Indoor-outdoor pollutant concentration modelling: a comprehensive urban air quality and exposure assessment

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Abstract
This paper is devoted to the investigation of the relationship between concentrations of traffic-related pollutants at pedestrian level in the street and indoor pollutant concentrations inside different rooms of different floors of a standard building. CFD modelling covering the whole urban environment, including the interior of a target building, is used to explicitly simulate wind flow and pollutant dispersion outdoors and indoors. A wide range of scenarios considering different percentage and location of open windows and different wind directions is investigated. A large variability of indoor pollutant concentrations is found depending on the floor and configuration of the open/closed windows, as well as the wind direction and its incidence angle. In general, indoor pollutant concentrations decrease with floor, but this decrease is different depending on the scenario and the room investigated. For some conditions, indoor concentrations higher than the spatially averaged values in the street (up to a ratio of 1.4) are found in some rooms due to the high pollutant concentrations close to open windows. This behavior may lead, on average, to higher exposure inside the room than outside although, in general, indoor pollutant concentrations are lower than that found in the street at pedestrian level. Results are averaged for all scenarios and rooms being the average ratio between indoor and outdoor concentrations 0.56 ± 0.24, which is in accordance with previous studies in real buildings. This paper opens to a unified approach for the assessment of air quality of the total indoor and outdoor environment.

Keywords Computational fluid dynamics (CFD) · Building in urban environment · Vertical indoor pollution variation · Ventilation through open windows · Indoor/outdoor concentration ratio · Traffic-related pollutants

Introduction
The impact of air pollution on human health has become an important problem in cities due to the high pollution levels and the increased percentage of people living in urban areas. More than half of the global population lives in cities, a percentage that is even higher in some areas such as Europe (> 70%), and it is foreseen that it will continue to increase in the next years (WHO 2018). In urban areas, vehicular traffic is often the main source of air pollutants. Since air ventilation in streets is significantly inhibited compared with open spaces (Buccolieri and Hang 2019; Peng et al. 2020), higher pollutant concentrations may occur, increasing population exposure to air pollution.

The assessment of such exposure to air pollution in urban areas is important to understand its potential impact on human health but remains a major challenge. Population exposure is usually related to outdoor air pollution, being correlated with a variety of health endpoints (Brunekreef and Holgate 2002; WHO 2016). To derive the exposure and its corresponding impacts on health, measurements recorded at air quality monitoring stations are used (Pope et al. 2009; Adar et al. 2010; Naddafi et al. 2012; Elliot et al. 2016). However, the spatial representativeness of measurements in urban environments is usually limited (Santiago et al. 2013) because the large variability of pollutant concentrations (such as nitrogen oxides (NOx) and particulate...
matter (PM)) within streets (Vardoulakis et al. 2003, 2011; Di Sabatino et al. 2013; Gromke and Blocken 2015; Borge et al. 2016, 2018; Santiago et al. 2017a, 2020). Alternatively, health impact assessments may rely on concentration values predicted by mesoscale chemical-transport models (Boldo et al. 2014; Izquierdo et al. 2020). Although the accuracy of the mesoscale models is increasing, they can provide only spatially averaged (over the grid cells) values (Buccolieri et al. 2021). Considering these limitations, the question that naturally arises is:

Is the concentration measured in the streets (or modelled by a mesoscale model) representative of the amount of pollutant to which people are exposed?

The answer to this question is complex and sophisticated methodologies must be used to assess the link between exposure and concentration distribution depending on differences between outdoor and indoor environments, atmospheric conditions, and urban morphology.

Models able to simulate pollutant dispersion at high resolution are necessary to obtain accurate estimates of the spatial distribution of pollutants both outdoor and indoor. Recently, a street-canyon model has been used by Van Brusselen et al. (2016) to investigate population exposure to several pollutants in Antwerp (Belgium). More complex models like computational fluid dynamic (CFD) models have been also applied to estimate population exposure to nitrogen dioxide (NO₂) in Pamplona (Spain) (Rivas et al. 2019; Santiago et al. 2022a) and to NOX in an urban area of Madrid (Spain) (Santiago et al. 2021).

Furthermore, the sole analysis of flow and dispersion outdoor may not be sufficient to assess the total exposure to air pollution since people spend most of their time indoors. For instance, Lai et al. (2004) found that participants in a personal exposure study spent 89.4% of their time indoors. Some studies (e.g., Fantke et al. 2017) used effective indoor-outdoor population intake fraction to estimate exposure. Specific attention has also been paid to the role of ventilation (Tham 2016; Śmiełowska et al. 2017; Li et al. 2017; Kelly and Fussell 2019). In general, the relation between outdoor and indoor air pollution varies depending on factors such as climate, emission sources, human activity, urban morphology or building ventilation. The source of indoor pollution can be indoor (smoking, cooking, etc.) or outdoor in case of infiltration due to penetration and ventilation (natural and forced) (Li et al. 2017). The relationship between indoor and outdoor pollutant concentrations has been demonstrated to be highly variable. Chen and Zhao (2011) found in their review that the relationship between indoor and outdoor particles concentrations varies within an enormous range depending on many factors. The recent review by Hu and Zhao (2020) indicated that indoor/outdoor NO₂ concentrations ratio differs between countries and regions, thus highlighting the differences in indoor NO₂ source strength and ventilation intensity. The influence of neighbouring structures on natural ventilation has been found important as well (King et al. 2017; Buccolieri et al. 2019). Some general patterns can be derived from these studies. For instance, if the building packing density is large, there is a reduction in pressure difference across buildings and thus the force driving the ventilation, limiting the possibility to use natural ventilation. Modelling approaches with different complexity have been applied to investigate the relationship between indoor and outdoor air pollution. Meng et al. (2005) used a single compartment mass balance model combined with measurements to assess indoor and personal PM₂.₅ concentrations in 212 residences. For air pollution exposure assessment, air exchange rate empirical and physically based models have been developed (Breen et al. 2014). To take into account the spatially and temporally resolved air exchange rate to investigate acute air pollution-related morbidity, Sarnat et al. (2013) used a hybrid modelling approach for outdoor concentrations and a simple air exchange rate estimation. The hybrid model fused spatially interpolated background concentrations and results from the stationary local-scale air quality model AERMOD (Cimorelli et al. 2005). To obtain more accurate estimations, even at the expense of computational load, CFD models are applied to ventilation problems (Jiru and Bitsuamlak 2010). Some studies simulated the outdoor environment through CFD models, and the indoor environment and the indoor-outdoor exchange through a simpler approach (e.g., building simulation tools) using the boundary conditions from CFD (Jiru and Bitsuamlak 2010; Song et al. 2018). Other works are based on the simulations of the whole domains through CFD models. However, most of them have been usually applied to simple cases, e.g., one block with several openings (Blocken 2018). Few cases consider more realistic buildings located in an urban environment. Among these studies applied to more complex cases are Cheung and Liu (2011) and Yang et al. (2015). Cheung and Liu (2011) simulated the impact of neighbouring structures on natural ventilation in a building cluster using a CFD model. Buildings were considered as one block with several open windows. Yang et al. (2015) investigated the effect of traffic pollution on indoor pollutant concentrations at different floors of naturally ventilated buildings in a street canyon taking into account different opening percentages of windows.

The present paper intends to take one more step towards a comprehensive assessment of urban air quality modelling and population exposure assessment. CFD modelling is used to explicitly consider important factors that change
the indoor/outdoor concentrations like the room floor or the configuration of open windows. In the present study, realistic rooms are simulated. Unlike Yang et al. (2015), rooms located at the windward side of the buildings are not connected to the rooms located at the leeward side; hence, pollutants from one street do not enter the other street through the building. In addition, this study is not focused on a street canyon but an urban environment composed of a regular array of buildings. To provide a better estimation of the concentrations people are exposed to, the main objective of this paper is to investigate the relationship between concentrations of traffic-related pollutants at pedestrian level in the street and indoor concentrations inside different rooms of different floors of a standard building of apartments in an urban environment. This study focuses on natural ventilation, and the main novel contributions are as follows:

• The realistic modelling of the target building and the explicit effect of room location and open windows on indoor concentrations. CFD simulations are performed to cover not only the whole urban environment around buildings but also the indoor of the target building (structured in realistic rooms on different floors). This approach, which is not usually considered in the literature, allows to explicitly compute outdoor concentrations with high spatial resolution and indoor concentrations in different rooms of a standard building. Wind flow patterns around the target building and the ventilation of the rooms (velocities and flows across the windows) are discussed to explore the relationship between indoor and outdoor concentrations depending on several factors (wind direction, configuration of open windows, and room location).

• The analysis of the variation of outdoor and indoor concentration depending on different factors (room floor and location, open windows and wind direction), which has not been extensively studied in previous works (Bo et al. 2017). The detailed CFD simulations and the wide range of simulated scenarios allow for explicitly estimating this variability in urban environments. The fact that indoor concentrations are investigated in rooms located on different floors and for different sides of the building is a novel aspect that has not been previously addressed. In addition, this study provides beyond state-of-art knowledge, by considering different configurations of open windows in the building façades and its impact on the ratio between indoor and outdoor concentrations.

The studied urban configuration and simulated scenarios are presented in the “Description of scenarios” section. CFD model is described and evaluated in the “Model description, simulation setup and model evaluation” section. The “Results” section presents the analysis of outdoor and indoor pollutant concentrations for different wind directions (subsections “Pollutant concentrations for wind direction perpendicular to the array (0° scenarios)” and “Influence of wind direction on pollutant concentrations” sections) and the population exposure (“Discussion” section). Discussion and conclusions are given in the “Summary and conclusions” section.

Description of scenarios

An idealized urban configuration representative of a real neighbourhood of high buildings separated by avenues is investigated in this paper. It is composed of an array of $7 \times 7$ cubes (Fig. 1). The height of buildings (H) is 35 m and the ratio between the height of buildings and the width of the streets (W) is 1. Then, the packing density (i.e., the planar area index which is the ratio of the plan-built area occupied by roughness elements to the total area under consideration) is 0.25. This value is within the range of planar area indexes that typically occur in urban areas (Grimmond and Oke, 1999). Hence, the neighbourhood dimensions are $455 \times 455$ m. Flow around an array of cubes with a packing density of 1 was previously studied using wind-tunnel measurements by Brown et al. (2001) and this experimental dataset, which was previously used to evaluate CFD simulation performance (e.g., Lien and Yee 2004; Santiago et al. 2007), allows to assess the CFD modelling in the present paper. The interior of the central building (“target building” hereinafter) is modelled in detail. It is composed of 10 floors and 4 rooms per floor with several windows. The rooms are independent of each other and not connected through doors (Fig. 1). Following the Spanish Technical Code for Building Construction (CTE), a 30% window to wall ratio (WWR) is considered, which we assume representative of Southern European cities. The thickness of wall buildings is neglected. The emissions are located on two roads for each street (red area in Fig. 1).

Different scenarios with open and/or closed windows are investigated:

• all the windows closed (no infiltration assumption)
• all the windows open
Fig. 1  a Array of buildings with indication of the target building (central position) and emission sources coloured in red. X-direction façades and Y-direction façades are coloured in blue and orange, respectively. b Target building for WinOpen100 scenarios. c Target building for WinOpen50X scenarios. d Target building for WinOpen50Y scenarios. e Target building for WinOpen50XY scenarios. Open windows are coloured in yellow and closed windows in brown (for the scenarios refer to Table 1).

Table 1 Description of the investigated scenarios

| Wind direction (°) | Open windows in the building (%) | Open windows in X-direction walls (%) | Open windows in Y-direction walls (%) | Scenario         |
|-------------------|---------------------------------|--------------------------------------|--------------------------------------|------------------|
| 0                 | 100                             | 100                                  | 100                                  | 0_WinOpen100     |
| 50                | 100                             | 0                                    | 100                                  | 0_WinOpen50X     |
| 50                | 0                               | 100                                  | 0                                    | 0_WinOpen50Y     |
| 50                | 50                              | 50                                   | 50                                   | 0_WinOpen50XY    |
| 0                 | 0                               | 0                                    | 0                                    | 0_WinClosed      |
| 22.5              | 100                             | 100                                  | 100                                  | 22.5_WinOpen100  |
| 50                | 100                             | 0                                    | 100                                  | 22.5_WinOpen50X  |
| 50                | 0                               | 100                                  | 0                                    | 22.5_WinOpen50Y  |
| 50                | 50                              | 50                                   | 50                                   | 22.5_WinOpen50XY |
| 0                 | 0                               | 0                                    | 0                                    | 22.5_WinClosed   |
| 45                | 100                             | 100                                  | 100                                  | 45_WinOpen100    |
| 50                | 100                             | 0                                    | 100                                  | 45_WinOpen50X    |
| 50                | 0                               | 100                                  | 0                                    | 45_WinOpen50Y    |
| 50                | 50                              | 50                                   | 50                                   | 45_WinOpen50XY   |
| 0                 | 0                               | 0                                    | 0                                    | 45_WinClosed     |
| 67.5              | 100                             | 100                                  | 100                                  | 67.5_WinOpen100  |
| 50                | 100                             | 0                                    | 100                                  | 67.5_WinOpen50X  |
| 50                | 0                               | 100                                  | 0                                    | 67.5_WinOpen50Y  |
| 50                | 50                              | 50                                   | 50                                   | 67.5_WinOpen50XY |
| 0                 | 0                               | 0                                    | 0                                    | 67.5_WinClosed   |

- and three scenarios with 50% of windows open
  - all windows open in X-direction façade and closed in Y-direction façade
  - all windows open in Y-direction façade and closed in X-direction façade
  - 50% of windows open in X- and Y-directions

For each scenario four wind directions (WD = 0°, 22.5°, 45°, 67.5°) are simulated. All scenarios are described in Fig. 1 and summarized in Table 1. All scenarios are simulated for the same meteorological conditions (see the “Model description and simulation setup” section).
Model description, simulation setup, and model evaluation

Model description and simulation setup

CFD simulations (performed with STAR-CCM+ code) are based on Reynolds-averaged Navier–Stokes (RANS) equations with realizable $k$-$\varepsilon$ turbulence model, where $k$ is turbulent kinetic energy and $\varepsilon$ is the dissipation rate for turbulent kinetic energy. Large-eddy simulations (LES) are more accurate, but a much higher CPU cost is required and entails higher simulation complexity (Blocken 2018). Thus, in this study, the RANS approach is selected as a compromise between accuracy and computational resources required (Santiago et al. 2010; Dejoan et al. 2010; Cheung and Liu 2011; Yang et al. 2015). Pollutant is considered non-reactive, and it is modelled using a transport equation where diffusivity is related to turbulent Schmidt number $(Sc)$. The optimum value of $Sc$ is between 0.2 and 1.3 depending on flow properties and geometry (Tominaga and Stathopoulos, 2007). The decrease or increase of $Sc$ allows increasing or decreasing the diffusivity, respectively. In this paper, a value of $Sc = 0.3$ was used (Sanchez et al. 2017; Santiago et al. 2017b, 2020). The equations are solved with a segregated solver using a second-order numerical discretization.

The computational domain is built following the best practice guidelines of COST Action 732 (Franke et al. 2007; Di Sabatino et al. 2011). The domain height is 11 H and the distance between buildings and inlet and outlet boundaries was larger than 15 H. Symmetry conditions are imposed at the top of the domain and ground, building walls and closed windows are modelled as wall boundary conditions with wall functions. As for the ground, a roughness length $z_0 = 0.03$ m is set. The roughness of the walls of the building is neglected (smooth walls). This value is selected taking into account the relationship between equivalent sand-grain roughness height and aerodynamic roughness length, the first cell height close to the ground and the wall law limitation (Blocken et al. 2007). No infiltration of pollutants through closed windows is assumed. Neutral inlet vertical profiles of wind speed $(u)$, turbulent kinetic energy $(TKE)$, and $\varepsilon$ are used (Eqs. 1–3).

\[
\begin{align*}
    u(z) &= \frac{u_*}{\kappa} \ln \left( \frac{z + z_0}{z_0} \right) \\
    TKE &= \frac{u_*^2}{\sqrt{C_\mu}} \\
    \varepsilon &= \frac{u_*^3}{\kappa (z + z_0)}
\end{align*}
\]

where $\kappa$ is von Karman’s constant (0.4), $u_*$ is the friction velocity, and $C_\mu$ is a model constant (0.09). These profiles are widely used in CFD simulations over urban environments (Richards and Hoxey 1993; Buccoliieri et al. 2011; Santiago et al. 2017a). To simulate different inlet wind directions, wind speed profiles are imposed with different angles at the inlet boundaries of the numerical domain. The friction velocity is fixed as $u_* = 0.22$ m s$^{-1}$ indicating a velocity logarithmic profile at the inlet with 3.2 m s$^{-1}$ at 10 m. Similar inlet wind speeds were used in other studies (e.g., Santiago et al. 2017a; Sanchez et al. 2017; Rivas et al. 2019). Around the target building, the spatially-averaged wind speed at pedestrian level (at 3 m height) obtained in the CFD simulations ranges between 0.4 and 0.7 m s$^{-1}$ depending on the simulated case. In this paper, the only pollutant source considered is traffic. Traffic emissions are homogeneously distributed along the streets where two roads with 3 lanes are modelled (Fig. 1). In addition, it is assumed that the pollutants are emitted from a volume with a height of 1 m above the ground (emission area) to consider the initial dispersion. The study is based on hourly scenarios and unsteady simulations of 1 h are carried out with indoor pollutant emissions and initial indoor concentrations set as 0 in all scenarios. The time step used is 1 s. However, it is found that the steady state was reached (or almost reached) for unsteady simulations in all scenarios. Therefore, the results are similar for both approaches (steady and unsteady). Therefore, simulated indoor concentrations are due to the transfer of traffic-related pollution from the outdoor.

Grid sensitivity and model evaluation

A grid sensitivity test is performed with three different computational grids taking as examples 0_WinClosed and 0_WinOpen100 scenarios. Previous studies (Lien and Yee 2004; Santiago et al. 2007) found that 12 cells in each direction were sufficient in resolving the flow around the cubes for this configuration. More than 16 cells in each direction are used, applying mesh refinements close to the surfaces (walls, windows, ground, and emissions) to capture the dispersion of pollutants and the effects of open windows accurately. Inside the array of buildings, all grids are composed of an irregular polyhedral mesh of around 2.5 m in each direction with refinement around the emission area, building walls, and windows. Two prism layers of 0.5 m around these surfaces are added. All gaps (e.g., windows) are resolved with at least 8 cells. The surfaces of the target building, windows, and emission areas are meshed with refinements of about 0.75 m.
in the coarse grid, 0.5 m in the medium grid, and 0.25 in the fine grid. The cell size growth rate from these refinements is 1.05. For coarse grid, each room, emission areas (as previously defined), and outdoor domain are approximately resolved with $8000 \times 10^6$, and $7.3 \times 10^6$ computational cells, respectively. Regarding the medium mesh, each room, emission area, and outdoor domain have 16,000, $2.2 \times 10^6$, and $9.3 \times 10^6$, respectively. And for the fine mesh, they had 21,000, $10.2 \times 10^6$, and $20.5 \times 10^6$ cells, respectively. Then, the total number of cells are $8.6 \times 10^6$, $12.3 \times 10^6$, and $31.7 \times 10^6$ for the coarse, medium, and fine meshes, respectively. Streamwise velocity ($U$), vertical velocity ($W$), and turbulent kinetic energy (TKE) at different vertical profiles around the central building for the three grids are compared. These variables are normalized with streamwise velocity and TKE at $3H$. The flow obtained around the buildings is similar for all meshes. For example, Fig. 2 shows the similar vertical profiles in the middle of the 3rd street (position 8 in the Fig. 3) obtained for the three grids. In addition, the pollutant transfer into the building indoor (initial indoor concentration = 0) is checked by comparing the results obtained using the three computational grids. 0_WinOpen100 is simulated with the three computational grids and the spatial average concentrations within each room of the central building (40 rooms) are compared. The average of differences between the concentrations in each room provided by medium and fine grids is 1%, the maximum being 5%. Therefore, taking into account that the wind flow around the buildings and the pollutant transfer to the indoor of the target building is similar for the medium and the fine meshes, the medium grid is selected for this study as a compromise between accuracy and computational cost.

Flow around the cubes is then evaluated by using wind-tunnel measurements (Brown et al. 2001). This experimental dataset has been previously used to evaluate CFD simulation performance (e.g., Lien and Yee 2004; Santiago et al. 2007). A vertical

![Fig. 2](image1)

Vertical profiles of a normalized streamwise velocity ($U_{\text{norm}}$), b normalized vertical velocity ($W_{\text{norm}}$), and c normalized turbulent kinetic energy (TKE$_{\text{norm}}$), in the middle of the 3rd street. These variables are normalized with streamwise velocity and TKE at $3H$.

![Fig. 3](image2)

Measurement locations considered to model evaluation.
clockwise vortex in the middle of the canyon is obtained. The center of the vortex is displaced to the center of the street canyon because the street canyon is not two-dimensional. This vortex shape was also found in the experiments of Brown et al. (2001) and the modelling studies of Lien and Yee (2004) and Santiago et al. (2007). Vertical profiles of streamwise velocity (U), vertical velocity (W), and turbulent kinetic energy (TKE) at several locations in the middle of the central row of buildings were compared (Fig. 3). These variables are normalized with streamwise velocity and TKE at 3H (U_norm, W_norm, and TKE_norm) and the model results at heights below 1.5H are evaluated by using fractional bias (FB), the normalized mean-square error (NMSE), the fraction of prediction that is within a factor of two of the observations (FAC2), and the correlation coefficient (R) (Eqs. 4–7):

\[ FB = \frac{\bar{O} - \bar{M}}{0.5(M + O)} \] (4)

\[ NMSE = \frac{\sum_{i=1}^{n} (M_i - O_i)^2}{\sum_{i=1}^{n} (M_i O_i)} \] (5)

\[ FAC2 = \text{fraction of data that satisfies } 0.5 \leq \frac{M_i}{O_i} \leq 2.0 \] (6)

\[ R = \frac{\sum_{i=1}^{n} \left[ (O_i - \bar{O}) (M_i - \bar{M}) \right]}{\sqrt{\sum_{i=1}^{n} (O_i - \bar{O})^2} \sqrt{\sum_{i=1}^{n} (M_i - \bar{M})^2}}^{0.5} \] (7)

where \( M \) are the modelled values extracted from CFD simulation and \( O \) are the observed values recorded in the wind-tunnel experiment. The bar over \( M \) and \( O \) indicates the average value of modelled and observed values. Note that FAC2 is only computed for TKE as it takes only positive values, while U and W do not. Results for these statistic metrics are shown in Table 2. In addition, the scatter plots of modelled variables vs observations are shown in Fig. 4.

The statistical analysis shows a good model performance with a slight underestimation of TKE. This fact may be due to two factors related to the differences between model setup and wind-tunnel experiments. The first difference is

![Fig. 4 a Scatter plot (modelled vs observed data) of the normalized streamwise velocity (U_norm); b same as a but for the normalized vertical velocity (W_norm); d same as a) but for the normalized turbulent kinetic energy TKE_norm](image)

Table 2 Model evaluation.

|          | NMSE | FB   | FAC2 | R   |
|----------|------|------|------|-----|
| U_norm   | 0.04 | 0.13 | -    | 0.99|
| W_norm   | 0.11 | 0.04 | -    | 0.94|
| TKE_norm | 0.19 | 0.36 | 0.83 | 0.85|
| Perfect model | 0   | 0    | 1    | 1   |
| Acceptable performance (Chang and Hanna 2004; Goricsán et al. 2011) | NMSE < 1.5 | −0.3 < FB < 0.3 | FAC2 > 0.5 | R > 0.5 |
the inlet profile of wind speed and TKE is different between the model (Eqs. 1–3) and the experiments. In the present study, neutral inlet vertical profiles of wind speed and turbulent kinetic energy imposed are described in Eqs. 1 and 2. However, in the wind tunnel experiment, the mean streamwise velocity can be described by a power-law profile and the experimental turbulent kinetic energy profile developed in the wind tunnel is slightly different from that described in the Eq. 2. The normalized results minimize the differences between variables; however, this small influence can be still visible. The second difference is the size of the building array—7 rows of buildings in the model and 11 in the experiments. The limit of the array can induce a slight influence on the results in the central row of buildings, and it is different depending on the size of the array. This fact can also be still visible in the normalized results.

**Results**

In this section, the street concentrations of traffic-related pollutants at the pedestrian level are related to the concentrations in different rooms of different floors of a standard building of apartments in an urban environment. The objective is to investigate the indoor concentration levels (generally not known) when compared to outdoor ground-level concentration (usually estimated) of pollutants. For this purpose, since indoor concentrations depend on wind flow and dispersion of pollutants around the building as well as the ventilation across the windows, these issues are also discussed. In the “Pollutant concentrations for wind direction perpendicular to the array (0° scenarios)” section, perpendicular wind scenarios are studied and the effect of wind direction is analyzed in the “Influence of wind direction on pollutant concentrations” section. In the “Discussion” section, population exposure is discussed.

To provide the results in a more generalizable way, the modelled concentrations at any location \((x, y, z)\) is normalized:

\[
C_{\text{norm}}(x, y, z) = \frac{C(x, y, z)u_*}{Q}
\]

where \(C(x, y, z)\) is the modelled concentration at the location \((x, y, z)\), \(u_*\) is the friction velocity of the inlet wind velocity profile and \(Q\) is the source emission rate in kg m\(^{-2}\) s\(^{-1}\).

**Pollutant concentrations for wind direction perpendicular to the array (0° scenarios)**

The interaction of the atmosphere with urban obstacles induces complex wind flow patterns in the street which drives the pollutant dispersion. An area of \(2H \times 2H\) with the target building in the middle (one unit of the array of buildings) is selected to investigate wind flow and pollutant dispersion. In these scenarios, pollutant emissions are...
located at ground and the inlet wind direction is orthogonal to the street canyons. The wind flow in street canyons shows a vertical clockwise vortex in the middle of the canyon, which results in a general decrease of concentration with height and higher concentrations at the leeward wall of buildings than that at the windward wall (Fig. 5). Similar pollutant distributions were found by other studies (Santiago et al. 2007; Angelidis et al. 2012; Martilli et al. 2015). The centre of the vortex is displaced to the centre of the street canyon as the street canyon is not two-dimensional. This shape of the vortex was also found in the experiments of Brown et al. (2001) and the modelling studies of Lien and Yee (2004) and Santiago et al. (2007). Wind flow and pollutant distribution in the street is different at each height (Fig. 6), which influences the indoor concentration of each room when windows are opened. In the bottom part of the street ($z = 3$ m above ground level, a.g.l.), a flow out of the canyon laterally and towards the leeward wall is produced.
by the divergence close to the ground of the downward wind flow at the windward face of the building. This fact explains that the maximum pollutant concentrations is located outside of the canyon (Santiago et al. 2007). In the middle of the street canyon (e.g., on the 5th floor), part of the air enters the canyon laterally creating two horizontal counter-rotating vortices at this height. At the top of the building (e.g., on the 10th floor), the flow is nearly parallel to the roof. At both heights, the maximum pollutant concentrations is located at the leeward wall, but the concentrations are lower than close to the ground.

This study focuses on estimating the pollutant concentrations to which population may be exposed, so not only the outdoor pollutant concentrations at pedestrian level ($z = 3$ m a.g.l.) but also the concentrations inside rooms of the target building is investigated. In this study, it is taken 3 m as pedestrian level because is the height where usually air quality monitoring stations measures pollutant concentrations.

**Fig. 7**

a) Wind flow around the study building at $z = 3$ m for 0_WinOpen100 scenario.
b) Normalized concentrations around the study building at $z = 3$ m for 0_WinOpen100 scenario.
c) Same as a but for 0_WinOpen50X scenario.
d) Same as b but for 0_WinOpen50X scenario.
e) Same as a but for 0_WinOpen50Y scenario.
f) Same as b but for 0_WinOpen50Y scenario.

The black line at the pedestrian level indicates the zone where the movement of pedestrians is allowed (sidewalks and pedestrian crossings).
and these measurements are widely employed to assess air quality. Thus, we will now examine cases with open windows.

It can be observed that the wind flow around the target building at pedestrian level is slightly altered due to the presence of nearby open windows (Fig. 7), so the differences of outdoor concentrations at the pedestrian level among scenarios are small. Comparing 0_WinClosed with the other scenarios with open windows, the maximum difference of the spatial average concentrations is lower than 2%. This suggests that opening windows in a building scarcely influences outdoor average pollutant concentrations, which is expected because windward and leeward façades of the building are not connected through the rooms and pollutants of one street does not enter to the contiguous street through the building. In this case, the volume of indoor air is much smaller than the volume of outdoor air and therefore its influence should be negligible. Therefore, outdoor exposure, considered as proportional to the spatial average outdoor concentration at pedestrian level, is similar regardless of the open window configuration.

On the contrary, indoor concentrations are different depending on an open window scenario. Pollutant concentrations in each room are dependant on the ventilating flow that rooms receive by having open windows, therefore indoor concentrations are strictly dependant on the façade orientation, the building floor and the location and the size of open windows. To illustrate this point, wind flow and pollutant dispersion at 3 m (first floor rooms) are investigated for 0_WinOpen100, 0_WinOpen50X, and 0_WinOpen50Y scenarios (Fig. 7). In this subsection, the discussion focuses on rooms A and C, because, results for rooms B and D are equivalent to those obtained for rooms A and C, respectively.

For the 0_WinOpen100 scenario, air enters the rooms A and C mainly across the windows of X-façade and flows out across windows of Y-façade being the air exchange rate across the windows slightly higher for room C \((\text{ACH} = 16.6)\) than for room A \((\text{ACH} = 15.8)\). ACH is air changes per hour and refers to the number of times that air is replaced in each room every hour. However, for 0_WinOpen50X and 0_WinOpen50Y, air flows in and out of the rooms only across windows of same façade (X-façade for 0_WinOpen50X and Y-façade for 0_WinOpen50Y). In both scenarios, air exchange rates through the windows are lower (for 0_WinOpen50X, \(\text{ACH} = 8.6\) and 4.8 through windows of rooms A and C, respectively; and for 0_WinOpen50Y, \(\text{ACH} = 3\) and 1.9 through windows of rooms A and C, respectively).

Concentration is larger in room C than in room A for all scenarios. This fact is due to room C being located at the leeward side of the street canyon where the concentrations are larger than for the windward side. The concentration in this room is similar for all scenarios because the concentration close to the windows of both façades are also similar. However, the situation is different in room A where the concentration is larger for 0_WinOpen50Y. This behaviour is related to the pollutant concentrations close to the windows and the flow rate through them. In this case, pollutant concentrations are higher close to Y-façade than close to X-façade, and while the airflow, and consequently the pollutants, enters the room across the windows of X-façade for 0_WinOpen50X and 0_WinOpen100 scenarios, for the 0_WinOpen50Y it occurs through the windows of Y-façade. Wind speed inside the rooms depends on the scenario and room location and a typical mean speed average is \(0.10 \pm 0.05 \text{ m s}^{-1}\).

To quantify these differences, the volume average concentrations in each room of each floor \((\text{C}_{\text{room}})\) are computed and compared with the surface average concentrations at pedestrian level in the street \((\text{C}_{\text{out}})\). As previously stated, this is taken at 3 m at the pedestrian level because this is usually the height at which air quality monitoring stations measure pollutant concentrations which are then widely employed to assess air quality. The ratio between both concentrations \((\text{C}_{\text{room}}/\text{C}_{\text{out}})\) at different floors for each scenario is shown in Fig. 8. In all cases, \(\text{C}_{\text{out}}\) is higher than \(\text{C}_{\text{room}}\) and, in general, the concentration decreases with increasing floor height. Inside Rooms A of the lowest four floors, the ratio \(\text{C}_{\text{room}}/\text{C}_{\text{out}}\) ranges from 0.35 to 0.52 for 0_WinOpen100, 0_WinOpen50X and 0_WinOpen50Y scenarios. This ratio decreases as the number of floors increases until it reaches a value of about 0.2 for the last floor. However, non-monotonic changes in concentration with height for 0_WinOpen50X and 0_WinOpen50XY scenarios are found due to the variation of wind flow and pollutant distribution around the building with height.

For the 0_WinOpen50Y scenario, \(\text{C}_{\text{room}}/\text{C}_{\text{out}}\) is higher (0.8) for the lowest two floors. As discussed previously, this behavior is related to the pollutant concentrations close to the windows and the flow rate through them. For the lowest floors of room A, pollutant concentrations are higher closer to the Y-façade than the X-façade; for the 0_WinOpen50Y scenario pollutants enter room A across windows of Y-façade.

While in the case of room C the trend is different, and in all scenarios, the ratio is close to 1 for the lowest floors. From the fifth to the tenth floor, the ratio for the 0_WinOpen50Y scenario decreases from 0.6 to 0.2 approximately. However, for the other three scenarios, the ratio ranges from 0.5 to
Influence of wind direction on pollutant concentrations

This section aims to expand the results to other wind directions (22.5°, 45°, 67.5°, see Fig. 1a). Different from the perpendicular wind scenarios, rooms A and C are not equivalent to rooms B and D, respectively; therefore, the concentration in all four rooms is investigated.

Pollutant distribution at pedestrian level is strongly different depending on wind direction (Fig. 9). At the pedestrian level, maximum concentrations are found in the horizontal vortex around the buildings because the residence time of pollutants emitted on the roads increases in these recirculation zones. Compared with the 0_WinClosed scenario, the average concentration at pedestrian level in the street is similar for 22.5_WinClosed and 67.5_WinClosed scenarios (differences around 3%). However, for the 45_WindClosed scenario, the average concentration increases by about 20% mainly due to the accumulation of pollutants in the wakes produced by the building in both façades. On the other hand, as for WD = 0° scenarios, it is observed that for these three wind directions, opening windows in a building scarcely influences the outdoor pollutant concentration. Wind flow, and consequently outdoor pollutant concentration, underwent slight modification close to the open windows in some scenarios (Figs. 10, 11, and 12); the maximum difference...
between average outdoor concentrations at the pedestrian level for scenarios with the same wind direction with and without open windows is less than 3%.

Concerning indoor concentration, unlike 0° scenarios, in some of these scenarios, \( \frac{C_{\text{room}}}{C_{\text{out}}} \) is greater than 1 for some rooms of the lowest floors (Figs. 13 and 14). This indicates that indoor concentration in these rooms is higher than the average outdoor concentration at the pedestrian level. It is important to note that, although the pollutant source is outdoor, these cases are possible because the indoor concentrations are compared with the spatially averaged concentration in the street at pedestrian level (and not with the maximum concentration in the street). The rooms receive pollutants from outdoor through the open windows, so indoor concentrations depend on flow through open windows and concentration close to them. Pollutant distribution at pedestrian level is strongly heterogeneous and, in these cases, pollutant concentrations near the open windows are...
larger than the average in the street inducing high indoor concentrations, also larger than the average in the street, but lower than the outdoor concentration close to the open windows.

For WD = 22.5° (Fig. 13), $C_{\text{room}}/C_{\text{out}}$ is greater than 1 in room C of the two lowest floors for 22.5\_WinOpen50X and the lowest floor of room D for the cases with open windows at X-façade. For this wind direction, the wake induced by the buildings produces an accumulation of pollutants in the X-façade of the leeward wall of the building (Fig. 10). Therefore, indoor concentration in rooms C and D is larger as the windows of X-façade are open and pollutants enter across these windows. For room C of the first floor, the maximum indoor concentration is obtained for the 22.5\_WinOpen50X scenario because outdoor air only enters across X-façade windows being $A CH = 2.6$. For a similar reason, the minimum is for the 22.5\_WinOpen50Y
scenario where room C receives pollutants across the windows of Y-façade being $\text{ACH} = 1.6$. Although the windows of X-façade are also open, room C concentration is lower for the 22.5_WinOpen100 scenario than for the 22.5_WinOpen50X scenario because the outdoor air enters across Y-façade windows and flows out through X-façade windows ($\text{ACH} = 13.9$). Regarding room D of the first floor, Y-façade is located on the leeward side of the building, and consequently, the concentration close to this façade is larger than in room C. For this reason, room D concentration for the 22.5_WinOpen50Y scenario is higher than room C concentration for the same scenario. For this wind direction, the maximum of room D concentration is obtained for the 22.5_WinOpen100 scenario where air flows across windows of both façades with an $\text{ACH} = 7.6$ (70% of flow through X-facades windows and 30% through Y-facades windows). For the 22.5_WinOpen50X scenario, $C_{\text{room}}/C_{\text{out}}$ in room D is
also greater than 1. In this case, ACH (the flow across the X-façade windows) is 4.2. Regarding rooms A and B, they have similar concentrations for all scenarios that decrease with height. Taking the average overall concentration for rooms on each floor, $C_{room}/C_{out}$ for each floor is similar for 22.5_WinOpen100, 22.5_WinOpen50XY, and 22.5_WinOpen50X scenarios. Its values range from 0.91–0.85 for the first floor to 0.38–0.31 for the last floor. However, for the 22.5_WinOpen50Y scenario, lower values are found and $C_{room}/C_{out}$ decreases with floor height from 0.70 to 0.23. Finally, considering the concentration averaged over the four rooms for each floor and over all open window scenarios, the ratio $C_{room}/C_{out}$ ranges from 0.85 for the first floor to 0.31 for the last floor and the standard deviation for each floor varies between 0.17 and
For 45° wind direction, the highest values of $C_{room}/C_{out}$ are obtained (Fig. 14). It reaches a value of 1.17 in room B of the first floor for the 45_WinOpen50Y scenario and room C of the first floor for the 45_WinOpen50X scenario (ACH = 3.8). For room D of the first floor, $C_{room}/C_{out}$ is greater than 1 for all scenarios being the maximum (1.42) for 45_WinOpen100 scenario. 45_WinOpen100 scenario has the X-façade windows opened; however, the wind flow enters room C across Y-façade windows (ACH = 13.7). For similar reasons, the minimum concentration of this room is obtained for the 45_WinOpen50Y scenario since Y-façade windows are open and X-façade windows are closed. Room B and room C have symmetric behavior, the highest concentration around room B is located in Y-façade. The highest indoor concentration is obtained in room D (located at leeward of the building) since high-polluted areas are found in both façades of the room. The maximum concentration is for the 45_WinOpen100 scenario where air flows into the room through the windows of both façades (ACH = 13). Regarding room A, it is located at the windward of the building and pollutant concentration at both facades is similar and lower than facades of the other rooms. For this reason, indoor concentration is similar for
all scenarios and lower than in the other rooms. The average overall indoor concentration for rooms on each floor is similar for all scenarios. \( C_{\text{room}}/C_{\text{out}} \) at each floor averaged over all scenarios ranges from 0.87 to 0.30 and the standard deviation at each floor varies from 0.28 to 0.1. ACH for rooms of all floors is shown in Appendix (Fig. 17). The results for 67.5° wind direction are analogous to those of the 22.5° case.

**Discussion**

This section aims to evaluate theoretical population exposure and its associated implications. To achieve this objective, an average concentration map is computed from the simulated scenarios. It is assumed that this map corresponds to the average concentrations over a theoretical time period, that is taken as a comparison reference. This assumption is done because the main focus of the present paper is to compare indoor vs outdoor concentration levels (including indoor concentration variability) and the corresponding differences between indoor and outdoor exposure estimates. CFD simulations require huge computational resources, and unsteady simulations of the time evolution of pollutant concentrations over long-time periods are not usually feasible. To address this issue, numerical
methodologies are used to compute long-term average pollutant concentrations. This kind of methodologies are based on combining the results of a set of CFD simulations for different wind directions (e.g., Santiago et al. 2017a; 2022b). For long-term average concentration estimates, there are several methodologies like WA-CFDRANS (Santiago et al. 2017b), which consists of a weighted combination of the simulated hourly scenarios considering wind speeds (pollutant concentrations are inversely proportional to wind speed) and directions. In addition, hourly traffic emissions are also considered. In the present paper, the results of our simulated scenarios are averaged assuming that each scenario provides hourly concentrations and this combination is the average concentration maps for a theoretical period. In future studies focused on real urban environment, more factors (e.g., annual meteorology, background concentrations, hourly traffic factors or indoor pollutant sources) could be taken into account for computing long-term average concentrations maps. Annual meteorology of the studied urban area would be considered to obtain frequencies of wind direction and wind speed for the weighted average. Background concentrations can be also considered for the annual average concentration computations. Their values can be obtained from urban background monitoring stations or mesoscale modelling and added to the concentrations from local emissions. In addition, the impact of indoor pollutant emissions on long-term average concentrations can be considered in future analysis simulating different scenarios with indoor pollutant sources in the different rooms. These sources can be modelled through pollutant sources in the pollutant transport equation and the results of the new scenarios can be used for computing long-term average concentrations. However, for traffic-related pollutants like particulate matter (PM) (at least Black Carbon) and NOx, indoor emissions should be negligible unless there are open burning activities (e.g., fireplaces) or cooking with wood or another biomass.

The first approach (approach 1) to estimate population exposure is to consider that all people are exposed to the average concentration at the pedestrian level during the time period studied. This assumption is the most used in the previous studies and it is employed as the reference value. The second approach (approach 2) is to assume that people are exposed to the average concentration over only the sidewalks at pedestrian levels. The third approach (approach 3) is to consider that people are uniformly distributed inside the building. Results of the previous sections show that the relationship between outdoor and indoor concentrations depends on several factors like the height of the floor, location of the room, wind direction and the distribution of open windows in the building façade. Thus, concerning the third approach, the following assumptions about indoor concentration and meteorological conditions are considered:

- Averaged indoor concentrations over all open window scenarios are considered.
- At each floor, indoor concentrations are averaged over all rooms and the standard deviation of concentrations is also computed to assess the variability of concentration, and so exposure.
- The frequency of each wind direction and the wind speed is the same during time period studied. This assumption means that there is no prevalent wind direction and results for all wind directions are combined.

Exposure estimates computed through approach 1 and 2 are similar because of the small differences between the average concentration over the whole study area and over the sidewalks. The differences are below 4%. In this case, people are considered to be exposed to the average concentrations. However, the exposure estimated by using indoor concentrations (approach 3) is lower. The ratio between approach 3 and by using the approach 1 is 0.56 ± 0.24, where 0.24 is the standard deviation. These results are in agreement with previous studies in real buildings. Meng et al. (2005) showed that the contribution of outdoor sources on indoor PM$_{2.5}$ concentration was 60% on average. Monn et al. (1997) found a PM$_{10}$ indoor/outdoor (I/O) ratio of 0.7 approximately where human activity was low and it increased to I/O ratios higher than 1.8 where human activity was larger. Nitrogen dioxide (NO$_2$) ratios ranged from 0.4 to 0.7 in the absence of NO$_2$ indoor sources, and it increased to I/O ratios greater than 1.2 where gas-cooking was present.

From the results of the present paper, the indoor exposure decreases reaching a value between 0.80 and 0.32 of the outdoor exposure. However, the population exposure throughout the day is a combination of outdoor pollutant concentration and indoor pollutant concentration. For instance, considering that people spent 89.4% of their time in indoor environments (Lai et al. 2004), the personal exposure during a day would be 0.61 ± 0.21 of the outdoor exposure. In this case, only traffic emissions are considered, and indoor exposure would increase when indoor sources like cooking or smoking would be taken into account.

**Summary and conclusions**

The main objective of this paper is to investigate the relationship between the concentration of traffic-related pollutants at pedestrian level in the street and concentration inside different rooms of different floors of a standard building of apartments in an urban environment. A novelty of this research is the realistic modelling of the target building since wind flow and pollutant dispersion in the interior of a standard building, while the urban environment around it is simulated through CFD modelling. The building has 10 floors, and it is modelled with 4 rooms...
per floor not open to each other. This realistic configuration is simulated for a wide range of scenarios considering different percentages and locations of open windows and different wind directions.

Results of indoor and outdoor concentrations show a strong variability depending on the floor and room location at each floor, as well as wind direction and the arrangement of open/closed windows. To provide a general view of the relationship between indoor and outdoor concentration, results are averaged for all scenarios and rooms, obtaining an average indoor-outdoor ratio of 0.56 with a standard deviation of ±0.24. These results are in agreement with previous studies in real buildings.

The results of the present paper show that indoor concentration in each room due to traffic emissions is highly dependent on the floor, the configuration of open windows and wind direction. For all cases, indoor concentrations decrease as the room floor increases. For some cases, concentrations in the lowest floor rooms reach a value larger than the average concentration in the street (e.g., indoor/outdoor concentration ratio of room D of the first floor for 45_WinOpen100 reaches a value of 1.42). As explained before, this ratio can be higher than 1 under certain conditions because indoor concentration is compared with the spatially-averaged concentration in the street at pedestrian level (and not with the maximum concentrations in the street). This means that in these cases the concentrations to which the population are exposed is, on average, higher inside the room than outside in the street. Therefore, to reduce the population exposure to traffic-related pollutants, mitigation strategies should be also addressed to improve indoor air quality. In future, the use of passive mitigation measures should also be investigated to improve indoor population exposure. To address this issue, these measures should be designed to reduce air pollution entering building rooms, with special attention to the rooms of the lowest floors. The rooms receive pollutants from the outdoor through the open windows, so indoor concentration depends on flow across open windows and outdoor concentration levels close to them. Then, indoor/outdoor concentration ratio higher than 1 is produced in rooms where pollutants are accumulated near at least one outdoor façade of the room, and the open windows induce the air to flow into the room from these highly polluted façades. In general, these rooms are found for some scenarios with non-perpendicular wind direction for the building side where outdoor concentration for the room façades is high (e.g., lowest floors, leeward walls, recirculation areas) and the windows of these façades are open. In future research, this kind of information could be used to design a smart system of opening and closing windows to optimize natural ventilation and reduce population exposure.

This paper focuses on natural ventilation and there are some limitations for several situations. Indoor and outdoor thermal effects and the possibility to add mechanical ventilation systems can modify air exchange rate, and consequently indoor concentrations. The present study intends to take one more step towards realistic indoor air quality modelling. However, future studies should be addressed to include in the simulations more physical effects like the indoor and outdoor thermal effects (e.g., modelled by means of thermal sources in model equations) or mechanical ventilation systems (e.g., modelled through momentum and turbulent sources). This study focuses on traffic-related pollutants and indoor pollutant sources are neglected. However, the presence of indoor pollutant emissions can modify the total indoor concentrations, and consequently the ratio between indoor-outdoor concentrations. In addition, there are uncertainties associated to that indoor pollutant sources. For traffic-related pollutants like particulate matter (PM) (at least black carbon) and NOx, indoor emissions should be negligible unless there are open burning activities (e.g., fireplaces) or cooking with wood or another biomass. In future studies, it would be helpful to investigate the impact of this kind of sources on indoor concentrations. These sources can be modelled in simulations through pollutant sources in the pollutant transport equations.

Overall, the present study connected outdoor and indoor concentrations of traffic-related pollutants finding that indoor air quality should be considered for the assessment of total population exposure. Indoor concentrations, and consequently population exposure, strongly depends on several variables like floor and room location on each floor, as well as wind direction and the arrangement of open/closed windows. In addition, the relationship between indoor and outdoor concentrations cannot be applied for every urban structure, and ventilation patterns for different building configurations may substantially change indoor exposure for the same outdoor pollution level. Therefore, more configurations including specific details of the building, the nearest outdoor obstacles like trees and distance of pollutant source from façade should also be investigated in future research.
Appendix

Fig. 15  

a Air changes per hour (ACH) for room A of each floor for 0_WinOpen100 scenario.
b Same as a but for room C.
c Same as a but for average concentration over the four rooms. The black line indicates the average over the four rooms for each floor and all scenarios, and the horizontal bars are the standard deviation.
Fig. 16  a Air changes per hour (ACH) for room A of each floor for 22.5\_WinOpen100 scenario. 
b Same as a but for room C. 
c Same as a but for average concentration over the four rooms. The black line indicates the average over the four rooms for each floor and all scenarios, and the horizontal bars are the standard deviation.
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**Data Availability** This datasets generated during the current study are available from the corresponding author on reasonable request.

**Declarations**

**Ethical approval** Not applicable.

**Consent to participate** Not applicable.

**Consent to publication** Not applicable.

**Conflict of interest** The authors declare no competing interests.
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