

Numerical Simulation of Dispersion in an Urban Street Canyon: Comparison between Steady and Fluctuating Boundary Conditions

S. M. Kwa, S. M. Salim

Abstract— Over the years, the reliance on CFD to investigate air flow and pollutant dispersion has increased significantly and the majority of these studies have employed Steady Wind Boundary Conditions (SWBC) at the inlet of the computational domain. In reality, wind fluctuates both spatially and temporally and the numerical simulations do not accurately represent field or experimental measurements when the inlet condition is assumed to be constant. Therefore, the aim of the current research is to address the limitations of these existing studies, by developing Fluctuating Wind Boundary Conditions (FWBC). The FWBC are then compared to SWBC in order to determine their suitability in the investigation of air flow and pollutant dispersion in urban street canyons. Three-dimensional (3D) numerical simulations are performed using Large Eddy Simulation (LES). The FWBC produces more realistic results when compared to the frequently employed SWBC.

Index Terms—Computational Fluid Dynamics (CFD), Fluctuating Wind Boundary Condition (FWBC), Large Eddy Simulation (LES), pollutant dispersion, urban street canyon

I. INTRODUCTION

AS the world population increases and urbanization sees rapid growth in all regions of the globe, concerns of air quality are of paramount interest given its repercussions on public health [1-3]. Despite substantial advancements in fuel and engine technology to curb car exhaust, the deteriorating air quality in urban areas are still largely dominated by traffic emissions [4]. This decline in outdoor air quality is one of the major contributors for the worsening public's health in urban areas and is more evident in high density cities such as Hong Kong, New York and Tokyo. Largest pollution concentrations occur in street canyons due to low air ventilation where presence of buildings neighboring the street causes pollutant accumulation at pedestrian level. Previous studies have shown that long-term exposure to traffic-generated pollutants is the main factor of various adverse health problems.

The atmospheric boundary layer flow in urban regions is complex; hence appropriate tools are required to

characterize the resulting flow field and accompanying processes such as pollutant dispersion and thermal distribution. Three main approaches are typically used to examine the governing physics of air flow and pollutant dispersion. These are on-site full-scale experiments [5-7], model-scale experiments in the form of wind tunnel investigations [2, 8, 9] and numerical modeling such as Computational Fluid Dynamics (CFD) [10-15].

CFD is rapidly gaining track as tool of choice for investigating fluid problems in a wide array of industries [16, 17] especially with the advent of ever increasing computer resources. Conventional wind tunnel experiments are being substituted by numerical simulations owing to the substantial savings in cost and time, in addition to providing practical solutions to evolving challenges of urban air quality [11, 15, 18]. The emergence of CFD in replacing traditional experimental investigation methods coincides with the setbacks of using the latter method. Full-scale experiments are not only expensive and time-consuming, but are also highly difficult to operate over a large range of variables. Additionally, model-scale experiments are not able to model internal flows appropriately. Despite these setbacks, wind tunnel and field measurements can still and often are used to validate the numerical results from CFD simulations. This validation exercise is an indispensable feature of research and numerous validation studies have been carried out over the years [19-23].

A number of numerical investigations on airflow and pollutant dispersion in urban street canyons have been accomplished and these are well reported in the literature, with many of them based on CFD. Majority of these studies has only considered Steady Wind Boundary Conditions (SWBC) at the inlet [11, 24, 25]. And the drawback of assuming a steady profile is that constant wind velocity and turbulent kinetic energy is defined which is not always consistent with on-site field and wind tunnel measurements [20, 21]. The temporal and spatial variations of the prevailing wind flow introduces further disturbances downstream which is not accurately accounted for when employing a SWBC [26] at the inlet. The instantaneous fluctuation of the wind velocity is greater within the urban street canyon in comparison to the mean recirculation. In many previous CFD studies only the mean wind velocity and the prevailing wind direction (i.e. SWBC) are used to define the wind boundary conditions [25 - 31].

Zhang et al. [26] determined that air flow in an urban street canyon is an unsteady flow due to the real-time upstream wind conditions. Correct representation of the

Manuscript received December 15, 2014.

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atmospheric boundary layer (ABL) flow in the computational domain is therefore important for the purpose of obtaining more realistic predictions of air flow and pollutant dispersion in the realm of urban air quality investigations.

With these in mind, the objective of the present study is to synthesize Fluctuating Wind Boundary Conditions (FWBC) from unsteady simulation and compare it against the conventionally used SWBC to observe the difference in the flow field development and pollutant dispersion process within an urban street canyon. This is an extension to the work presented by Kwa and Salim [32].

Three-dimensional (3D) numerical simulations are performed using Large Eddy Simulation (LES) in ANSYS FLUENT. LES has previously been found to perform better than Reynolds-Averaged Navier-Stokes (RANS) modelling because of its ability to account for the fluctuations in the flow variables. This allows for the transient mixing process to be well captured hence improving the prediction of the pollutant distribution [11, 28, 29]. LES directly resolves the bulk of the energy-containing eddies while the universal small-scale eddies are filtered out and appropriately modelled. On the other hand, RANS turbulence closure schemes define turbulent fluxes based on time-averaging, using Reynolds isotropic decomposition and Boussinesq approximation [40]. Further elaboration on the two different modelling approaches is well defined by Salim et al. [28].

In order to determine the suitable inlet boundary condition, comparisons are made between results from FWBC profile used in the present study and SWBC profiles previously implemented by Salim et al. [11].

It is observed that the FWBC profiles produces much more realistic results better mirroring real behavior of ABL flows with the potential to contribute significantly to the current body of research on air flow and pollutant dispersion in urban street canyons.

II. METHODOLOGY

A. Computational Domain

In a previous study, Salim et al. [11] carried out CFD simulations implementing SWBC and validated against data from wind-tunnel experiments by Gromke and Ruck [35-37]. The current investigation considers the same computational domain to allow for comparison with previous numerical and experimental results. In fluid mechanics investigations, sub-scale models are often used to reduce cost and time associated with full-scale systems. With an isolated street canyon of length $L = 180$ m, street width $W = 18$ m and two flanking buildings of height $H = 18$ m and width $B = 18$ m, the model is scaled by 1:150 similar to the wind tunnel experimental model. The computational domain is discretized using 1.2 million hexahedral elements following the wall y^+ approach [38, 39]. Majority of the mesh elements are positioned within the vicinity of the street canyon and the flanking builds to accommodate a finer resolution in regions where the flow variables vary tremendously.

B. Boundary Conditions

Fig. 1 illustrates the computational domain and implemented boundary conditions for the present study. At the entrance and exit of the domain an inlet and outlet are defined, respectively. Non-slip conditions are applied at the building walls and floors and to impose a parallel flow, symmetry are designated at the upper boundary and sides of the computational domain to impose zero shear slip conditions in the viscous flows [11] to mimic the ABL flow.

The initial simulation is performed using a SWBC profile to replicate the study by Salim et al. [11] and wind tunnel experiment by Gromke and Ruck [35]. The inlet velocity profile is by a power law profile.

$$u(z) = 4.7 \left(\frac{z}{0.12} \right)^{0.3} \quad (1)$$

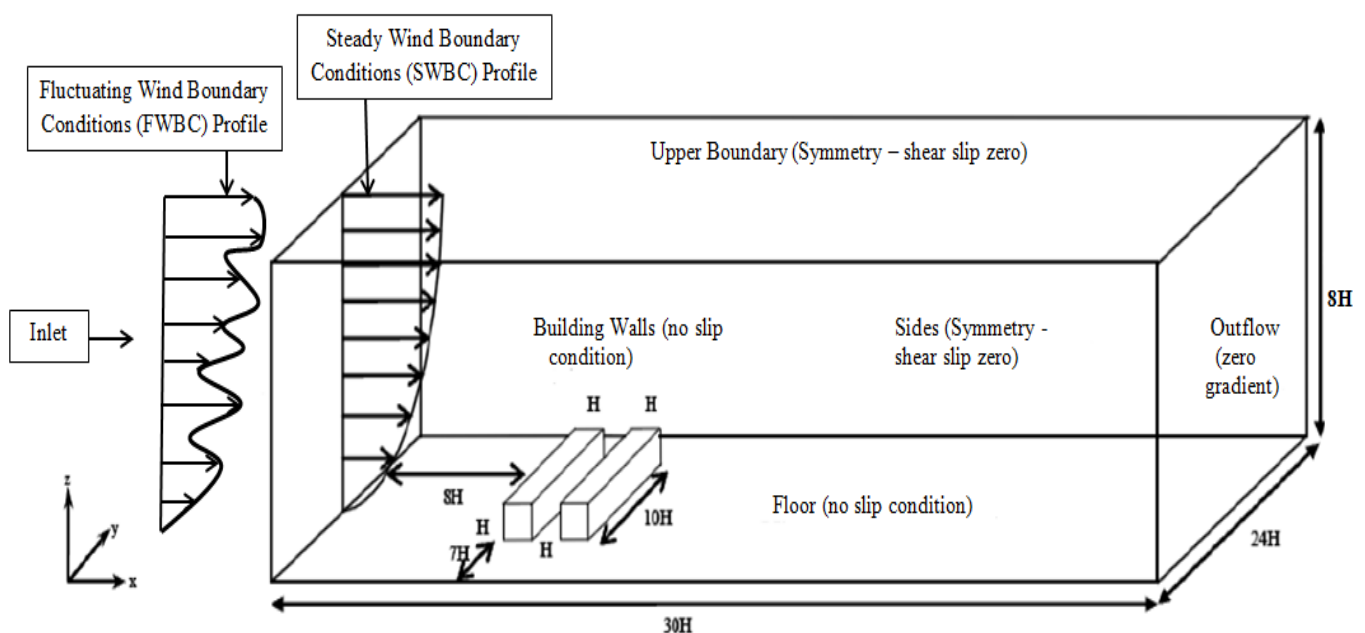


Fig. 1. Computational domain and boundary conditions for CFD simulation setup in ANSYS FLUENT

The turbulent kinetic energy, k and dissipation rate, ε profiles are specified as

$$k = \frac{u_*^2}{\sqrt{C_\mu}} \left(1 - \frac{z}{\delta}\right) \quad (2)$$

and

$$\varepsilon = \frac{u_*^3}{\kappa z} \left(1 - \frac{z}{\delta}\right) \quad (3)$$

with u being the vertical velocity profile, z being the vertical distance, δ being the boundary depth layer (≈ 0.5 m), u_* being the friction velocity ($= 0.54$ m/s), κ being the von Kàrmàn constant ($= 0.4$) and lastly $C_\mu = 0.09$. The similarity between the velocity and turbulent kinetic energy profiles from the simulated user defined functions (UDF) and CODASC are shown in Fig. 2

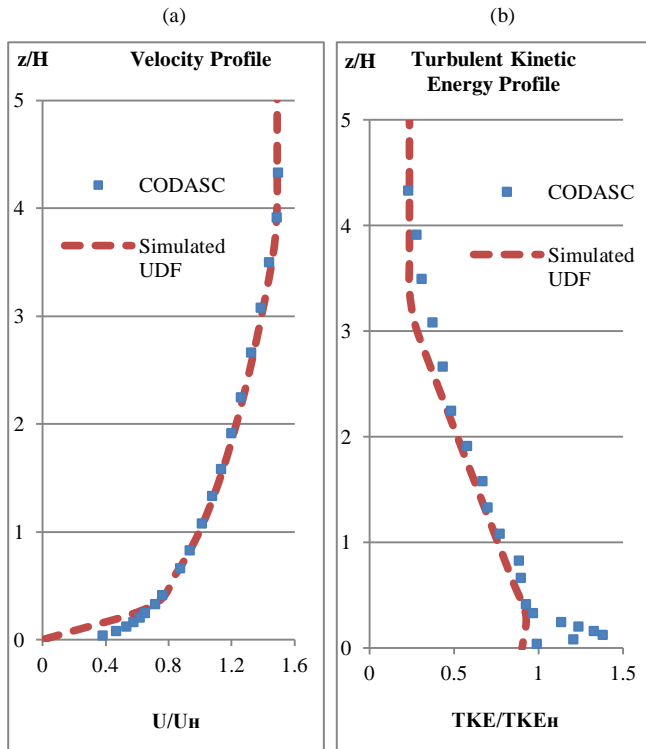


Fig. 2. (a) Velocity and (b) TKE profiles for the inlet boundary conditions showing similarity between CODASC profile [13] and simulated UDF profiles

LES generates fluctuating profiles of flow variables at the outlet. The differences in the velocity profiles generated from the SWBC and FWBC scenarios are illustrated in Fig. 3. It is observed that the flow profiles vary considerably and even the slightest temporal variation results in perceptible changes at the outlet.

Two approaches are tested in the investigations related to the FWBC. The first is through the use of a single fluctuating profile at a specific instant while the second approach involves applying multiple fluctuating profiles in the carrying out the simulation run. These different approaches employed in the study are summarized in Table 1:

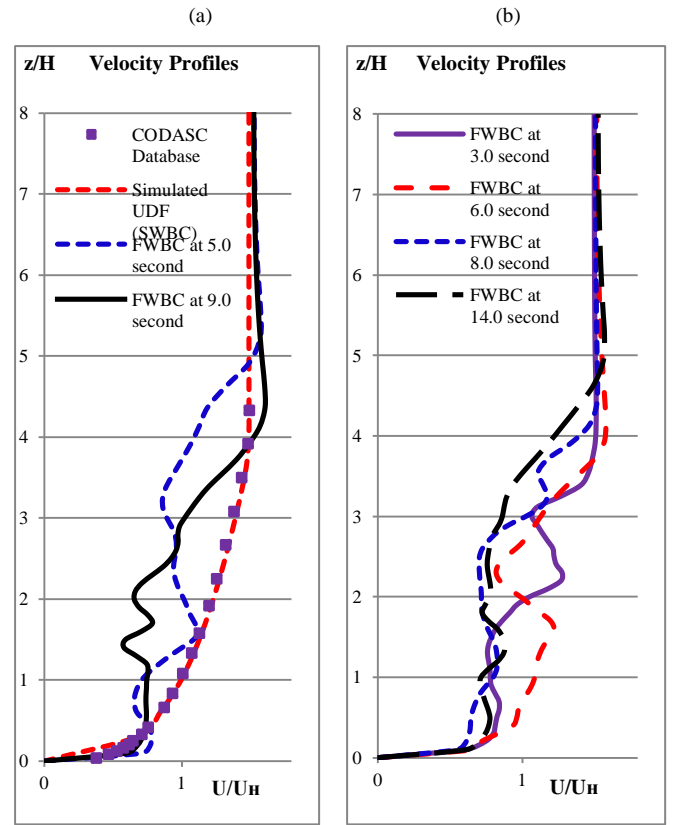


Fig. 3. Velocity profiles based on CODASC database [33], SWBC [11] and FWBC (at outlet)

TABLE 1. FLUCTUATING PROFILES USED IN SIMULATIONS

Simulations	Fluctuating Profiles from Fig. 3
Simulation 1	5.0 second
Simulation 2	9.0 second
	0-10 second flow-time in ANSYS FLUENT = 3.0 second
	10-20 second flow-time = 6.0 second
Simulation 3	20-30 second flow-time = 8.0 second
	30-40 second flow-time = 14.0 second

C. Flow Simulation

In the aforementioned numerical studies, LES has been shown to perform better in simulating turbulent flows for urban air quality studies hence is also employed in the present investigation in order to resolve both temporal and spatial fluctuations. The equations for continuity and momentum are:

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0 \quad (4)$$

and

$$\frac{\partial \bar{u}_i}{\partial t} + \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_j^2} - \frac{\partial \tau_{ij}}{\partial x_j} \quad (5)$$

The dynamic Smagorinsky-Lily sub-grid scale model is used together with 2nd order upwind discretization schemes for species and energy transport equations. This options increases simulation accuracy and reduces numerical diffusion [40]. SIMPLEC and PRESTO! schemes are selected and the scaled residual criteria for all flow

properties are set at 1×10^{-3} . A dimensionless time-step of 0.0025 is used in line with previous studies.

For the single fluctuating profiles simulations, the initial simulation is performed for 6000 time-steps. Upon reaching statistical steady-state, the flow statistics are reset and data sampling initiated. Additional 6000 time-steps are executed bringing the total to 12000 time-steps. This corresponds to approximately 40 flow-through times and a physical time of 30 seconds.

For the multiple fluctuating profiles scenario, each of the four profiles is performed consecutively for 4000 time-steps, totalling to 16000 time-steps. This translates to a physical time of 40 seconds and approximately 52 flow-through times.

D. Dispersion Modeling

Sulphur hexafluoride (SF_6) is used as tracer gas and the emission rate, Q is set at 10 g/s to replicate the study done by Salim et al. [11] and wind tunnel experiment from CODASC [33]. Regions of the pollutant sources are marked in the computational domain as line sources in order to model the traffic exhausts. This is achieved by demarcating sections of the volume in the geometry and defining the encompassing cells as different fluid zones. Their positions are illustrated in Fig. 4.

The advection-diffusion (AD) method is employed for modeling the dispersion of pollutant species. In turbulent flows, this is computed as

$$J = -(\rho D + \frac{\mu_t}{Sc}) \nabla Y \quad (6)$$

where D is the molecular diffusion coefficient for the pollutant in the mixture, μ_t is the turbulent eddy viscosity, Y is the mass fraction of the pollutant, ρ is the mixture density

and Sc is the turbulent Schmidt number.

III. RESULTS AND DISCUSSIONS

The study's aims to determine the change in airflow and pollutant dispersion when the conventionally used SWBC in previous investigations are replaced with the current FWBC generated in this study.

Dispersion and distribution of the pollutants are observed through species concentration contours along the leeward wall (Wall A), windward wall (Wall B) and the mid-plane of the street canyon.

Fig. 5 illustrates the results of mean concentration contours along Wall A and Wall B, comparing simulation data obtained using both FWBC and SWBC and previous WT measurements from CODASC [37]. It can be seen that the SWBC profile produces pollutant concentration distribution similar to WT, particularly in the vicinity of the centerline ($y/H=0$) along both Wall A and Wall B, underlining them as the most critical zone where maximum pollutant concentration occurs. A similar observation was reported by Salim et al. [11].

In the case of using FWBC, the contours differ noticeably from those simulated with the conventional SWBC and measured in the WT experiment. For the results obtained with the 5.0 second fluctuating profile, the pollutant concentrations are more prominent towards the right of the centerline ($y/H \approx 1.5$), whereas results produced by the 9.0 second fluctuating profile are more concerted towards the left of the centerline ($y/H \approx 1.3$). Pollutant concentrations produced in the multiple FWBC profiles case are focused at the region towards the right of the centerline ($y/H \approx 0.6$).

These indicate that the pollutant dispersion in urban street canyon can vary vastly when a FWBC is employed, and the maximum concentration is not necessarily concerted at the centerline as reported in previous studies using SWBC and in WT experiments with steady inlet flow. Therefore, it is important to use real-time meteorological data when

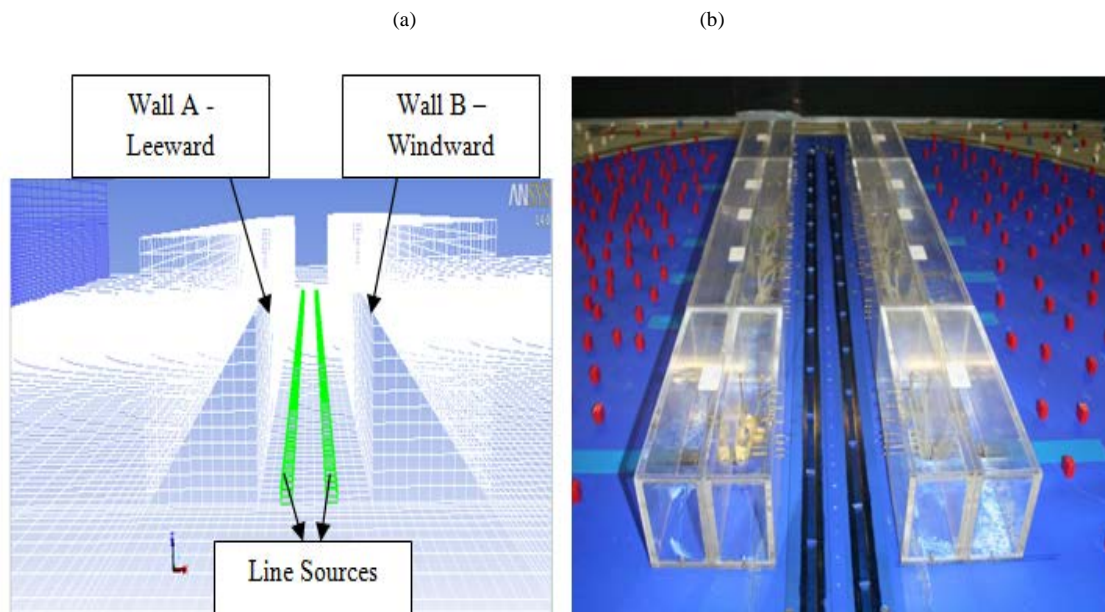


Fig. 4. Position of line sources from (a) computational domain (FLUENT), showing similarity with (b) wind tunnel setup (CODASC database) [33]

performing numerical investigations of urban airflow and pollutant dispersion.

Additionally, it is observed that the magnitude of the pollutant concentrations predicted by the FWBC simulations is significantly lower as compared to the results generated using SWBC and in the WT experiment. These variations can be explained by analyzing the velocity profiles along both walls.

Fig. 6(a) demonstrates that the velocity profiles are consistently the same at all locations ($y/H = 0$, $y/H = 2.5$ and $y/H = -2.5$) when employing a SWBC. On the other hand, the velocity profiles for all the FWBC cases (i.e. Fig. 6 (b)-(d)) are fluctuating along both ends of the wall. These differences in velocity cause pollutant concentrations to vary at different locations. The locations along which higher velocities occur produces lower pollutant concentrations.

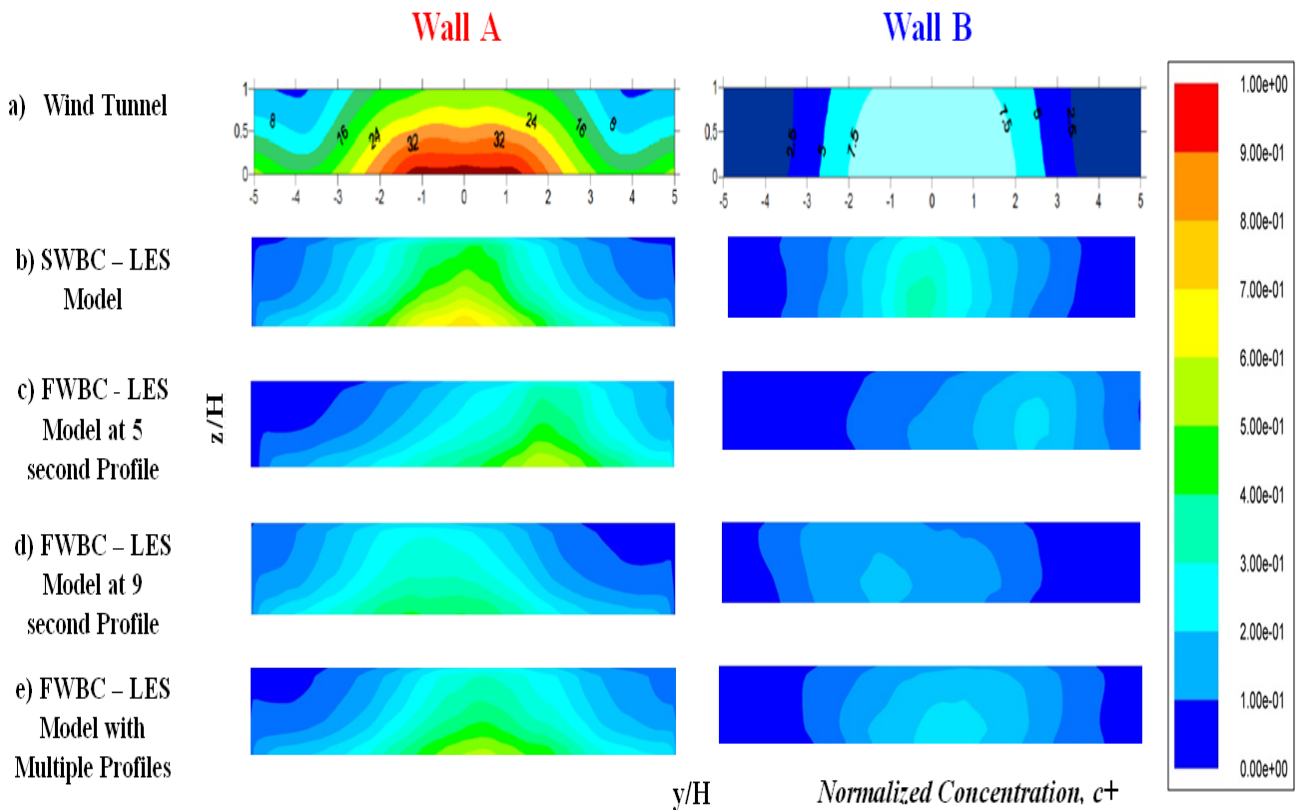


Fig. 5. Mean concentration contours on leeward (Wall A) and windward (Wall B) showing comparison between (a) WT data from CODASC database [13] (b) SWBC (c) FWBC at 5.0 second (d) FWBC at 9.0 second and (e) Multiple FWBC profiles

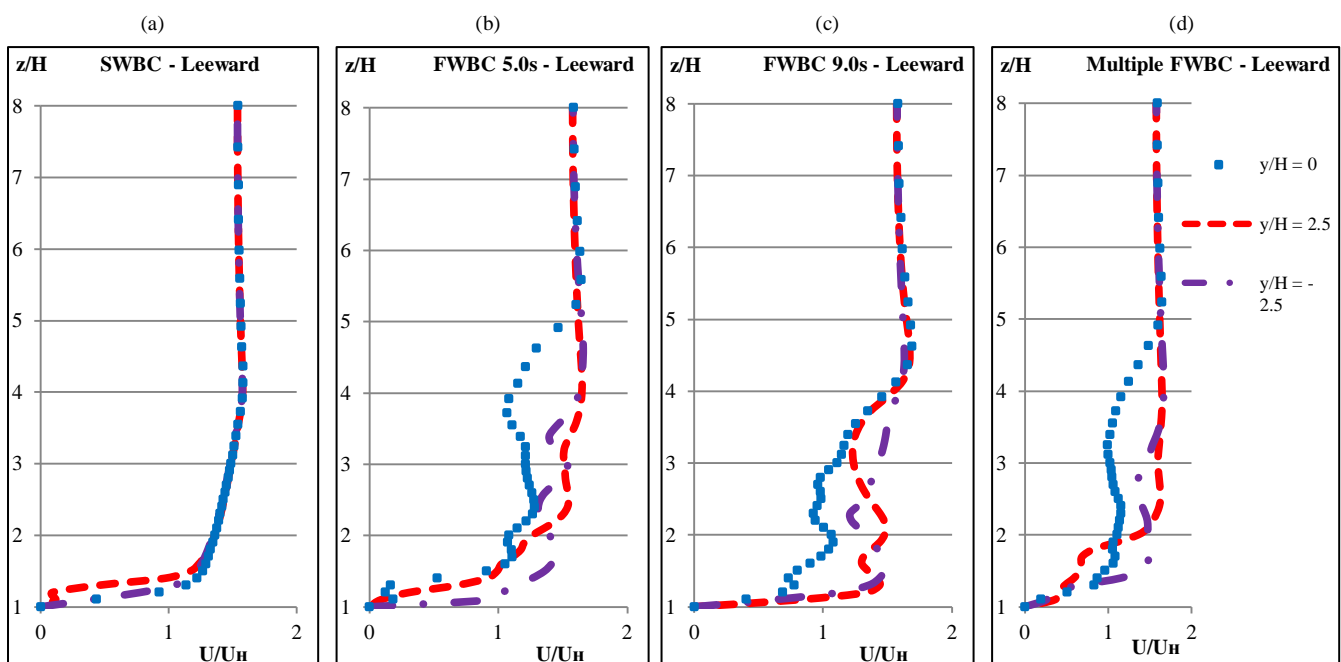


Fig. 6. Velocity profiles along leeward wall ($y/H = 0$, $y/H = 2.5$ and $y/H = -2.5$) comparing between (a) SWBC (b) FWBC at 5.0 second (c) FWBC at 9.0 second and (d) Multiple FWBC profiles

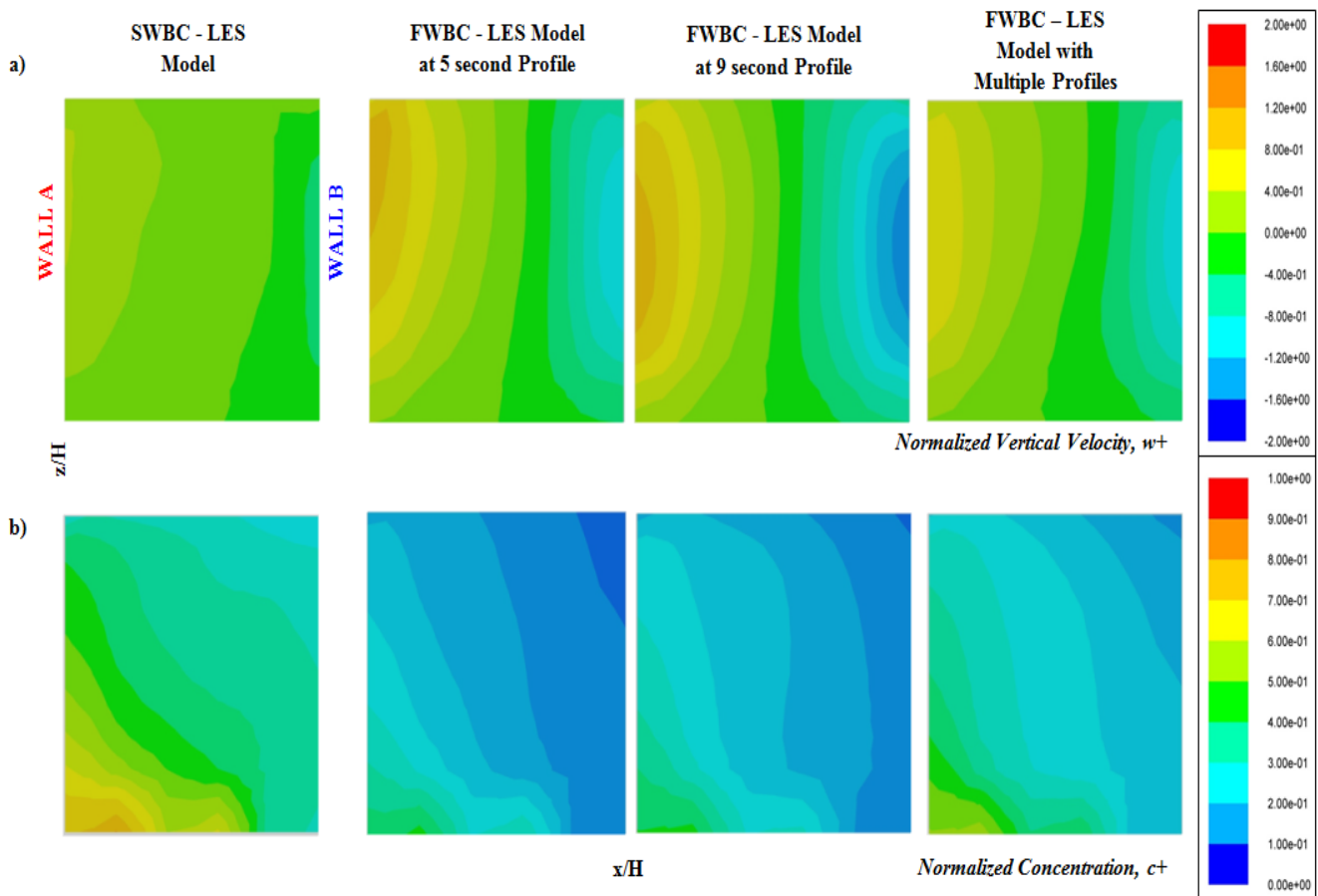


Fig. 7. (a) Mean normalized vertical velocities, w and (b) mean normalized concentration contours, c^+ at the mid-plane of the street canyon, comparing between SWBC, FWBC at 5.0 second, 9.0 second and multiple FWBC profiles

Predictions obtained from SWBC and FWBC profiles are compared in Fig. 7 based on the mean normalized vertical velocities and concentration contours along the mid-plane ($y/H = 0$) within the street canyon. It is observed that the spread of pollutants along the mid-plane between SWBC and all the FWBC simulations are similar with the only notable difference being that SWBC produces higher magnitude of pollutants at the bottom left corner towards the leeward wall. However, there are differences in the vertical velocities contours along the mid-plane. SWBC produces lower maximum magnitudes of negative and positive vertical velocities within the canyon. In contrast, all three FWBC simulations produce high maximum magnitudes of positive and negative vertical velocities near both leeward and windward side of the canyon, prompting the pollutant concentrations to be lower near the bottom left corner of leeward wall as compared to SWBC.

Fig. 8 further illustrates the velocity magnitude across the computational domain, comparing between SWBC and FWBC simulations. For SWBC, the velocity contours produces consistent magnitude throughout the upstream side. All three FWBC simulations generated different magnitudes of velocities upstream. For FWBC at 5.0 second, it is noted that there is a larger region of high velocity magnitude located at the bottom area after the street canyon as opposed to the top. This is different as compared to the result of FWBC at 9.0 second which has a larger region of high velocity magnitude located at the top. The simulation with multiple FWBC showed almost consistent velocity magnitude at the top and bottom region beyond the

street canyon area, similar to that in SWBC. The differences in the velocity regions for all three FWBC cases inevitably cause variations in pollutant concentration distribution in and around the street canyon vicinity.

In actual situations, the pollutant dispersion may vary significantly in both time and space. Fig. 9 shows the instantaneous solutions of normalized concentration contours along Wall A and Wall B. The LES results of both SWBC and FWBC on both walls support the statement by Louka et al. [41], where time-evolution of concentration field illustrates significant variations in peak concentrations. On top of illustrating significant changes of pollutant concentration at different flow-time in ANSYS FLUENT, the results in Fig. 9 further validates the results obtained from Fig. 5, showing similar pattern in terms of concentration contours. For example, it can be seen that for FWBC at 5.0 second, the pollutant concentrations are more prominent at the region to the right of the centerline for both walls. This is applicable to all the instantaneous solutions presented ($t = 10$ second, $t = 20$ second and $t = 30$ second). Similar trend is observed from the results of FWBC at 9.0 second whereby maximum pollutant concentrations occur at region to the left of the centerline.

Relationship between pollutant dispersion and flow field development along mid-plane of the street canyon is also presented in Fig. 10. For FWBC at 5.0 second, the magnitude of velocity leaving the canyon at $t = 10$ second is relatively small and as a result of this, the pollutants are more prominent near the bottom corner of Wall A.

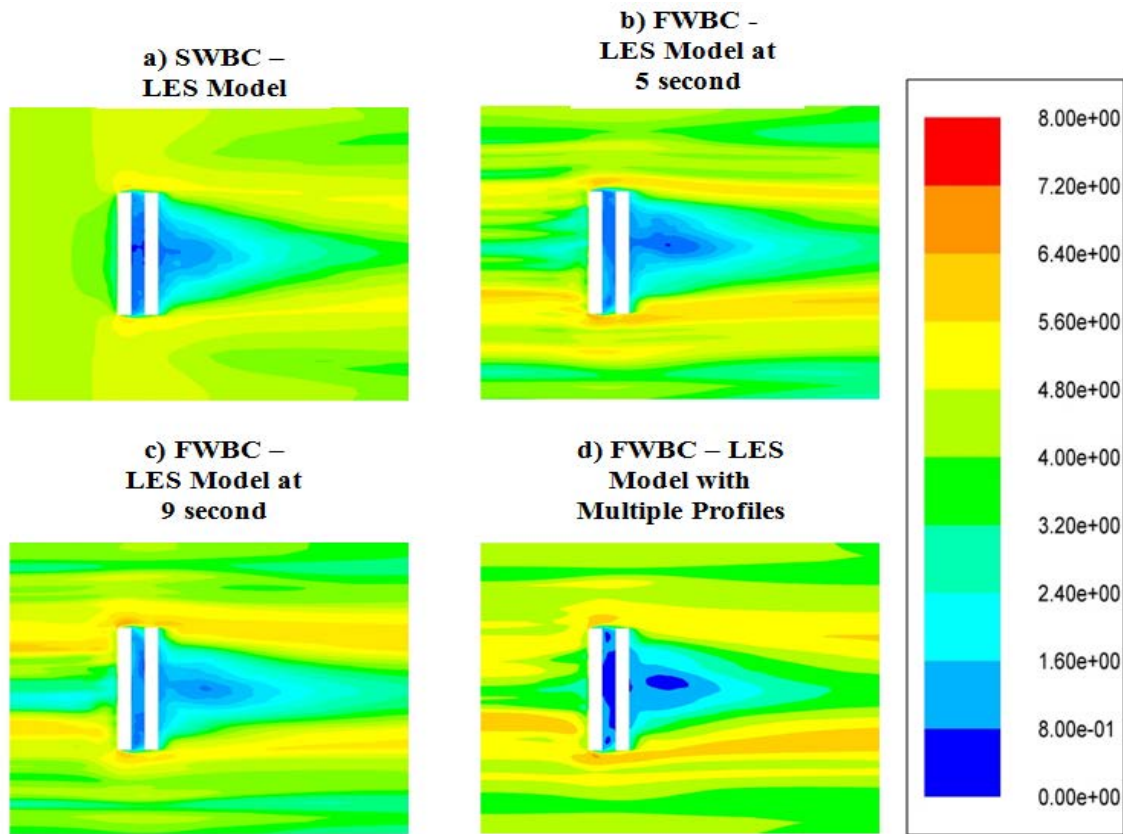


Fig. 8. Mean velocity magnitude contours across the computational domain for (a) SWBC (b) FWBC at 5.0 second (c) FWBC at 9.0 second and (d) Multiple FWBC profiles

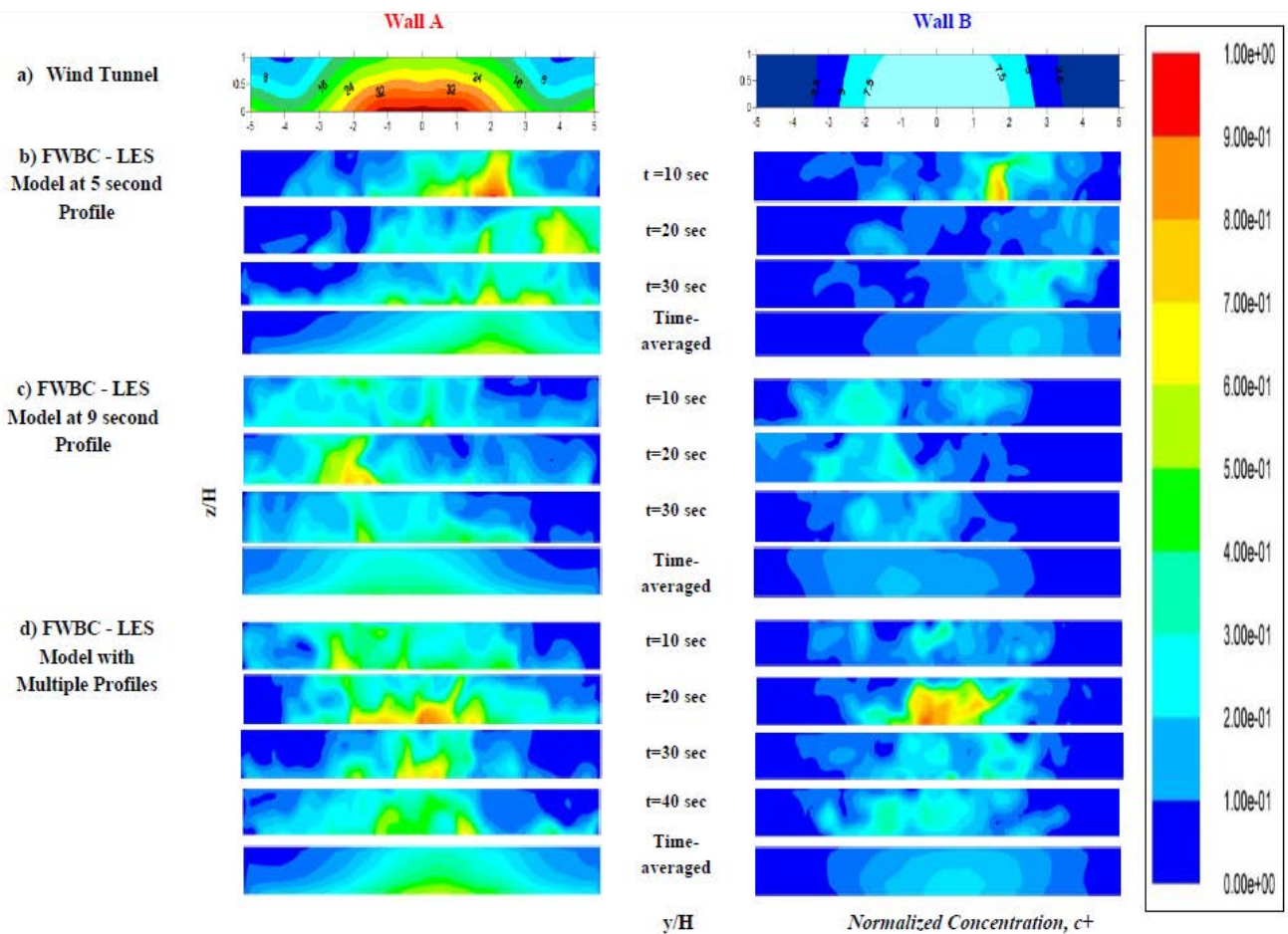
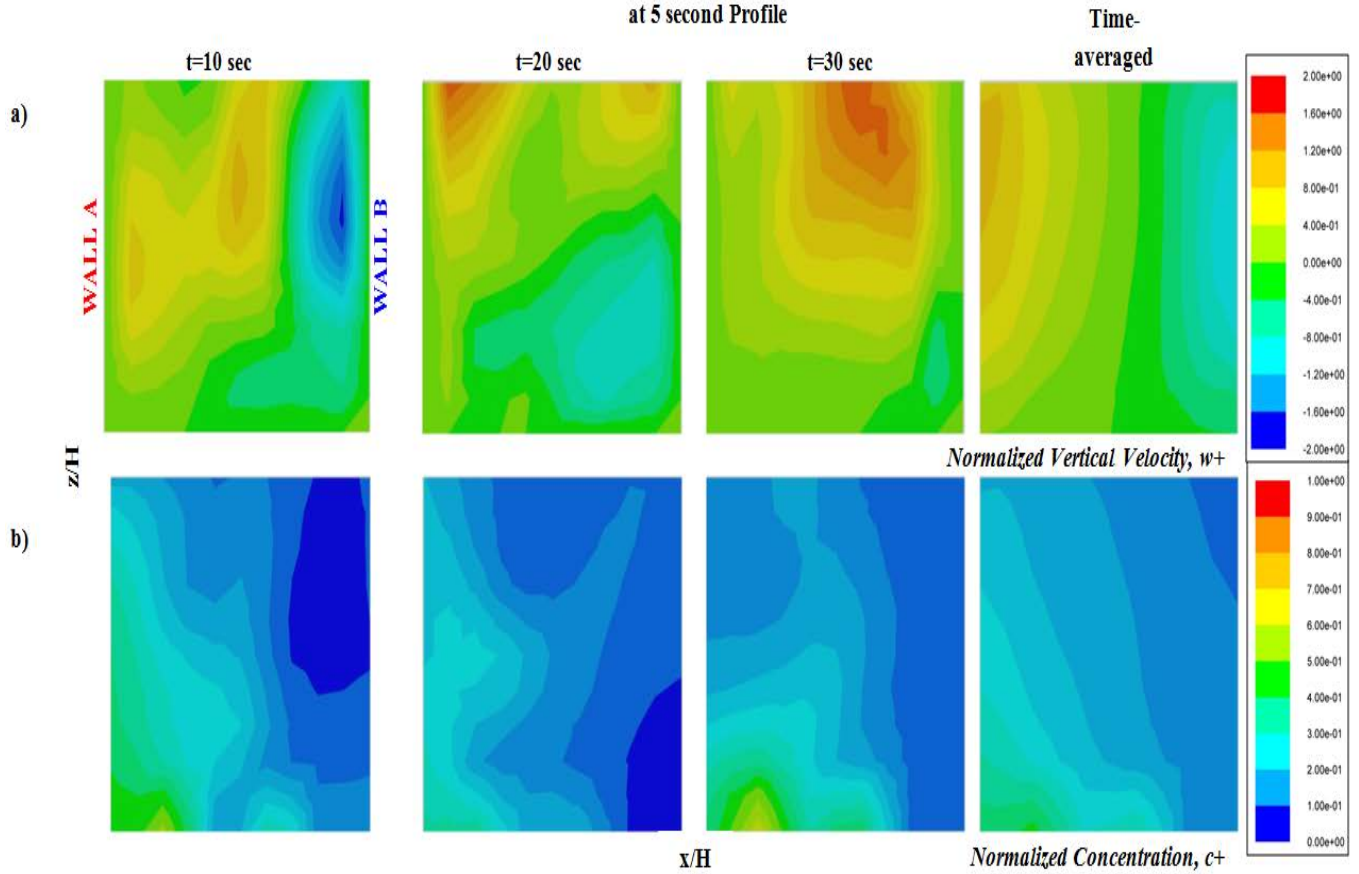


Fig. 9. Instantaneous normalized concentration data for (b) FWBC at 5.0 second (c) FWBC at 9.0 second and (d) Multiple FWBC profiles on Wall A and Wall B obtained with LES model compared to mean time-averaged data from (a) WT data from CODASC database [16]

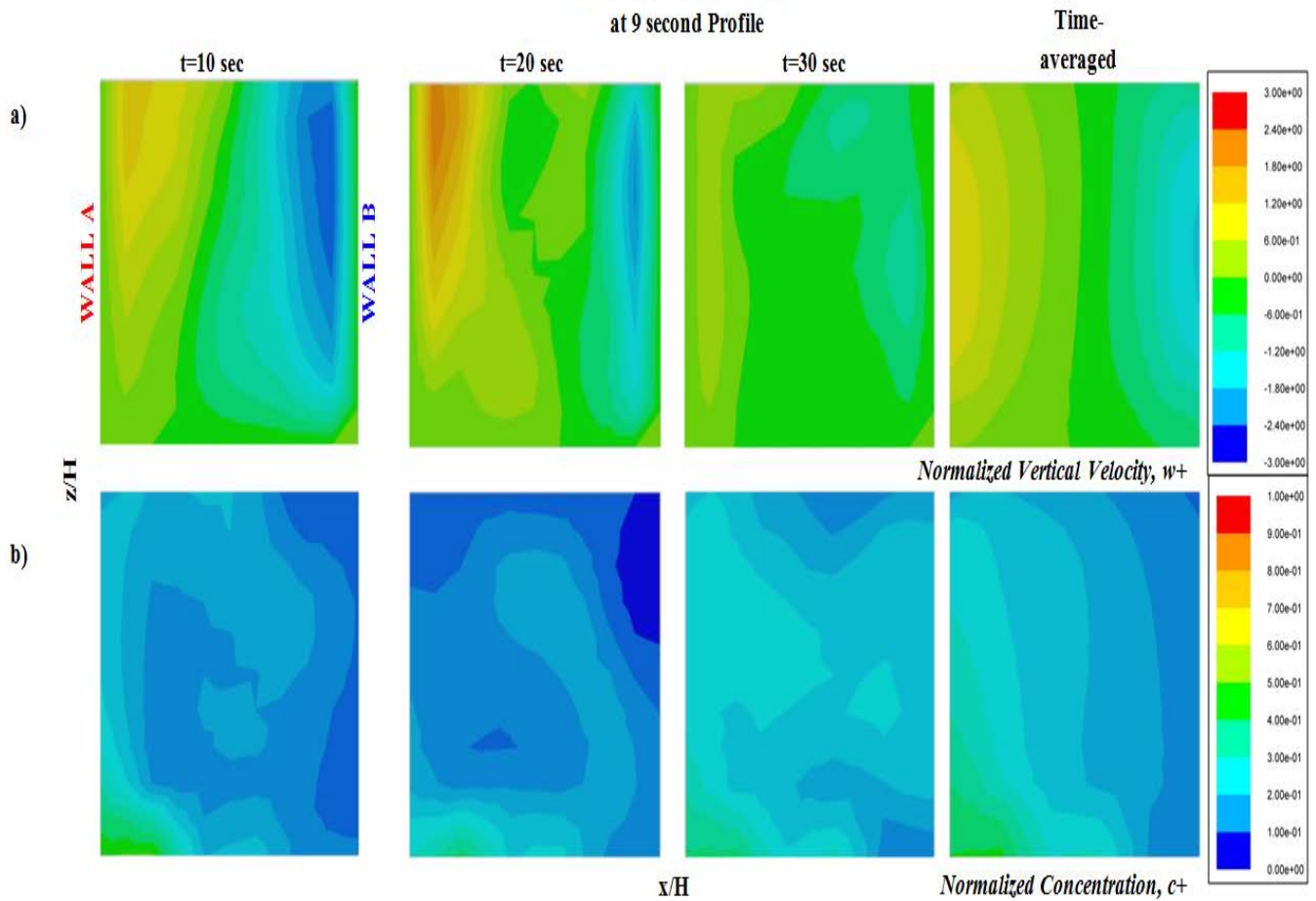
A) FWBC - LES Model

at 5 second Profile



B) FWBC - LES Model

at 9 second Profile



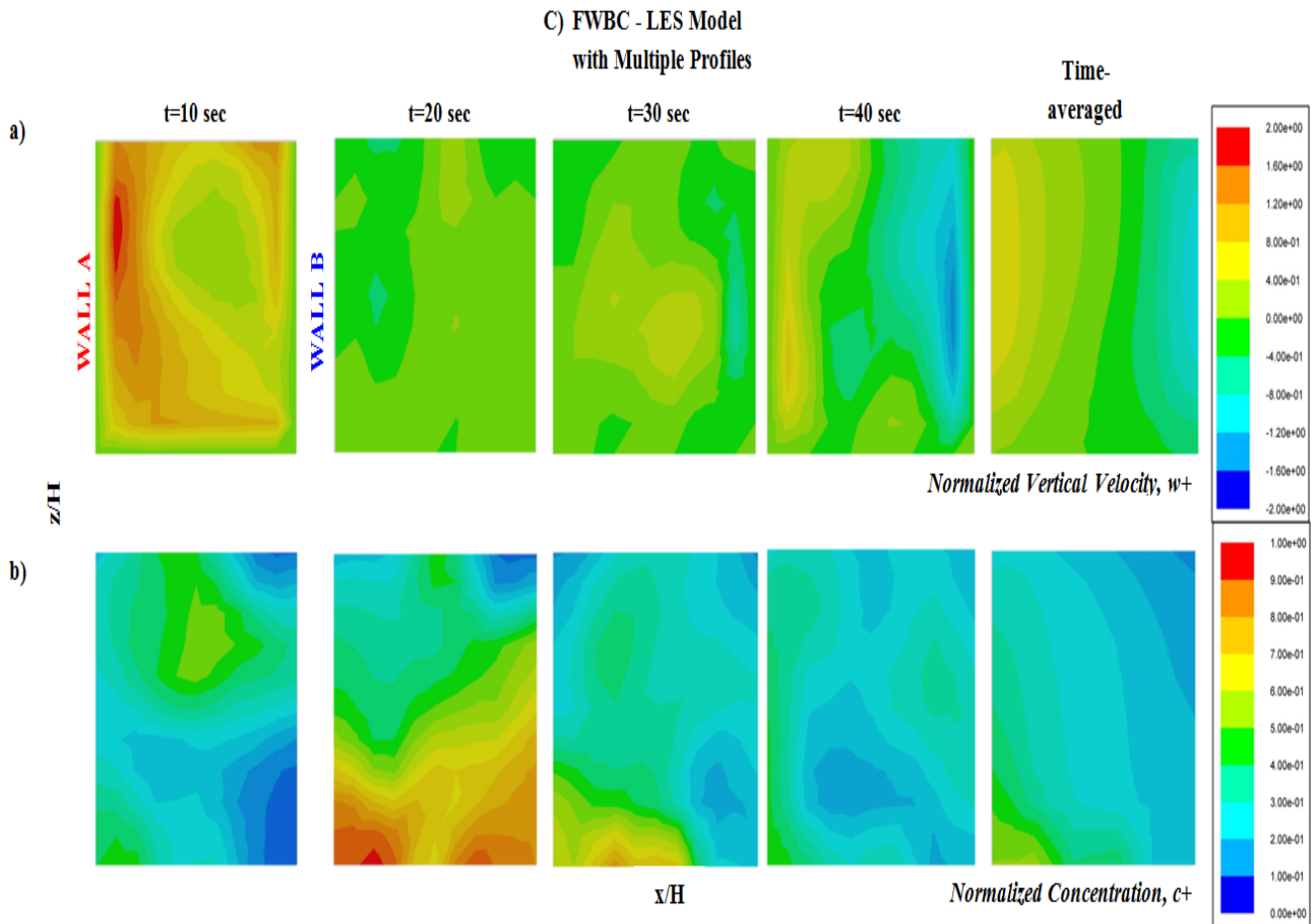


Fig. 10. (a) Instantaneous normalized vertical velocities contours, w and (b) instantaneous normalized concentration contours, c^+ at mid-canyon plane for (A) FWBC at 5.0 second (B) FWBC at 9.0 second and (C) Multiple FWBC profiles

However, at $t = 30$ second, the velocity leaving the canyon is relatively high, especially at the top right region of the canyon. Despite this difference, the pollutant concentration is similar to that at $t = 10$ second. For FWBC at 9.0 second, all three instantaneous solutions ($t = 10$ second, $t = 20$ second and $t = 30$ second) showed analogy when it comes to the relationship between magnitude of velocity and pollutant concentration. The region where low velocity magnitude occurs is where most of the pollutants accumulate. For multiple FWBC cases, at $t = 10$ second, highest velocity is achieved along Wall A while most pollutants are concentrated in the mid-canyon region. On the other hand, at $t = 20$ second, velocity magnitudes are evenly spread across the mid-canyon plane. But, very high pollutant concentrations are observed along the ground throughout the mid-canyon plane. These further proves that the flow field varies significantly over time, independent of each other.

IV. CONCLUSION

Computational Fluid Dynamics (CFD) simulations were performed to study air flow and pollutant dispersion in urban street canyons using Large Eddy Simulation (LES) model. Two different velocity profiles, namely Steady Wind Boundary Conditions (SWBC) and Fluctuating Wind Boundary Conditions (FWBC) were employed to determine their suitability in conducting air flow and pollutant dispersion simulations in urban street canyons. Majority of published studies employed SWBC which could be a source

of inaccuracy as temporal variations of wind velocities are not taken into account. SWBC assumes a horizontally homogeneous wind velocity profiles which is not always consistent with on-site field and wind tunnel experiments. The present study illustrates the importance of implementing the more realistic FWBC in characterizing air flow and pollutant dispersion. It is imperative to consider the fluctuating component in wind velocity as real-time meteorological data are time dependent. The use of FWBC helps to provide more realistic predictions similar to real urban conditions.

In order to better predict the outcome of air flow and pollutant dispersion process, it is vital to take into account the temporal and spatial variations in the velocity profile. On top of that, WT testing could be replicated following fluctuating velocity profiles to obtain better experimental data for future validations based on meteorological data.

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