Supplementary Material

S1. Grid sensitivity test

The grid sensitivity test is carried out using three different meshes. The BASE scenario for 0º wind direction is simulated using these meshes. Previous studies [65,66] found that 12 cells in each direction are enough for resolving the flow around the cubes for this configuration. More than 16 cells in each direction were used, applying mesh refinements close to the surfaces (walls, windows, ground and emissions). The surfaces of the central building and the emission area are meshed with refinements of about 0.75 m, 0.5 m and 0.25 m for the coarse, the medium and the fine grids, respectively. The growth rate of cell size from these refinements is 1.05. The total number of cells is 8.3 x 10^6, 11.5 x 10^6 and 30.7 x 10^6 for the coarse, medium and fine meshes respectively. Figure S1 shows the grids around the central building. Streamwise velocity (U), vertical velocity (W) and turbulent kinetic energy (k) for the three grids are compared at different vertical profiles around the central building (lines 1, 2 and 3 of Figures S1). Figure S2 shows that the vertical profiles of all variables are similar for the three grids at each location. This fact indicates that the flow around the buildings is similar for the three meshes. In view of these results, the medium grid is selected for simulating the set of simulations as a compromise between accuracy and computational cost.

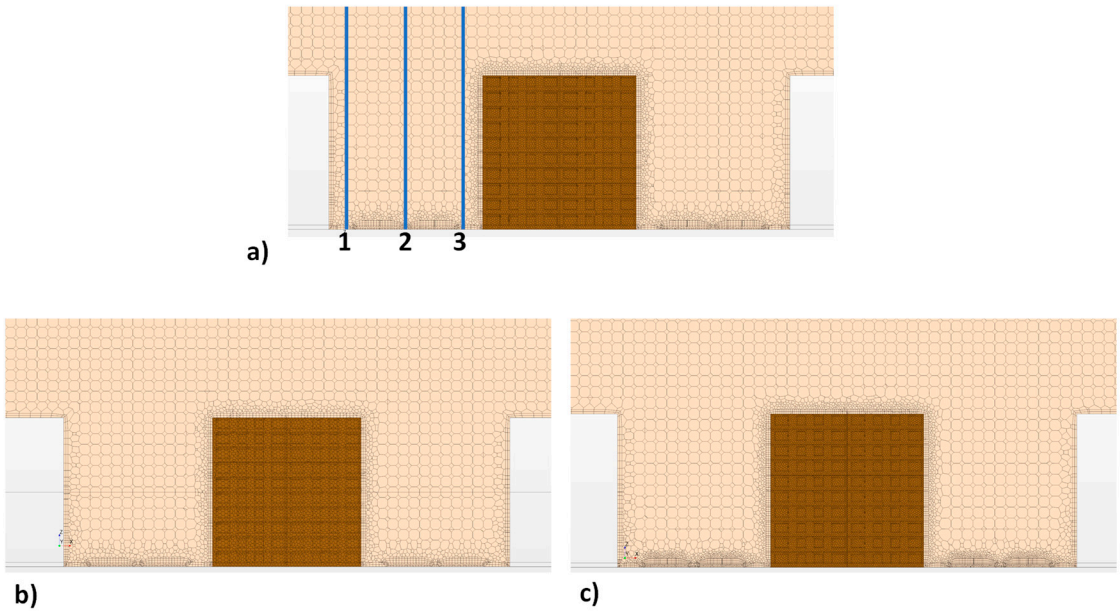

Figure S1. Mesh details of: (a) medium mesh, (b) coarse mesh and (c) fine mesh. Blue lines are the locations where the results are compared.

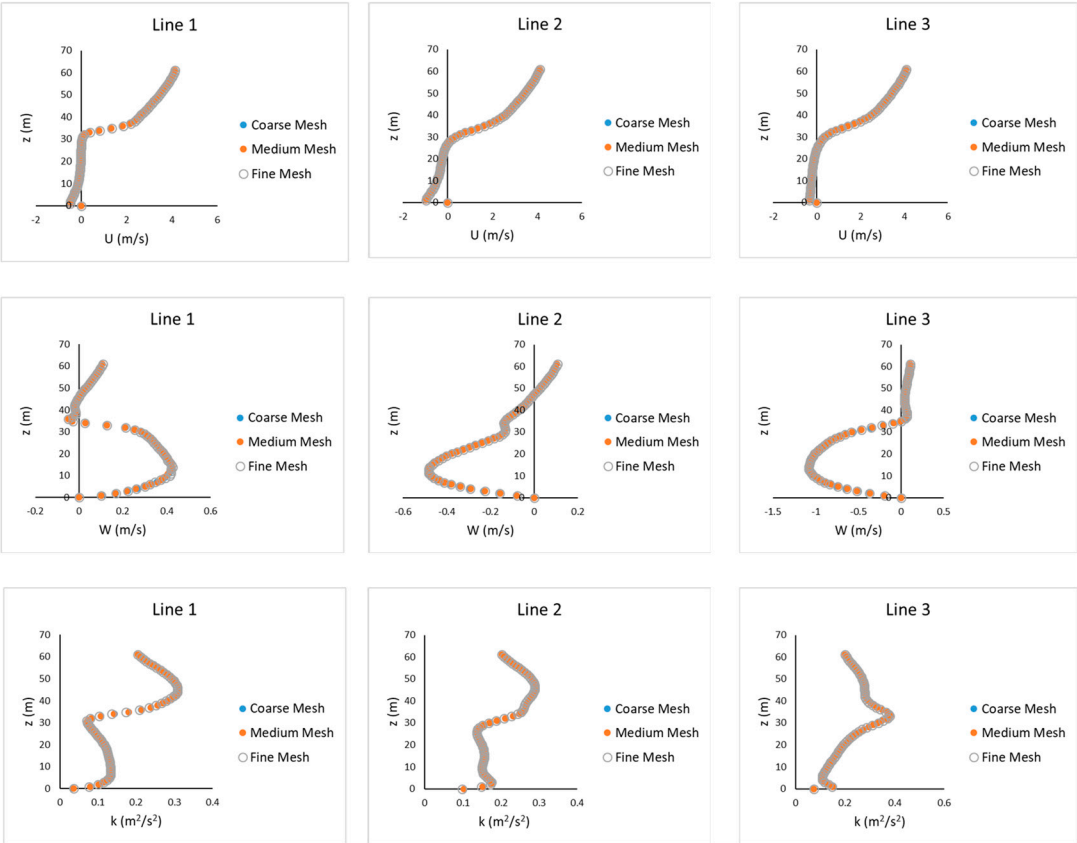

Figure S2. Vertical profiles at line 1 (column 1), line 2 (column 2) and line 3 (column 3) of streamwise velocity (U) (row 1), vertical velocity (W) (row 2) and turbulent kinetic energy (k) (row 3) for the three grids.

S2. Model Validation

Flow around the buildings for the BASE scenario is validated by using data from wind-tunnel [64], which has been previously used to assess CFD simulation performance in previous studies such as [65,66]. Streamwise velocity (U), vertical velocity (W) and turbulent kinetic energy (k) are evaluated at different locations in the middle of the central row of buildings (Figure S3). Measurements at heights below 1.5H are used for this comparison. Wind inlet profiles of simulations and wind-tunnel experiment are different and, for the comparison, U an W are normalized with U at 3H and k with k at 3H. Statistical metrics such as fractional bias (FB), the normalized mean-square error (NMSE), the fraction of prediction that are within a factor of two of the observation (FAC2) and the correlation coefficient (R) (Equations 1-4) are computed.

$$FB = \frac{\bar{O}-\bar{M}}{0.5(\bar{M}+\bar{O})}, \tag{1}$$

$$NMSE = \frac{\sum_{i=1}^{n}(M_i-O_i)^2}{\sum_{i=1}^{n}(M_i O_i)}, \tag{2}$$

$$FAC2 = fraction\ of\ data\ that\ satisfies\ 0.5 \leq \frac{M_i}{O_i} \leq 2.0, \tag{3}$$

$$R = \frac{\sum_{i=1}^{n}[(O_i-\bar{O})(M_i-\bar{M})]}{\left[\sum_{i=1}^{n}(O_i-\bar{O})^2\right]^{0.5}\left[\sum_{i=1}^{n}(M_i-\bar{M})^2\right]^{0.5}}, \tag{4}$$

where M and O are the modelled values extracted from CFD simulation and O are the observed values measured in the wind-tunnel experiment, respectively. The bar over O and M indicates the average value of modelled and observed values. The FAC2 is only computed for k because it is needed that the variable evaluated takes only positive values and U and W takes positive and negative values. Table S1 shows the values of statistical metrics and Figure S4 shows the scatter plots (modelled vs observed data) for U, W and k. Their values indicate a general good model performance with a slight underestimation of turbulent kinetic energy. All statistical metrics fall within the ranges proposed by [67] for urban environments and the more restricted intervals proposed by [68] with the exception the FB for k, which is slightly outside (0.3 vs 0.36). These differences are due to the differences between model set-up and wind-tunnel experiment. The inlet wind profiles and the size of the building array (7 rows of buildings in the model and 11 in the experiment) are different. It is concluded that the flow around the buildings for the BASE scenarios is well reproduced.

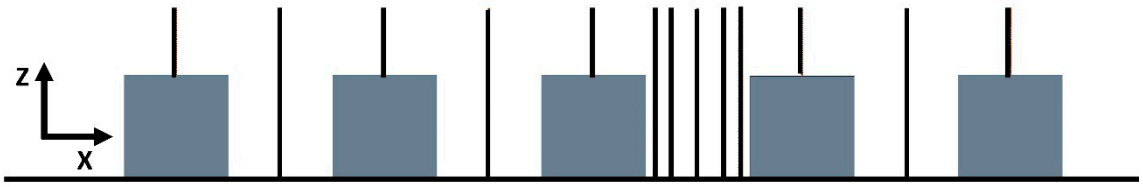

Figure S3. Location of measurements used in the model performance evaluation.

Table S1. Values of statistical metrics for the BASE scenario validation

	NMSE	**FB**	**FAC2**	**R**
(ideal value)	**(0)**	**(0)**	**(1)**	**(1)**
U_{norm}	0.04	0.13	-	0.99
W_{norm}	0.11	0.04	-	0.94
k_{norm}	0.19	0.36	0.83	0.85

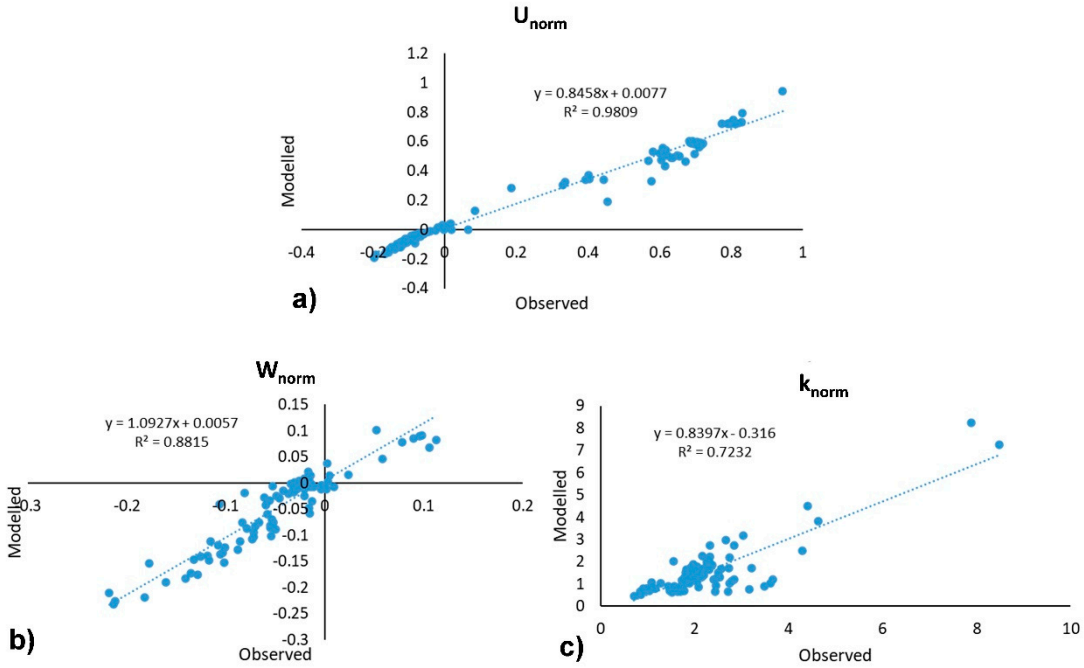

Figure S4. Scatter plot for normalized streamwise velocity (U_{norm}), normalized vertical velocity (W_{norm}) and normalized turbulent kinetic energy (k_{norm}).

Vegetation modelling cannot be evaluated over the same vegetation scenarios studied in the present paper since experimental data are not available for these configurations. However, previous studies validated the same vegetation model in several urban environments both in simplified and real configurations [32,40,41,56]. Krayenhoff et al. [56] evaluated the vegetation modelling (results in Supplementary material of [56]) using wind-tunnel experiments for a "continuous forest" [72] and a "forest edge" [73]. Flow through a continuous forest was simulated and mean horizontal velocity, turbulent kinetic energy and mean shear were compared with the experimental data from [72]. Forest characteristics correspond to cd = 0.2, LAD = 0.159 m^2 m^{-3} and a vegetation canopy height of 10 m. In general, the model captures the trends of the observations. The flow at the edge of a forest was also simulated and vertical profiles of horizontal velocity and turbulent kinetic energy at different locations were compared with data from wind-tunnel experiment [73]. In addition, results from another RANS model [74] and a large eddy simulation (LES) model were also included in the comparison. This forest had a LAI (Leaf area index, LAD*VegetationHeight) = 2. Overall, the performance of our model was acceptable, and no worse than the results obtained by [74] with RANS simulations for tuned coefficient of vegetation model, or [75] with LES simulations. In particular, better agreement is obtained for wind speed than for turbulent kinetic energy. These validations were presented in [56] and [41]. In addition, the current vegetation modelling applied to a scenario with vegetation in an urban environment was evaluated by using the CODASC experimental data [76,77]. A street canyon composed of two building with and without vegetation was simulated for an inlet wind flow perpendicular to the axis of the street. The ratio between the height of buildings (H) and the width of street (W) was 1 and between the length of the street (L) and the street width was 10. Vegetation was located along the street with the top at roof level and the size was 0.5H x 0.66H x 10H (streamwise x vertical x lateral). Two different tree porosities corresponding to a pressure loss coefficient (λ) in

wind-tunnel dimensions of 80 and 200 m^{-1} (0.53 and 1.33 m^{-1} at full scale) were simulated. These values correspond to LAD = 2.6 and 6.6 m^2 m^{-3} taking into account c_d = 0.2. Pollutant emissions were modelled by a line source in the street. Numerical domain was built following the best practice guidelines of COST Action 732 [57]. The distance between the inlet and street canyon and between the street canyon and the outlet were 7H and 15H respectively. Domain was meshed with a resolution of H/30 in the studied zone. Simulations with several turbulent Schmidt numbers were performed obtaining the best results for 0.3. Normalized concentrations close to both walls of the street canyon were compared with wind-tunnel measurements and statistical metrics (NMSE, FB, FAC2 and R) were computed (Table S2). Concentrations were slightly overestimated, however similar results were obtained by other studies performed using similar RANS models [-35,78,79] and LES models [80] over the same configuration. Table S2 shows that the statistical metrics were within the ranges proposed by [67] for all cases with similar agreement for cases with and without vegetation. Therefore, it was concluded that the aerodynamic effects of vegetation are reproduced by our vegetation modelling approach. This model evaluation was presented by [41].

Table S2. Values of statistical metrics for the model evaluation using CODASC experiment. Results taken from [41].

	NMSE	FB	FAC2	R
No Vegetation	0.04	-0.04	0.92	0.95
λ = 80 m^{-1}	0.12	-0.05	0.93	0.92
λ = 200 m^{-1}	0.17	-0.06	0.91	0.89

In addition, NOx dispersion in a real neighborhood with trees in the street was simulated by [40] with the same vegetation modelling approach used in the current paper. Model performance was evaluated by using data recorded in an air quality monitoring station (AQMS) located in the neighborhood. Time series of concentrations were compared and statistical metrics (NMSE, FAC2 and R) were computed to evaluate the model performance. Table S3 shows a good agreement between observed and modelled results with a slightly better fit when deposition is considered. All statistical metrics were within the ranges proposed by [68].

Table S3. Values of statistical metrics for the model evaluation using AQMS data from a real neighborhood of Pamplona, Spain. Results taken from [40].

	NMSE	FAC2	R
Vegetation considering deposition	0.27	0.73	0.71
Vegetation without deposition	0.28	0.72	0.71

Vegetation model was also evaluated in a real vegetation barrier composed of a hedgerow and two trees [32]. Dispersion of black carbon (BC) emitted by traffic and the aerodynamic and deposition effects on concentration were simulated. Hedgerow was 1 m-height and 0.8 m-width and its LAD was 4.29 m^2 m^{-3}. LAD of both trees was 0.5 m^2 m^{-3}, however the dimensions were

different. The tallest tree was 10 m-height and the smallest was 4 m-height. BC concentration was measured at three points at 0.4 m-height during an experimental campaign. One point was taken as reference (upwind to the barrier) and the other two points was located, one just after the hedge (green point) and the other at the same distance from road but without vegetation that shelter the pollutant dispersion. Modelled concentration reduction (27.8% in blue point and 45.4 in green point) obtained for perpendicular winds to the barrier was similar to average concentration measured (20% in blue point and 44.4 in green point). Further model evaluations were performed in other previous studies. Pollutant concentrations (NO_x, NO_2, PM_{10}) were appropriately modelled in real environments with urban vegetation that used the same vegetation model to simulate the effects of trees on air quality [15,19,24,62]. In conclusion, the vegetation model used in the current paper is suitable to simulate the vegetation effects on air quality.