MODELAIR – DELIVERABLE

D2.3 – REVIEW AND RESULTS OF ACTIVITIES IN TC2

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Type
R = Report
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Abstract

Air pollution remains a critical societal challenge, consistently identified as a leading cause of mortality and adverse health effects. Computational Fluid Dynamics (CFD) has emerged as a powerful tool for analysing air pollutant dispersion, particularly in complex urban environments. This study investigates Atmospheric Boundary Layer (ABL) flows over the ULB Solbosch campus using an advanced CFD framework. The CAD model of the campus, sourced from the Brussels Datastore, was used to construct a computational domain with a 1.3 km radius, ensuring full development of incoming flows. The mesh, generated with snappyHexMesh, comprises 92 million cells with a resolution ranging from 20 cm to 30 m, capturing both large-scale flow features and fine-scale details.

To provide realistic boundary conditions, meteorological data from the Brussels Airport weather station was incorporated into the simulation. Model validation was conducted using data from QSENSE-Air air quality sensors positioned across the campus, collecting measurements every 10 minutes throughout March 2023. Data from three sensors, filtered based on meteorological station statistics for dominant wind directions, offered robust validation for the CFD results.

The simulations employed the k–ω SST turbulence model implemented in the open-source OpenFOAM software. This framework demonstrated its capability to accurately resolve the complex interactions within urban canopy. The findings underscore the effectiveness of high-resolution CFD in supporting environmental decision-making, particularly for urban air quality management. Future applications may extend this methodology to other urban scenarios, contributing to the development of Reduced-order Models (ROMs).

DOCUMENT HISTORY

Keywords: Computational Fluid Dynamics, ABL Flows, Environmental Modeling.

Acronyms

AP: Associated Partner

BEN: Beneficiary

CFD: Computational fluid dynamics

COO: Coordinator

ABL: Atmospheric Boundary Layer

CFD: Computational Fluid Dynamics

BIA: Building Influenced Area

NLEV: Non-linear Eddy-viscosity

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1. Introduction

Air pollution remains one of the most pressing challenges for modern society, consistently ranked among the leading causes of mortality and health complications by organizations such as the European Environmental Agency (2022), the Environmental Protection Agency (2022), and the World Health Organization (2016). To address this critical issue, environmental modelling plays a pivotal role by generating actionable insights that inform policymaking for air quality management and guide the development of advanced pollution mitigation technologies.

In this context, Computational Fluid Dynamics (CFD) has emerged as a powerful tool for conducting environmental studies. By solving the three-dimensional fluid dynamics equations, coupled with transport equations and rigorous turbulence modelling, CFD enables the detailed analysis of pollutant dispersion across diverse domains, including highly intricate environments such as urban canopies.

This study aims to enhance turbulence modelling frameworks for analysing Atmospheric Boundary Layer (ABL) flows on the ULB campus (Fig. 1) using the k–ω SST turbulence closure model. The methodology has been implemented in the open-source OpenFOAM CFD software and validated against sensor-collected data, ensuring both accuracy and practical relevance.

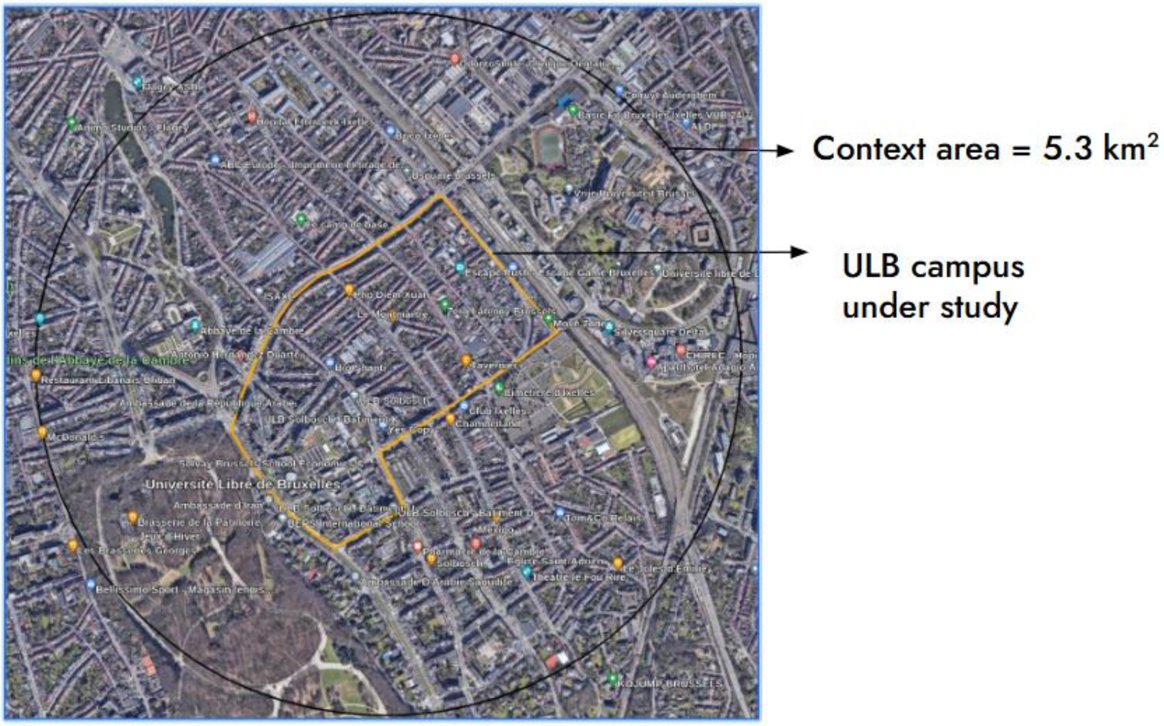


Figure 1. ULB campus under study and context area.

2. ABL k-ω SST model

The implementation of the general model for a homogeneous Atmospheric Boundary Layer (ABL) begins with the foundational equations describing a two-dimensional neutral ABL. This model is based on the assumptions of zero vertical velocity, constant pressure in both the vertical and streamwise directions, and uniform shear stress. These simplifications serve as the basis for deriving a consistent and computationally efficient representation of ABL dynamics.

$$\mu_t \frac{\partial u}{\partial z} = \tau_w = \rho u^{*2} \tag{1}$$

$$\frac{\partial}{\partial z}\left(\frac{\mu_t}{\sigma_k}\frac{\partial k}{\partial z}\right) + G_k - \rho\beta^* k\omega = 0 \tag{2}$$

$$\frac{\partial}{\partial z}\left(\frac{\mu_t}{\sigma_\omega}\frac{\partial \omega}{\partial z}\right) + \rho\frac{\gamma}{\nu_t}G_k - \rho\beta\omega^2 + 2(1 - F_1)\rho\sigma_{\omega_2}\frac{1}{\omega}\frac{\partial k}{\partial z}\frac{\partial \omega}{\partial z} = 0 \tag{3}$$

where G_k is the production term of turbulent kinetic energy and μ_t is the turbulent viscosity and β^* represents the equilibrium between turbulence production and dissipation in a homogeneous ABL flow:

$$G_k = \mu_t\left(\frac{\partial u}{\partial z}\right)^2 \quad ; \mu_t = \frac{a_1\rho k}{\max(a_1\omega, F_2 S)}; \beta^* = \frac{u_*^4}{k(z)^2} \tag{4}$$

while σ_k, σ_ω, β, $\sigma_{\omega 2}$ and a_1 are constants. ν_t is the kinematic turbulent viscosity, S represents the strain rate, F_1 is the blending function and F_2 is the function to limit the eddy viscosity. When cells are near the wall, $F_1 = 1$ and the Wilcox's $k - \omega$ model is applied while cells are away from the wall, $F_1 = 0$ and the standard $k - \epsilon$ model is implemented. Moreover, fully developed inlet profiles are usually imposed as boundary conditions in terms of velocity and turbulence characteristics computed to have an equilibrium boundary layer:

$$u = \frac{u^*}{\kappa} ln\left(\frac{z + z_0}{z_0}\right) \tag{5}$$

$$k(z) = C_1 ln(z + z_0) + C_2 \tag{6}$$

$$\omega(z) = \frac{u^*}{\sqrt{\beta^*}}\frac{1}{\kappa(z + z_0)} \tag{7}$$

Where u^* is the friction velocity reflecting the intensity of shear stress on the surface, z_0 is the roughness length and κ is the Von-Karman constant, the value of which usually is 0.41.

It is known that the consistency achieved with the comprehensive approach does not stand anymore when an obstacle is present in the domain. As a matter of fact, their formulations were derived employing the equilibrium and horizontal homogeneity assumptions, which is not applicable anymore in this zone. To solve this problem, we proposed the blending with another turbulence closure model in the so-called Building Influence Area (BIA), which is detected through the computation of the deviation from the undisturbed ABL flow. The transition from the undisturbed to the disturbed flow region can be considered by using either a polynomial or sinusoidal function:

$$\phi = \phi_{wake} + (1 - \delta^{\alpha})(\phi_{ABL} - \phi_{wake}) \tag{8}$$

$$\phi = \phi_{wake} + (\phi_{ABL} - \phi_{wake})[1 - 0.5(1 + \sin(\delta^*))] \tag{9}$$

where ϕ represents the quantities of flow fields in the transition area, $\delta^* = \pi \cdot \max(\delta - 0.5, 0.5)$ and δ is the max deviation among velocity, turbulent kinetic energy and dissipation rate defined as follows:

$$\delta = \max[\delta_u, \delta_k, \delta_\omega] \tag{10}$$

$$\delta_u = \min\left[A_u \left|\frac{u - u_{ABL}}{u_{ABL}}\right|, 1\right] \tag{11}$$

$$\delta_k = \min\left[A_k \left|\frac{k - k_{ABL}}{k_{ABL}}\right|, 1\right] \tag{12}$$

$$\delta_\omega = \min\left[A_\omega \left|\frac{\omega - \omega_{ABL}}{\omega_{ABL}}\right|, 1\right] \tag{13}$$

At this point, a Non-Linear Eddy-Viscosity (NLEV) model was proposed for the solution in the BIA region. This consists in extending the Boussinesq's hypothesis to higher order terms and, practically, to use a different formulation for C_μ, for which the expression by Ehrhard and Moussiopoulos (2000):

$$C_\mu = \min\left(0.15, \frac{1}{0.9S^{1.4} + 0.4\Omega^{1.4} + 3.5}\right) \tag{14}$$

In the SST $k-\omega$ framework, a new blending approach was implemented here. From a mathematical point of view, it consisted in applying the sinusoidal blending function in Eq. (3) to the $F1$ function of the SST $k-\omega$ model, as follows:

$$bF_1 = F_1 \cdot [1 - 0.5(1 + \sin(\delta^*))]^a \tag{15}$$

where $bF1$ indicates the blended $F1$ function. From a physical point of view, this means that the Standard $k - \varepsilon$ model was employed inside the BIA but keeping the viscosity limitation near the walls, since the function $F2$ was not blended, while the SST $k-\omega$ model was used in the undisturbed flow region.

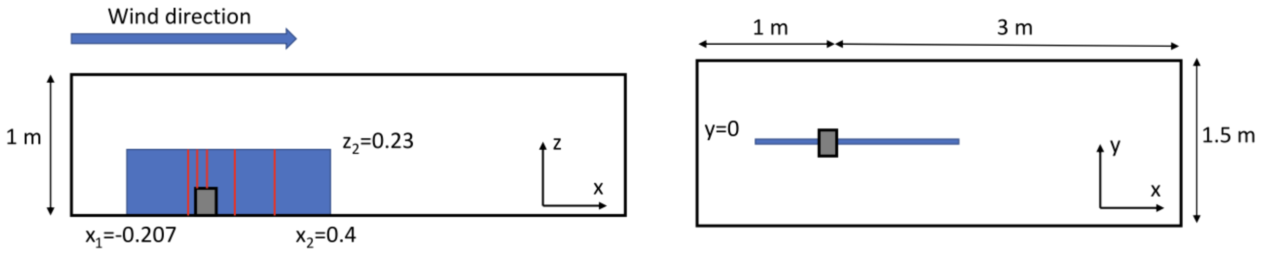
As a matter of fact, the sinusoidal blending function is zero in the BIA, thus giving $bF1 = 0$, which means to blend to Standard $k-\varepsilon$ equations. On the contrary, in the undisturbed flow region, the sinusoidal function goes to 1 and so the usual equations of the SST k–ω model are applied.

This novel blending technique was compared here with the above-mentioned blending to an NLEV model in the BIA, using the same expression in Eq. (14) for the variable $\beta*$ that is equivalent to $C\mu$, as stated above.

3. Model Validation on Flow over a single building – CEDVAL A1-1

For the validation on a single building test case, the CEDVAL A1-1 case (Leitl and Schatzmann, 2010) was chosen. This experimental test was performed by researchers of the University of Hamburg and it is one of the most common choices for validation studies of ABL models.

The test case consisted of a building with a height of H = 0.125 m, length L = 0.1m and width W = 0.15m immersed in a flow of a wind tunnel with a height of 1 m and a width of 1.5 m. The atmospheric boundary layer was the same of the empty fetch case and measurements were collected in a total number of 603 data points distributed in the domain from a location put 0.2 m upstream the building to one located 0.4 m downstream (for a total of 44 locations). Fig. 2 reports the dimensions of the computational domain together with the area in which measurements were collected, indicated in blue with the values of minimum and maximum x, y and z coordinates. The origin was set at the ground, in the center of the building. Fig. 2 also indicates the locations of the measurement lines chosen for the validation of CFD results. The first line was in front of the building, two lines were on the roof and the last two were in correspondence of the wake.

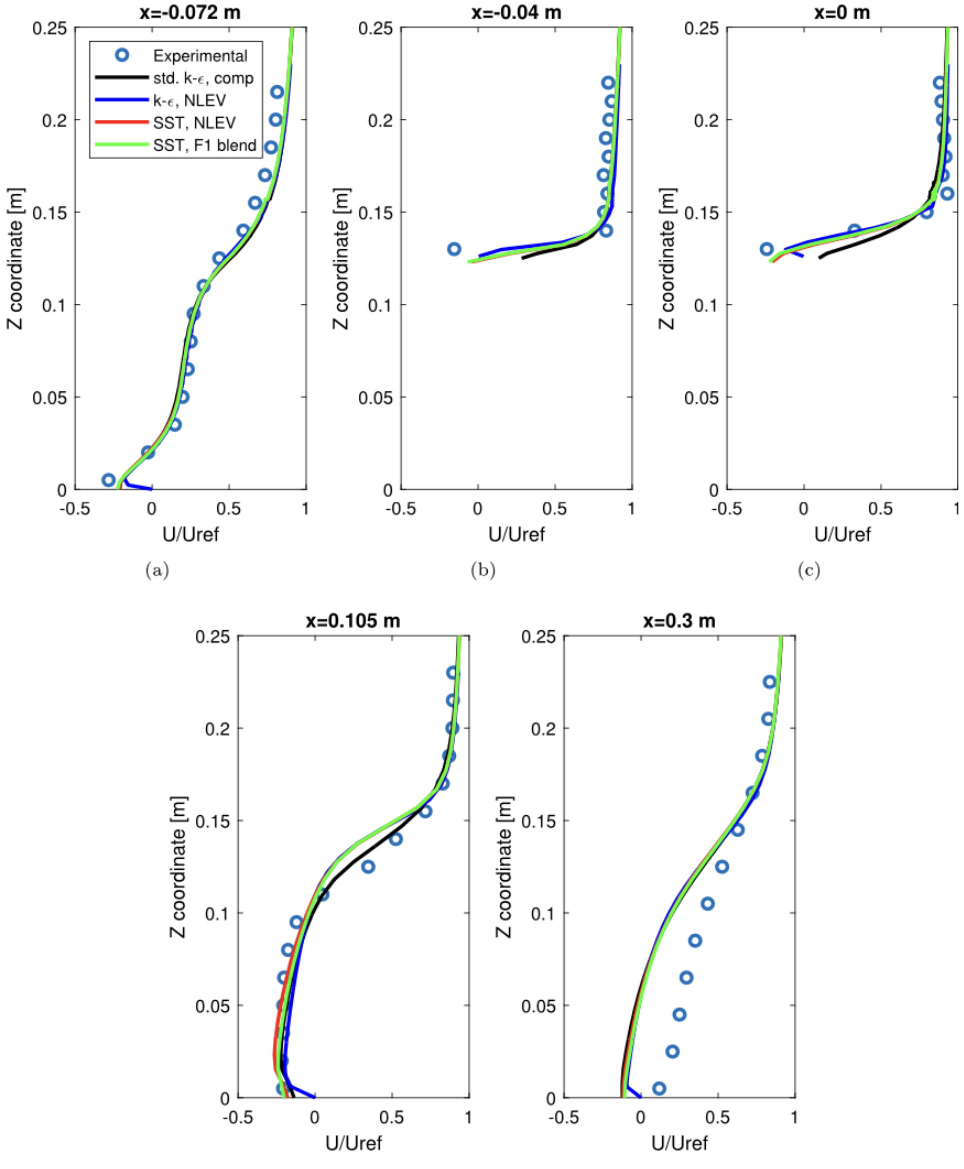


(a)

(b)

Figure 2. Scheme of CEDVAL A1-1 test case with indications of computational domain dimensions in the middle lateral view at y=0 (a) and the top view (b). The blue area represents the zone where measurements were taken with indications of the minimum and maximum coordinates in metres. In (a) the locations of the measurement lines are visible in red, i.e. (x=−0.072 m), (x=−0.04 m), (x=0 m), (x=0.105 m), (x=0.3 m) from the left to the right.

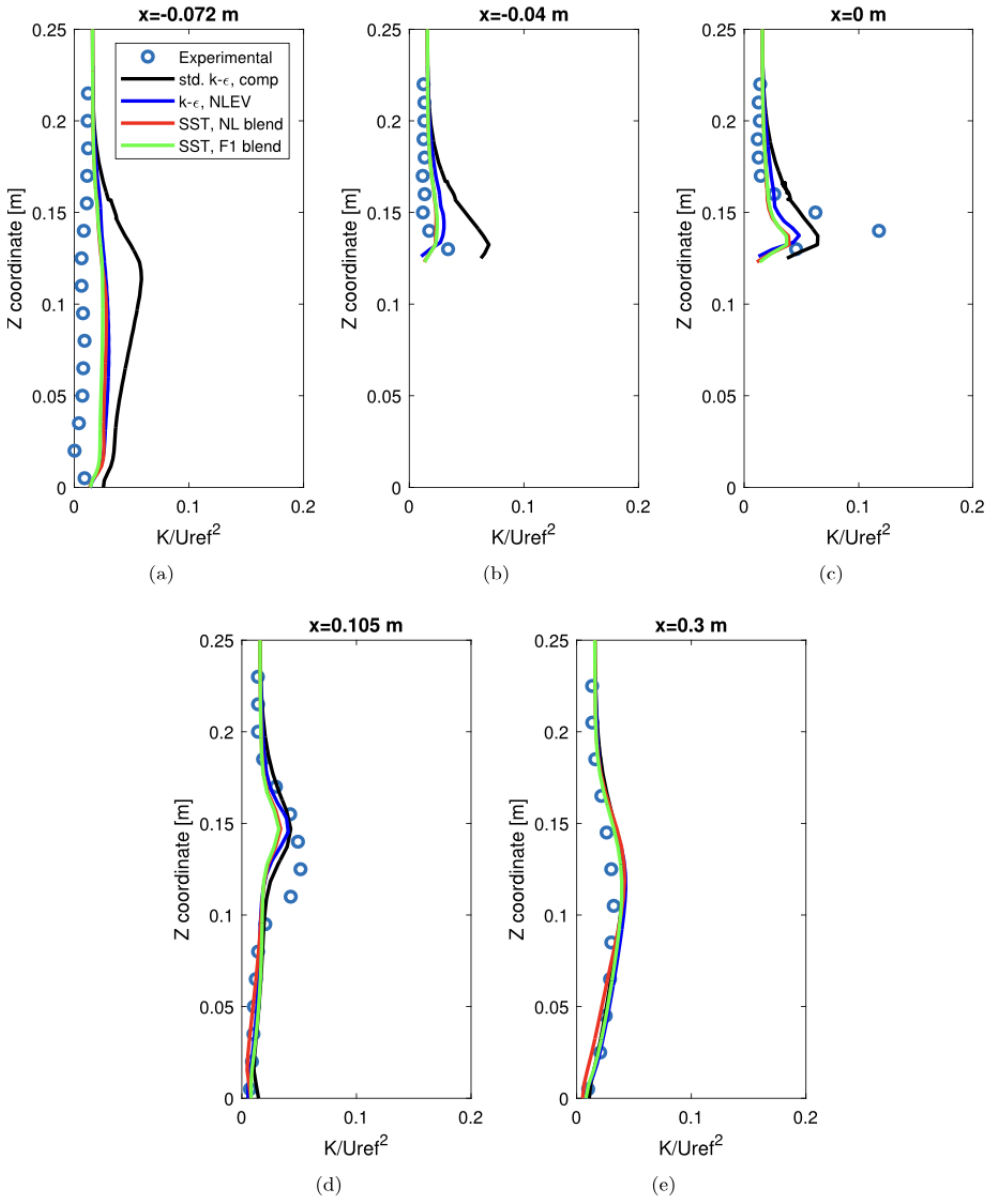
In this case, the ability of the new blending approach of detecting one obstacle is validated against experimental observations and verified comparing its results with the existing approach to blend to an NLEV model inside the BIA. Figs. 3 and 4 show wind profiles in terms of non-dimensional mean velocity and turbulent kinetic energy in the five locations where measurements were taken.



(a) (b) (c)

(d) (e)

Figure 3. Wind velocity profiles obtained using Standard $k-\varepsilon$ model, $k-\varepsilon$ with NLEV blending approach and SST $k-\omega$ with NLEV and blending of $F1$ function compared with experimental observations in the measurement's lines of CEDVAL A1-1 case.



(a) (b) (c)

(d) (e)

Figure 4. Wind turbulent kinetic energy profiles obtained using Standard $k-\varepsilon$ model, $k-\varepsilon$ with NLEV blending approach and SST $k-\omega$ with NLEV and blending of $F1$ function compared with experimental observations in the measurement's lines of CEDVAL A1-1 case.

From the point of view of velocity, all the models provide similar results. However, it is worth noting that SST $k-\omega$ model performs better especially near the terrain, meaning that the $k-\omega$ equations are more effective in this zone. As a matter of fact, considering the locations $x = -0.072$ m and $x = 0.105$ m, the Standard $k-\varepsilon$ model with the blending to the NLEV one provides values of $U\,/\,Uref = -0.17$ and $U\,/\,Uref = -0.13$ versus experimental values of −0.28 and −0.21, respectively; this corresponds to a relative percentage error of about 38% in both cases. The error reduces when considering the SST $k-\omega$ predictions to 28% and 3%, respectively.

If we look at the turbulent kinetic energy profiles, we can notice quite a large discrepancy of all the models with respect to experiments in the location x = 0 m (see Fig. 4(c)), which is exactly in the middle of the building. In particular, the peak observed in the experiments ($k \ / \ U_{ref}^2$ = 0.12) is not present in the CFD simulations, where the maximum is reached employing the comprehensive $k{-}\varepsilon$ model without blending ($k \ / \ U_{ref}^2$ = 0.06). All the other CFD models provide even smaller values, but this discrepancy could also be imputed to the low resolution of experimental measurements in this zone.

4. ULB campus study

The case study focuses on the ULB Solbosch campus, located at Av. Franklin Roosevelt 50, 1050 Brussels, as shown in Fig. 1. Meteorological data from the Brussels Airport weather station, depicted in Fig. 5, is utilized to generate the boundary conditions required for the CFD simulations.

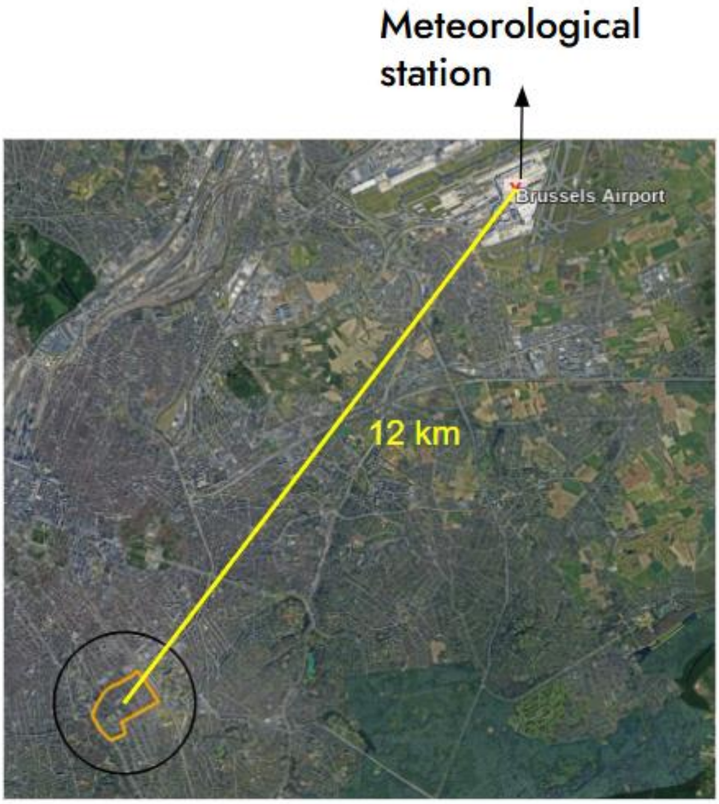


Figure 5. The distance of the Meteorological Station from ULB campus

The CAD model of the ULB Solbosch campus was obtained from the Brussels Datastore, as shown in Fig. 6. To set up the CFD simulation, a computational domain with a radius of 1.3 km was constructed to ensure the full development of the approaching flows. The characteristic length H for the case is 144 m. The mesh was generated using snappyHexMesh, resulting in a total of 92 million cells. The cell sizes range from a minimum of 20 cm to a maximum of 30 m, ensuring a fine resolution where needed and efficient computational performance.

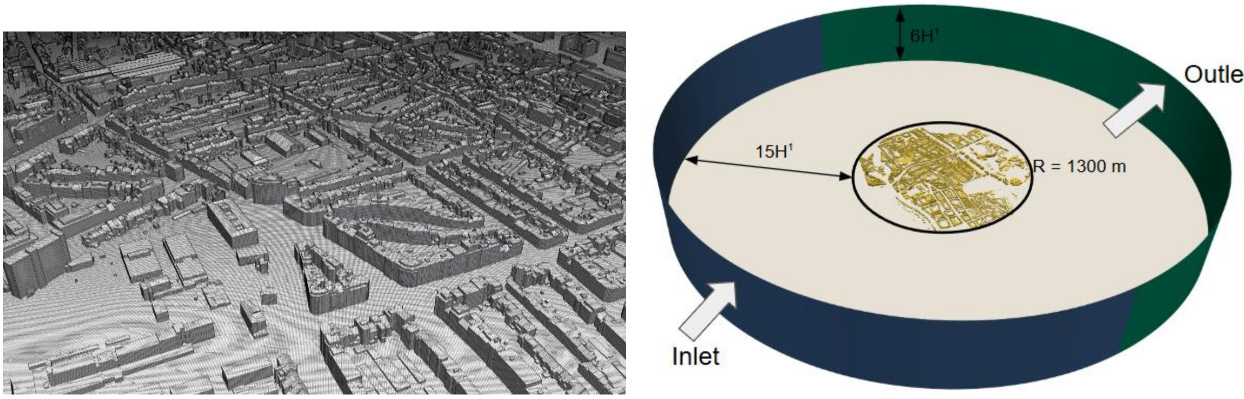


Figure 6. The CAD of the ULB campus and the case preparation.

Three directions: 180N, 210N and 240N are simulated via the ABL k-$\boldsymbol{\omega}$ SST model as well as the simpleFOAM solver in OpenFOAM v7.

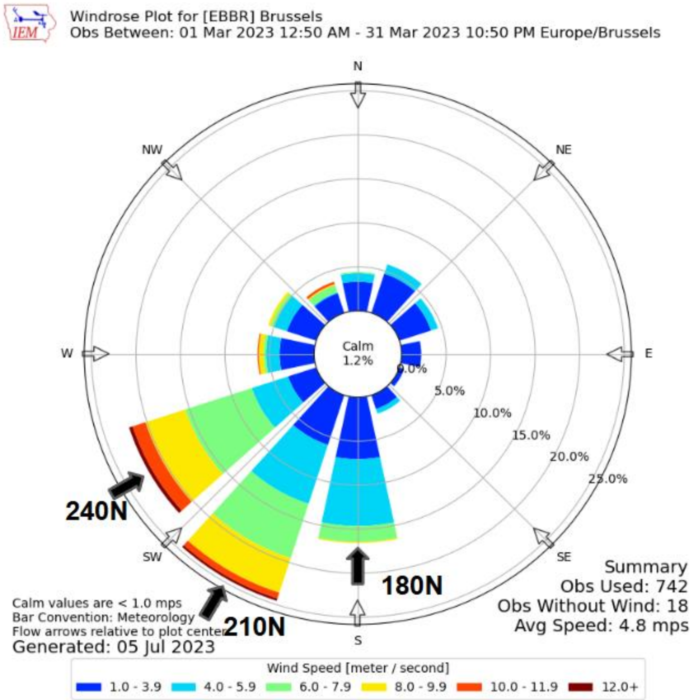
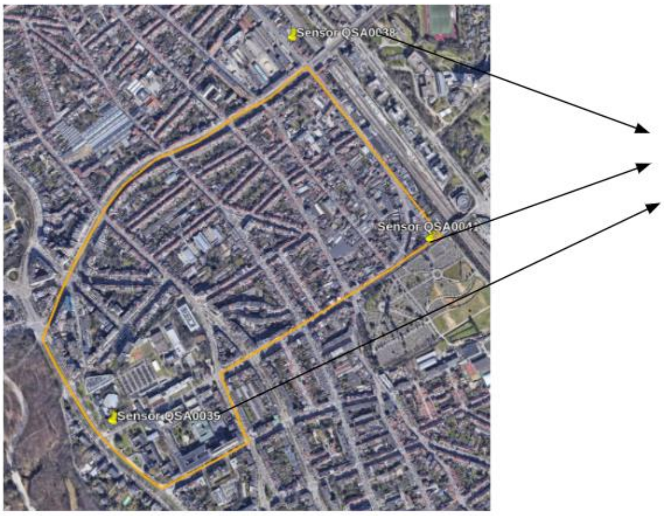


Figure 7. The wind rose plot of the meteorological data.

To validate the CFD simulation results, data from QSENSE-Air air quality sensors installed within the ULB campus was utilized. These sensors recorded data at 10-minute intervals over the sampling period from 1st March 2023 to 31st March 2023. Measurements from three sensors were processed and filtered using statistical data from the meteorological station, specifically for the three dominant wind directions, ensuring alignment with the simulated conditions.



- **Sensors** : QSENSE-Air air quality sensors
- **Sampling frequency** : 10 min
- **Data sampling period** : 1st March 2023 - 31st March 2023
- Obtained data filtered using the meteorological station statistics for the three wind directions (180N, 210N, 240N)

Figure 8. The information of the sensors used for validation.

5. Results

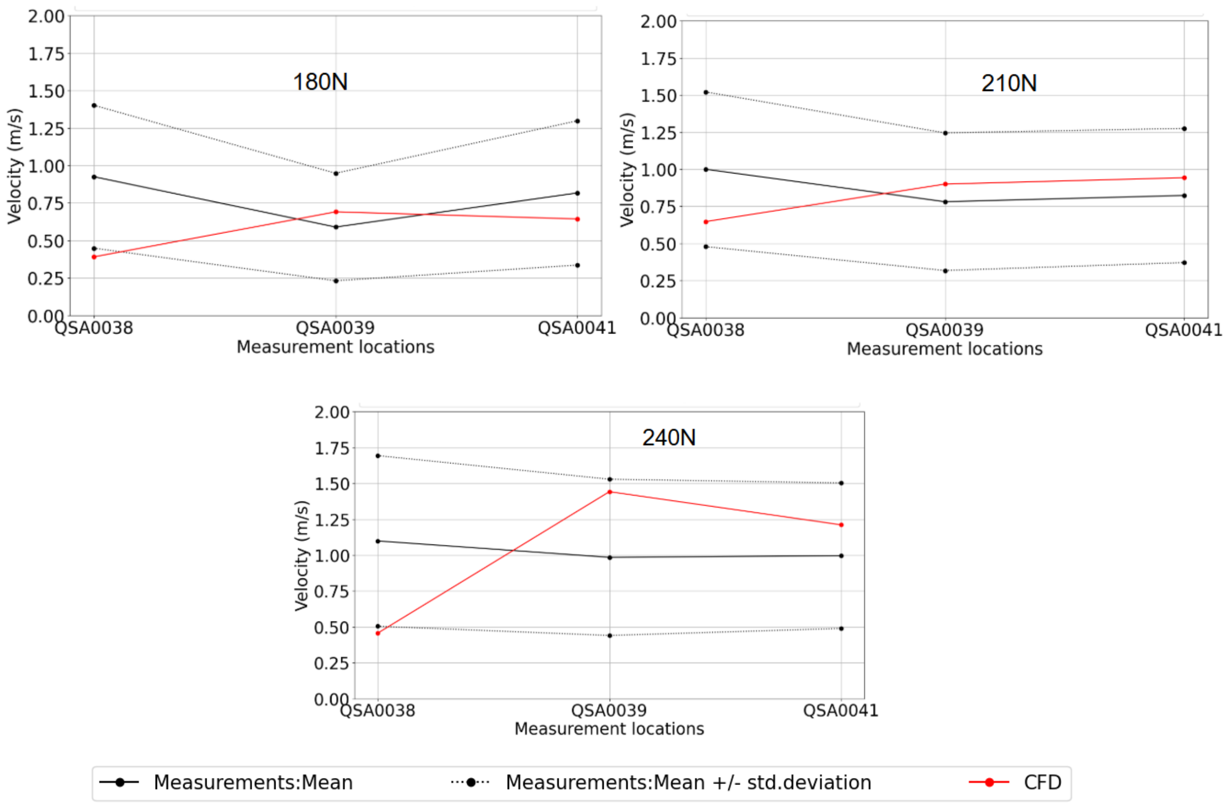


Figure 9. Comparison of CFD results and sensor data.

Fig. 9 compares velocity profiles from CFD simulations and field measurements at three urban sensor locations (QSA0038, QSA0039, and QSA0041) under wind directions of 180N, 210N, and 240N. The measured velocities show variability with standard deviation error bars, while CFD predictions exhibit steeper trends. At 180N and 240N, the CFD model overpredicts velocity at QSA0039 compared to measurements, whereas it aligns more closely at 210N, suggesting improved accuracy for that wind direction. QSA0039 consistently shows the highest variability, particularly under 240N, likely due to complex urban geometries or localized flow disturbances.

Discrepancies between CFD and measurements may arise from model simplifications, such as boundary conditions and turbulence models, or environmental factors like sensor placement and micro-scale urban effects. While the CFD model provides a useful baseline, further refinements and expanded field data validation are essential to enhance accuracy and address the influence of local flow phenomena.

Future work in uncertainty quantification for this study should focus on systematically evaluating the sources of discrepancies between CFD simulations and field measurements to enhance predictive accuracy. This includes performing sensitivity analyses on key model parameters, such as turbulence modeling, boundary conditions, and urban geometry resolution, to identify their impact on velocity predictions. Incorporating probabilistic approaches, such as Monte Carlo simulations or Bayesian inference, can help quantify uncertainties arising from input variability and model assumptions. Additionally, expanding the dataset with measurements under varying environmental conditions, including different wind speeds and directions, would provide a more robust basis for model validation.