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Simulation of near-field dispersion of pollutants using detached-eddy simulation ☆

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ABSTRACT

A numerical simulation is developed using the unsteady-state turbulence model on a structured highly refined grid to predict the wind-flow field and dispersion field of a pollutant emitted from a rooftop stack around a two-building configuration. The results obtained are compared with those of a steady-state model previously reported by the authors. The pollutant concentrations are examined on the roof where the stack is located as well as on the leeward wall of an upstream tower to the emitting building in order to evaluate how the pollutant is dispersed by the DES model compared to RNG model. DES results are discussed against those from RNG k–ε approach and wind tunnel. The study emphasises limits in reproducing correctly the wind flow and dispersion fields due to underestimation and/or overestimation of the Reynolds stress components and the steady-state methodology when using the RNG k–ε model. Despite such limits, the RNG model produces a similar average error, in terms of concentrations, to that obtained with the DES model.

1. Introduction

Pollution in the atmospheric boundary layer (ABL) is an important environmental problem which affects human health. Investigations of pollutant transport and dispersion have received a lot of attention in recent years, and become a focal point in environmental research because of the increasing interest for protecting the air quality [1]. Besides, this subject is of great concern especially in the urban environment when the crucial issue of well-being and human comfort are considered.

Turbulent wind flows have long presented a considerable obstacle to the accuracy and applicability of calculations in industrial applications [2]. The types of flows encountered in the field of wind engineering are no exception, and consist of many complex flow features which may contain recirculation zones and stagnation points [3]. Indeed, in the lower atmospheric boundary layer, specifically in cities around individual and/or groups of buildings, the superposition and interaction of the flow patterns induced by the buildings and the structures strongly affect the dispersion and govern the movement of pollutants [4]. Therefore, complicated and highly unpredictable dispersion phenomena are created. Clearly, understanding the process of pollution dispersion characteristics and its mechanisms still remains a great challenge for wind engineering researchers. Nonetheless, the scientific community has significantly contributed to daily life quality by controlling and maintaining air quality in buildings and offices within the acceptable norms typically established and authorised by governments and/or professional organizations [5].

Substantial research projects have been carried out and are available in the literature on the topic of pollutant dispersion. They have used a wide range of different methods (e.g. field tests, laboratory modelling, semi-empirical methods and numerical approaches) to evaluate the pollutant dispersion, identifying their advantages and disadvantages [6]. During the past years, especially in urban environment, pollutant dispersion has been studied extensively by means of both experimental and numerical approaches. Field measurements (e.g. [7,8]), wind tunnel testing (e.g. [9–13]), semi-empirical methods (e.g. [14,15]) and numerical modelling (e.g. [16–20]) have been performed, on the one hand, to get an insight into the complicated physical pollution processes, and on the other hand, to obtain a better comprehension of the coupled mechanisms occurring around buildings and/or cluster of buildings. Among these methods, numerical modelling with computational fluid dynamics (CFD) appears as one of the most accessible and largely spread approach to study the wind environmental problems because of the lower cost, the advantages and reliability of such approach.

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However, CFD simulations are not straightforward to perform and their results still require validation to establish extended acceptability [21]. Therefore, the need of validating numerical studies makes the experimental tests necessary.

Notwithstanding the widespread use of CFD studies, the quality of results depends mainly on many physical and numerical parameters which can compromise accuracy and reliability. From that point of view, many authors and organizations have developed practice guidelines (e.g. [22–30]) to establish a common methodology for verification and validation of CFD simulations in certain cases, and/or to assist and support the users in making a better implementation of CFD in other cases. In addition to the fundamental error of selecting an inappropriate physical model to simulate a flow field (i.e. steady or unsteady approach), there are basically two types of difficulties that can produce erroneous results in CFD [30]: (i) modelling errors (e.g. turbulence models and physical boundary conditions) and (ii) numerical approximation errors (e.g. grid design, discretization scheme and iterative convergence).

Regarding turbulence modelling errors, various turbulence models (i.e. steady Reynolds-averaged Navier–Stokes (RANS), unsteady RANS (URANS), large-eddy simulation (LES) and hybrid URANS/LES) reported in the literature are well known to the computational wind engineering (CWE) community, as they have been listed by many authors (e.g. [27,6]). Several studies have investigated and assessed the performance of such different turbulence models to predict the flow field around buildings (e.g. [31,32]). However all studies agree on the difficulty of some models and the differences between the various approaches to reproduce the complex and random character of the flow field. In addition, the dispersion field is closely related to the overall behaviour of the wind flow as stated by Tominaga and Stathopoulos [33]. Therefore, the choice of the turbulence model is revealed crucial to reproduce an accurate dispersion process, and, consequently, essential to understand the pollutant transport mechanisms.

The present study follows previous work of Lateb et al. [34] where various RANS k–ε turbulence models were compared (i.e. standard k–ε, re-normalised group k–ε and realisable k–ε referred as SKE, RNG and RLZ throughout, respectively). Previous work suggested that the limitations in RANS models to reproduce the experimental results are probably due to an incorrect estimation of Reynolds stress components and the steady-state methodology of the tested models. Thus, the purpose of this study is to reproduce the flow and dispersion fields compared to RANS approach using FLUENT software. The detached-eddy simulation (DES) model – referred as the most widely known hybrid URANS/LES by Franke et al. [27] – has been selected for the present study because of the well-established limitations of the two following models in resolving the internally induced fluctuations of flow and concentration fields [35], i.e. the high computational cost of LES and the low accuracy of URANS. For more details about the technique, advantages and applications of the DES approach, the reader can refer to works existing in the literature (e.g. [36–47]).

In this work, one case is considered because of the long time required by DES modelling. Regarding the objectives of this work cited above, the most critical case is selected, namely when the pollutant is emitted at high speed from the stack (i.e. $h_s = 1$ m and $M = 5$ where h_s is the stack height and M the momentum ratio which represents the ratio between the exhaust velocity of the pollutant w_e and the wind velocity U_H at the height of the BE building). Such case induces complex pollutant/flow-field interactions above the stack. Consequently, the capability of the DES model to reproduce the dispersion process is severely tested. It is worth noting that among the various RANS k–ε models tested by Lateb et al. [34], the RNG k–ε model provided the best agreement with the wind tunnel results conducted by Stathopoulos et al. [48] for the current considered case ($h_s = 1$ m and $M = 5$). DES results are thus compared with those from the RNG approach and wind tunnel experiments.

The paper is organised as follows. Section 2 summarises the computational details including the DES concept, the grid generation, the boundary conditions and the solution strategy. Section 3 demonstrates the consistence of both constructed grid and statistical averaging period. The results are described and compared to those of the RNG k–ε model and experimental data in Section 4. The analysis and discussion of results are presented in Section 5. Finally, the main findings of the study are summarised in Section 6.

2. Computational details

2.1. Detached-eddy simulation model

The strategy of DES model is such that switching from URANS to LES models is realised according to mesh definition and not to the local turbulent properties of the flow [49]. Thus the turbulent viscosity obtained depends on the local grid spacing, Δx_i, and the sub-grid scale (SGS) stresses are parameterized using a turbulent viscosity model. The RLZ turbulence model is selected to calculate the turbulent viscosity for both strategies (i.e. as URANS model in boundary layer regions and LES sub-grid scale model in massive separated regions) since the RLZ model is the only model available in FLUENT among the various RANS k–ε models tested by Lateb et al. [34]. In addition to the continuity and momentum equations, two others are added to estimate the turbulent viscosity, ν_t, at each cell. One equation for the turbulent kinetic energy, k, another for the turbulent dissipation rate, ε, and their detailed expressions can be found in work of Lateb et al. [50].

2.2. Grid generation

Since the present research is complementary to Lateb et al. [34] work, the same site is used. Therefore, the reader can refer to that work for more details about the configuration and the dimensions of the two buildings. The main difference in the grid generation of these two studies is the grid refinement required by this unsteady three-dimensional approach particularly in the separated flow regions where the LES model is used. The "wall function" is used as near wall treatment for the present study since it is the only approach available when using the DES model. Basically there are two overlapping layers over walls: an inner layer where viscous processes dominate, and an outer layer far from these effects [18]. The near wall treatment used bridges the viscosity-affected region between the wall and the fully turbulent region; therefore, on the one hand a substantial refinement of grid meshing is saved, and on the other hand the attached boundary layer regions are assured to be modelled by the URANS model.

The proceeding of refining the grid deals with three criteria. The spacing cells, Δx_i, should (i) be fine enough near wall regions to capture the high gradients which occur within the turbulent boundary layer, and to reach the slope $-5/3$, associated with the range of frequencies in which the energy cascade is dominated by the inertial transfer, (ii) be smaller than the turbulence length scales, defined previously as $l_{rke} = k^{3/2}/\varepsilon$, to make sure that the separated flow regions will be treated by the LES approach out of the turbulent boundary layer, and (iii) keep the spacing length perpendicular to each wall at least equal or larger than the two other spacing directions to eliminate the grey zone and thus avoiding a modelled-stress depletion (MSD) defined and noticed by Spalart et al. [51].

Starting from the grid used in Lateb et al. [34] and the results obtained with the steady RLZ model solution, Taylor microscale