid RANS/LES. The hybrid RANS/LES methods aim at combining the best of RANS (e.g., lower computational cost) and LES (e.g., resolving the unsteady, large-scale motions) turbulence models. Full realization of the potential of the hybrid RANS/LES approach requires that LES be used in regions of the flow to capture the physics the RANS model cannot, and RANS be used everywhere else for

computational efficiency. The transition between LES and RANS solutions can be continuous or discontinuous in space, leading to two main classes of hybrid RANS/LES methods, namely “global” and “zonal” hybrid RANS/LES approaches (Sagaut et al., 2013).

The global hybrid methods, e.g. detached eddy simulation (DES) (Spalart, 2009), rely on a single set of model equations, and a continuous treatment of the flow variables at the RANS/LES interface. They switch automatically from one method to another based on the physical and numerical (grid size) scales of the problem. The switch from RANS to LES mode in the global hybrid methods does not imply an instantaneous change in the numerical resolution. Therefore, according to Sagaut et al. (2013), *“these methods introduce a ‘grey-area’ in which the solution is neither ‘pure RANS’ nor ‘pure LES’.”*

As stated by Sagaut et al. (2013), *“The use of pre-defined ‘pure’ RANS and ‘pure’ LES zones in which classical RANS and LES models are utilized may alleviate this ‘grey-area’ problem. Zonal hybrid methods are therefore based on a purely discontinuous treatment of the RANS/LES interface.”* The coupling between RANS and LES solutions is challenging since the RANS solution does not provide any turbulent fluctuations that can be used to feed to the LES solution. In many cases, additional modeling to bridge the gap between the two methods is required. The RANS/LES interface can be in various forms. In the wall-modeled LES (WMLES) (Piomelli and Balaras, 2002), the inner part of the boundary layer is treated using a RANS model and the rest of the flow is solved using LES. Another common configuration for the RANS/LES interface is when an LES region is located downstream of a RANS region. Finally, the most general problem concerns the case where a local LES simulation is embedded into a global RANS simulation (Sagaut et al., 2013).

Considering the characteristics of the flow and pollutant dispersion around buildings (highly unsteady wakes, downwash effects, recirculation regions, and corner vortices at the vicinity of the building and a relatively steady flow upstream and far downstream), the embedded LES (ELES) seems to be an attractive choice balancing the computational accuracy and efficiency. It has been used to study complex turbulent flows including those around the Ahmed body (a simplified vehicle geometry) (Mathey et al., 2005), a hump (Davidson and Peng, 2013), and a cubical building (Jadidi et al., 2016a). Jadidi et al. (2016a) investigated the performance of ELES in comparison with LES in simulating the pollutant dispersion around a cubical building. They concluded that ELES provides comparable results with those of LES with almost 50% lower computational costs (Their LES and ELES simulations took 310 and 158 hours wall-clock time to complete, respectively, using 16 processors).

In the present ELES simulations, we use the two-equation Shear Stress Transport (SST) $k-\omega$ model in the RANS region:

$$\tau_{ij}^{\text{model}} = \tau_{ij}^{\text{RANS}} = -\nu_t \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \frac{2}{3} k \delta_{ij} \quad (4)$$

$$q_{ij}^{\text{model}} = q_j^{\text{RANS}} = - \frac{\nu_t}{Sc_t} \frac{\partial \bar{c}}{\partial x_j} \quad (5)$$

where ν_t is the turbulent eddy viscosity, k is the turbulent kinetic energy, and $Sc_t=0.7$ is the turbulent Schmidt number. This value has been chosen in this study based on a series of sensitivity tests confirming previous reports in the literature (Salim et al., 2011; Jadidi et al., 2016a). The eddy viscosity ν_t is obtained by solving two transport equations for the turbulent kinetic energy k and for the specific dissipation rate ω (rate of dissipation per unit of turbulence kinetic energy, often called turbulent frequency). These two equations in the SST k - ω model are obtained by blending the k - ω model near the surface and the k - ϵ model in the outer region, making the SST model a proper choice for wall bounded flows as well as those including stagnation points.

The turbulence closure in the LES region is obtained by using the Wall-Adapting Local Eddy-Viscosity (WALE) model (Nicoud and Ducros, 1999):

$$\tau_{ij}^{\text{model}} = \tau_{ij}^{\text{LES}} = - \nu_{SGS} \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \quad (6)$$

$$q_j^{\text{model}} = q_j^{\text{LES}} = - \frac{\nu_{SGS}}{Sc_{SGS}} \frac{\partial \bar{c}}{\partial x_j} \quad (7)$$

where ν_{SGS} is the subgrid scale eddy viscosity and $Sc_{SGS}=0.7$ is the subgrid scale Schmidt number. The WALE model uses the traceless symmetric part of the square of the velocity gradient tensor to calculate ν_{SGS} , and reproduces the proper scaling at the wall ($\nu_{SGS} = \alpha y^3$). Therefore, it is a suitable choice for wall-bounded flows such as the present problem.

As discussed above, the RANS solution does not provide any turbulent fluctuations that can be used to feed to the LES solution. Therefore, special treatments need to be considered at the interface where the flow leaves the RANS and enters the LES region (RANS-LES interface). Specifically, the RANS-modeled turbulent kinetic energy (TKE) should be converted to the resolved velocity scales. Here, we employ the random 2D vortex method as described in Mathey et al. (2006) to generate a time-dependent, perturbed condition at the RANS-LES interface. In this method, a perturbation is added to the RANS-modeled mean velocity profiles via a fluctuating vorticity field. This vorticity field is 2D in the plane normal to the mean flow direction. In each time step, the vortex positions are given randomly at the interface. The vortices are then given a random rotation sense such that the total TKE of vortices becomes the same as the mean value specified by the TKE profile at the RANS-LES interface. These vortices then induce a fluctuating velocity based on the Biot-Savart law. The use of this method requires the specification of the mean TKE and dissipation rate profiles at the interface, which are available from the RANS solution. At the

LES-RANS interface, where the flow reverts from LES to RANS, the RANS-modeled turbulent quantities are employed.

3.2. Numerical setup

The computational domain, shown in Fig. 1, extends $32H \times 24.67H \times 8.89H$ in the streamwise (x), lateral (y), and vertical (z) directions, respectively. The LES region embedded in this main domain extends $11H$, $6H$ (for 1:2:1) or $12H$ (for 1:8:1), and $3H$ in the x, y, and z directions. These choices are made based on the geometry of the wind tunnel as well as the “Best Practice Guidelines” of Franke et al. (2007, 2011). The profiles of mean velocity and TKE are applied as inlet conditions at the main inflow plane (boundary ① in Fig. 1) located $8H$ upstream of the stack. To obtain these profiles, a separate case of atmospheric boundary layer with no building and periodic boundary conditions at the inlet and outlet was simulated. In that simulation, roughness tabs were physically modeled to match the approach flow of the wind tunnel. The SST $k-\omega$ turbulence model was used to produce the equilibrium profiles of mean velocity and turbulence quantities that agree well with the wind tunnel profiles. These results are then extracted and used as inlet boundary conditions for the main simulations. Figure 2 shows vertical distributions of normalized streamwise velocity and TKE at three sections upstream of the building for case A. Comparison between profiles at $x/H = -8$ (main inlet) and $x/H = -3$ (RANS-LES interface) suggests that the vertical profiles of wind speed were sufficiently maintained leading up to the building. The only wind tunnel measurements upstream of the building were at $x/H = -1.5$, or $0.5 H$ upstream of the building. The simulated velocity at this section is in close agreement with wind tunnel data, capturing reversed flow near ground. Simulations also seem to capture the TKE enhancements in this region although some overpredictions are observed compared to wind tunnel data. The top and side boundaries (② and ③) are far enough from the building such that zero normal velocity and zero normal gradients of all other variables can be used with confidence. Zero static pressure and zero gradient conditions are used at the outflow boundary (boundary ④) located $24H$ downstream of the stack. The no-slip conditions are imposed on the building, stack, and the ground. Nevertheless, the surfaces of the building are defined as “smooth” walls, while the ground (boundary ⑤) is defined as a “rough” wall with an aerodynamic roughness height of $0.0169H$ (no physical roughness tabs were included in the main simulation). The two-layer zonal model for near-wall treatments is used. The vortex method, as described in Sec. 3.1, is used at the RANS-LES interface (boundary ⑥), while no special treatment is used at the LES-RANS interface (boundary ⑦) since the LES solution is already available there.

The domain is discretized with a computational grid, which produces a body-fitted, hex-dominant mesh based on octree decomposition of the domain. The cells around the edges of the building have an average size of $0.028H$, while cells around the source and stack have a much smaller size of $0.0035H$, which corresponds to approximately 36 cells around the equator of the source. This choice of the cell size results in a y^+ value between 5 and 13 for the majority of the building-adjacent cells. Away from the building, the cell size grows gradually to maximum $0.05H$ within the LES region, and then to maximum $0.44H$ in the RANS region. The grid is refined adjacent to the ground with a first cell height of $0.0044H$ and a growth rate of 1.25. Grid-dependency studies are performed for the configuration

associated with case A. Three computational grids, namely, coarse, medium, and fine with 2.19×10^6 , 3.28×10^6 , and 5.48×10^6 computational cells are employed to simulate case A. The concentration results are compared with wind tunnel measurements at various vertical, lateral, and streamwise sampling lines. The medium grid produced better agreement with wind tunnel data over the coarse grid, while the fine grid did not lead to significant improvement (less than 4%) over the medium grid. Therefore, the medium grid, shown in Fig. 3, is chosen as the final grid resolution. The total cell numbers for each of the six cases are given in Table 1.

Unsteady ELES simulations, initialized by converged steady RANS SST $k-\omega$ simulation results, are carried out in ANSYS-FLUENT 15.0. The time step size was chosen based on the general rule of ensuring the Courant-Friedrichs-Lewy (CFL) number to be less than 1.0. Four time step sizes were tested: $t^* = 0.02462$, 0.01231 , 0.00615 , and 0.00307 , where $t^* = U_0 \Delta t / H$. No continued improvement (less than 6% change in concentration results) was observed after refining t^* from 0.00615 to 0.00307 , therefore, 0.00615 is chosen as the final time step size in the present simulations. The mean flow and concentration fields are obtained by averaging the unsteady results over more than 15 through-flow times (the time required by the mean flow to pass through the domain once) corresponding to 100,000 time steps, after allowing an additional 20,000 time steps for spin-up time during the initial transient period. At each time step, the solution is considered to be converged when the residuals are lowered by two orders of magnitude, which usually takes 5-10 subiterations. Simulations are conducted using 512 processors, and typically took 30-60 hours wall-clock time to complete depending on the mesh size.

4. Results and Discussion

4.1. Flow fields

The flow around a building contains various complex aerodynamics features governing the pollutant dispersion. Therefore, it is important to first validate numerical results of the flow fields. Figure 4 shows vertical distributions of normalized streamwise velocity for case A at several centerline sections downstream of the building. It is seen that there is a generally very good agreement (less than 6% average difference and $R^2 = 0.99$) between the ELES results and wind tunnel measurements. Specifically, the vertical expansion of the reverse flow region is well predicted by ELES indicating that the level of mixing is well captured in the near-field region behind the building. A similar conclusion can be drawn by investigating the lateral distributions of normalized streamwise velocity (Fig. 5, top), where the velocity deficit profiles of ELES are in close agreement ($R^2 = 0.99$, 0.95 , and 0.96 at sections $x/H = 0.8$, 2 , and 3 , respectively) with experimental data. The distributions of spanwise velocity (Fig. 5, bottom) clearly show the inward entrainment of the flow associated with horseshoe and wake vortices. As expected, the increased level of mixing reduces the deficit of streamwise velocity and the spanwise entrainment farther downstream.

The vertical profiles of TKE are plotted in Fig. 6 at the same sections as Fig. 4. The local maximum near the ground is the result of high velocity gradients due to no-slip conditions, while a larger peak in TKE is seen away from the ground indicating the existence of a strong shear layer at the interface between the main flow and the recirculation region. The present

ELES simulations show good performance in capturing the location of and the extent of TKE production in this shear layer, although some overpredictions (as much as 35% at $x/H=3$) are seen at the further downstream sections. This is important for simulations of pollutant dispersion since it has been pointed out that the positions of ‘shear layers’ and ‘dividing streamlines’ largely control the patterns of mixing and transport in urban areas (Belcher, 2005).

4.2. Concentration fields

Vertical distributions of normalized concentration at two sections located 3 and 10 times the building height downstream of the stack are plotted in Fig. 7. The ELES results for cases A to F are compared with wind tunnel measurements at each section. In all the cases, pollutant concentrations show a local peak at $x/H=3$ associated with the plume centerline, while more uniform distributions are seen further downstream at $x/H=10$ due to mixing. The time-averaged ELES results agree fairly well with the experiments for all cases (R^2 in the range of 0.87 to 0.98). Specifically, the downward shifting of the plume centerline due to the building (downwash effect) is captured by ELES, where the location of the local maximum concentration is predicted in close agreement with data. Nevertheless, the level of local maximum concentration is generally underpredicted at $x/H = 3$. The largest deviation (as much as 37%) between ELES and wind tunnel data is seen for cases C and D (1:8:1 building) where a considerably larger backflow region and stronger vertical structures form behind the building. Near-ground ($z/H = 0.05$) lateral profiles of normalized concentrations from ELES and wind tunnel measurements at the same two streamwise locations ($x/H = 3$ and 10) are depicted in Fig. 8 (note that lateral profile wind tunnel measurements were not available for the case F). The ELES model is able to predict the lateral expansion of the plume, which is usually hard to simulate using RANS turbulence models with the gradient diffusion hypothesis (Gousseau et al., 2011). It should be noted, however, that the subgrid scale turbulent transport of concentration is still treated using the gradient diffusion hypothesis with a constant Sc_{SGS} . The deviations between ELES and wind tunnel data for concentration field in Fig. 7 and 8 may be attributed to this limitation of the present simulations, especially since the flow field predictions are in great agreement with data. Jadidi et al. (2016b) investigated Sc_{SGS} for a cubical building and showed that it may vary as much as fivefold within the domain. One approach to overcome this limitation is to use a dynamic Sc_{SGS} , which, in turn, increases the computational costs (~15% in the case studied by Jadidi et al. (2016b)).

In the context of exposure, the GLCs are most important and dispersion models are shown to considerably both underpredict (Perry et al., 2016) and overpredict (Schulman and DesAutels, 2013) GLC values for elongated buildings. Fig. 9 compares streamwise variations of near-ground ($z/H = 0.05$) concentrations obtained from ELES simulations with those from wind tunnel measurements (when available). The maximum GLC is associated with the location where the plume centerline reaches the ground. The ELES model results calculate the location and the magnitude of maximum concentration with fairly good agreement with wind tunnel data (average deviations of around 11%, 28%, 14%, 4%, and 8% for cases A, B, C, E, and F, respectively) indicating that building downwash effects are being well captured. For case B, with an acute wind angle, the concentration peak is

predicted to be closer to the building, while results are in better agreement under the perpendicular wind.

The evaluation and comparisons with wind tunnel data presented above show that the ELES can provide reliable results of flow and pollutant concentrations around elongated isolated buildings (at least for controlled flow conditions). Therefore, in the rest of the paper, we focus on using the ELES as a tool to investigate the characteristics of the source-building geometry. These investigations are based on the comparisons between the six cases in Table 1 for which the concentration profiles are presented in Figs. 7–9. In addition, the non-dimensional advective and turbulent concentration fluxes overlaid with the mean concentrations are depicted in Figs. 10 and 11 for all six cases. The advective and turbulent concentration fluxes represent the transport of pollutant concentrations by the mean flow and its fluctuations, respectively. In the present ELES simulations, the advective and turbulent concentration flux vectors are calculated based on the resolved LES fields:

$$q_{a,i} = \bar{u}_i \bar{c} \quad (8)$$

$$q_{t,i} = u'_i \bar{c}' \quad (9)$$

where $\bar{u}$ is the mean velocity vector, $\bar{c}$ is the mean concentration, u'_j is the fluctuating velocity vector, and c' is the fluctuating concentration. These two flux vectors are normalized by $U_0 C_0$ in Figs. 10 and 11. Comparisons between advective and turbulent concentration fluxes reveal interesting information about the mechanism of the plume spread. The advective flux vectors tend to move the bulk of the plume in each direction. For instance, it is seen that the emitted pollutant is mainly advected downstream by streamwise advective flux $\bar{u} \bar{c}$, while vertical advective flux $\bar{w} \bar{c}$ pushes the plume downward closer to the ground. In contrast, the turbulent fluxes, whose values are most significant at the boundaries of the plume, tend to expand the plume in each direction. As seen in Fig. 11, all three components of $q_{t,i}$ have opposite signs at the edge of the plume, indicating that the plume is being expanded by these components.

Furthermore, Fig. 12 illustrates the isosurfaces of the mean normalized concentrations representing the time-averaged shape of the plume, and the isosurfaces of Q (colored by the instantaneous concentrations) representing instantaneous coherent vortical structures around the building. Q , defined by $-\frac{1}{2}(S_{ij}S_{ij} - \Omega_{ij}\Omega_{ij})$, quantifies the local balance between shear strain rate S_{ij} and vorticity Ω_{ij} magnitude and its positive values corresponds to regions of the flow where rotation dominates strain rate.

Together, Figs. 7–12 give a comprehensive picture of the effect of building aspect ratio, wind direction, stack height, and stack location on pollutant distributions around elongated buildings. As expected, both vertical and lateral plume spreads increase for the 1:8:1 building due to a larger wake region forming behind it (compare Fig. 7A to 7C, Fig. 8A to

8C, and Fig. 12A to 12C). This subsequently shifts the GLC peak closer to the building as shown in Figs. 9A and 9C. Comparing streamwise advective fluxes in Figs. 10A and 10C shows a significantly larger recirculation region (where $\bar{u}\bar{c} < 0$) behind the 1:8:1 building, and comparison between spanwise components indicates a considerably larger lateral expansion. Turbulent fluxes on the planes shown in Fig. 11 are somewhat stronger for case A (1:2:1 building) due to being closer to the side edge of the building where vortical structures are generated (see the right column in Fig. 12). Nevertheless, it seems that the concentration pattern is mainly dictated by advective fluxes in these cases.

As shown in Fig. 12, an acute wind angle results in plume shifting, which is more significant for a higher aspect ratio (cf. case A with B and C with D) due to a larger recirculation region. Combined with the effect of mixing, this results in a widespread plume further downstream of the rotated 1:8:1 building (see Fig. 8D at $x/H = 10$). Furthermore, vertical advective concentration flux is much larger for a rotated building (cf. case A with B and C with D in Fig. 10) pushing the plume downward to a greater degree, which consequently results in higher GLCs for the rotated building (cf. Fig. 9A and 9B).

Comparisons between cases A and E illustrate the effect of source location on pollutant dispersion. When the source is moved to the downwind corner (point DC+ in Fig. 1), the plume is only partially affected by building downwash. Therefore, much lower GLCs are seen close to the building ($x/H < 3$) as shown in Figs. 8E and 9E. In addition, as depicted in Figs. 8E and 12E, the plume is slightly shifted towards the wake region where the pressure is lower. Similar observations can be made in Fig. 10, where streamwise advective fluxes have higher values for case A near the ground, while spanwise advective fluxes are considerably more negative (higher in magnitude) for case E indicating the tendency to shift the plume behind the building.

Finally, the effect of stack height is investigated comparing cases A and F. As shown in Fig. 7–9, a shorter stack results in considerably higher pollutant concentrations (by more than a factor of two) close to the building ($x/H < 5$). The pollutant is more affected by the building-generated turbulence in case F as indicated by Fig. 10 and 11. Note that the flow field is almost the same in cases A and F (flow disturbances due to the stack are negligible compared to those of the building). However, as shown in Fig. 10F, more pollution reaches the recirculating region behind the building, resulting in higher advective flux and more influence on the final concentration field.

5. The Path Forward

The dispersion processes in AERMOD and other Gaussian plume models are highly parameterized to account for the complex dynamics of plume dispersion around buildings described in the preceding section. Wind tunnel studies have been a major source of information from which to understand these physical processes and to develop dispersion model parameterizations (Schulman et al., 2000; Robins et al., 1997). High fidelity, scale-resolving CFD, supported by wind tunnel data as presented in this work, provides a means to examine these physical processes in greater detail and to improve Gaussian plume models' (e.g. AERMOD) ability to accurately model complex building downwash scenarios. We

have documented our effort in this context in an accompanying manuscript recently published (Monbureau et al., 2018). With comprehensive velocity and concentration fields, an examination of plume growth, plume trajectory, and the pollutant fluxes between various flow regions is possible to a degree not feasible with wind tunnel measurements alone. In addition, the ELES databases developed here allow for close examination of the partitioning plume mass between main plume and the portion entrained into the recirculation region downwind of the building, the average transport speeds for plumes, and the lateral motions induced when winds approach buildings at oblique angles. This expanded understanding of important parameterizations is possible over a range of conditions including building geometry, stack height and location, and wind direction. In order to fulfil these ultimate goals, limitations of this work including being restricted to isolated rectangular buildings, stack being attached to the building, and neutral atmospheric conditions should be addressed in future studies.

6. Conclusions

The performance of ELES in modeling the near-field pollutant dispersion around elongated buildings is examined. Simulations are compared with available wind tunnel measurements for six test cases, where four parameters are studied: building aspect ratio (2 and 8), source stack height (1.5 and 1.2 times the height of the building), source location with respect to the building (downwind middle and downwind corner), and building angle with respect to the wind (0° and 45°). In addition, an analysis of the pollutant transport in the turbulent flow field behind a building is presented and cases are compared within this context.

It is shown that ELES is able to model the complex flow and concentration fields reasonably well for all cases. Although some overestimation of TKE is observed, the mean flow field (streamwise and spanwise velocities) is simulated with very good agreement with experimental data. The time-averaged ELES concentration fields represent wind tunnel data fairly well. Nevertheless, utilizing gradient diffusion hypothesis (and a constant subgrid scale Schmidt number) is one limitation of the present simulations that may affect concentration results. Several important and complex phenomena such as recirculation region, inward entrainment of the flow, shear layer between the wake region and the main flow, enhanced lateral dispersion with the width of the building, asymmetry of the wake and the associated skewness of the plume for a rotated building, and enhanced entrainment of the plume into the wake for lower source heights are all well captured by the present ELES model. Through detailed analysis of velocities, concentrations, and advective/turbulent concentration fluxes, we showed how the changes in building aspect ratio, source stack height, and wind angle affect ground-level concentration that is the most important factor from the exposure and human health point of view.

Future research will focus on using this CFD-based “virtual test-rig” constrained by wind tunnel data (see Perry et al., 2016) to examine the building downwash phenomena for a much greater variety of building shapes, stack heights, and locations. Ultimately, the data from these simulations, along with relevant data from the previous and current wind-tunnel measurements, will be used to thoroughly analyze the flow and dispersion around buildings and to help develop improved parametrizations (see Monbureau et al., 2018).

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Figure 1.

Schematic diagram ((A) top view (B) side view) showing the building orientation and decomposition of the computational domain for ELES, and cross sections, where experimental data are presented in this paper: (C) vertical cross sections (Figures 2, 4, 6, and 7) (D) lateral cross sections (Figures 5, 8).

Figure 2.

Vertical profiles of normalized streamwise velocity (left) and turbulent kinetic energy (right) upstream of the building at $y/H=0$ plane for case A.

Figure 3.
Computational grid on a vertical plane at $y/H=0$ for case A; the whole domain (left) and mesh details near the stack and source (right).

Figure 4.

Vertical distributions of normalized mean streamwise velocity at $y/H=0$ (see Fig. 1C) plane for case A (line: model results; dots: wind tunnel measurements).

Figure 5.

Lateral distributions of normalized mean streamwise (top) and spanwise (bottom) velocities at $z/H = 0.5$ (see Fig. 1D) plane for case A (line: model results; dots: wind tunnel measurements).

Figure 6.

Vertical distributions of normalized turbulent kinetic energy at $y/H=0$ (see Fig. 1C) plane for case A (line: model results; dots: wind tunnel measurements).

Figure 7.

Vertical distributions of normalized pollutant concentration ($\chi = C/C_0$ and $C_0 = QH^{-2}U_0^{-1}$) at $y/H=0$ (see Fig. 1C) plane for cases A to F (line: model results; dots: wind tunnel measurements).

Figure 8.

Lateral distributions of ground-level ($z/H=0.05$; see Fig. 1D) normalized pollutant concentration for cases A to F (line: model results; dots: wind tunnel measurements).

Figure 9. Streamwise distributions of ground-level ($z/H=0.05$ and $y/H=0$) normalized pollutant concentration for cases A to F (line: model results; dots: wind tunnel measurements).

Figure 10.

Streamwise (left), vertical (center), and spanwise (right) normalized advective fluxes overlaid by contour lines of normalized mean concentrations at 0.5, 1.0, and 5.0. For each case, streamwise and vertical fluxes are plotted in $y/H=0$ plane and spanwise fluxes are plotted in $z/H=1.0$ plane.

Figure 11.

Streamwise (left), vertical (center), and spanwise (right) normalized turbulent fluxes overlaid by contour lines of normalized mean concentrations at 0.5, 1.0, and 5.0. For each case, streamwise and vertical fluxes are plotted in $y/H=0$ plane and spanwise fluxes are plotted in $z/H=1.0$ plane.

Figure 12.

Isosurfaces of normalized mean concentrations (at $\chi=0.2$) representing the average plume shape (left), and isosurfaces of $Q=0.5$ colored by instantaneous concentrations representing the coherent vortical structures and their interactions with pollutant concentrations (right).

Table 1

Test case configurations and the number of computational cells for each case

Case	Configurations (aspect ratio-wind direction-stack height-stack location)	LES zone cell count ($\times 10^6$)	RANS zone cell count ($\times 10^6$)
A	2-00-1.5-DM0	1.60	1.68
B	2-45-1.5-DM0	2.07	1.74
C	8-00-1.5-DM0	3.05	1.88
D	8-45-1.5-DM0	3.62	1.95
E	2-00-1.5-DC+	1.87	1.71
F	2-00-1.2-DM0	1.55	1.68