

1 **Shaping buildings to promote street ventilation: a large-eddy** 2 **simulation study**

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11
12 **Abstract** Proper ventilation of urban streets is important for safeguarding the health and comfort
13 of urban inhabitants. To compare the influence of different street canyon building geometries on
14 urban ventilation, large-eddy simulations (LES) have been performed under neutral stability
15 conditions. Five different street canyon building geometries have been tested: the i) flat roof, ii)
16 pitched roof, iii) round roof, iv) terraced building and v) building with balconies. The geometries
17 were configured as seven building arrays, with six street canyons in between them aligned in the
18 span-wise direction. The Air Exchange Rate (ACH) between the street canyons and the free
19 atmosphere has been computed for the different cases. The results show that the ACH is very
20 sensitive to the building geometry; therefore, it appears reasonable to suggest that buildings can
21 be shaped to promote urban ventilation. The paper also proposes an alternative ACH estimation
22 method based on the folded-normal distribution that is shown to produce very good estimates of
23 the LES-computed ACH. The new method uses vertical mean velocity and turbulence statistics
24 that can be obtained from less intensive Computational Fluid Dynamic (CFD) models. A
25 simplified two-reservoir Pollutant Concentration (PC) estimation methodology based on the
26 ACH results is also proposed.

27 28 **Keywords:**

29 Air Exchange Rate, Air Quality, Architectural Design, Large Eddy Simulation, Urban
30 Ventilation.

31 **1 Introduction**

32 The World Health Organization reported that in 2012, around 7 million people died prematurely
33 – one in eight of the total global deaths – as a result of air pollution. This finding more than
34 doubles previous estimates and confirms that air pollution is now the world’s largest single
35 environmental health risk (WHO, 2014). Since adverse air quality tends to be primarily an urban
36 problem, and given the very rapid pace of urbanization in this century (UNFPA, 2014),
37 maintaining good air quality in built areas is of paramount importance to safeguard the health
38 and comfort of urban inhabitants.

39 Air quality in cities is affected by ambient wind speed and direction, atmospheric stability, solar
40 radiation and anthropogenic pollutant emissions (Britter and Hanna, 2003). Thermal pollution
41 and chemical pollutant concentrations peak in cities, as opposed to the countryside, due to the
42 high and localized anthropogenic emissions, as well as to the topographical and surface material
43 properties of the urban fabric (Landsberg, 1981; Oke, 1987). Luke Howard, a British chemist and
44 meteorologist, was one of the first scientists to address this evidence through observational work
45 in the 1830s (Howard, 1838); and since then, research on urban air pollution has been on-going.
46 In the second half of the 20th century, the first comprehensive air quality policy was established
47 in the UK - the Clean Air Act of 1956 - which was followed by the US clean air act in 1963. Of
48 specific relevance to urban pollution, an effort to move polluting plants and manufacturing
49 outside of cities has been underway for decades. Vehicle circulation restrictions are also being
50 implemented in various cities. That is the case for Madrid, for example, with the newly approved
51 anticontamination protocol, or London, with the Low Emissions Zone (LEZ) regulation
52 established in 2008 (Transport of London, 2015). Similar policies are concomitantly being
53 implemented in other cities around Europe such as Paris, Milan or Budapest.

54
55 Nevertheless, since emissions are not the only factor contributing to pollution risk, regulations
56 that pertain to urban planning and architectural design considerations are also starting to be
57 implemented. The Hong Kong Air Ventilation Assessment (AVA) is one such regulation
58 formulated to assess the impact of architectural designs on the pedestrian wind environment (Ng,
59 2009; Ng, 2012). Such building design guidelines that promote urban ventilation by accelerating
60 pedestrian-level air flow and pollutant dispersion are becoming increasingly more important.
61 This is especially true for dense urban environments where urban ventilation is most

62 compromised (Oke, 1988b). However, despite Hong Kong's example, urban policies that
63 incorporate guidelines to promote urban ventilation are still scarce. The reasons for this are
64 numerous; one of the most important being the barrier posed by the technical expertise and effort
65 required for modelling of air flow and pollutant dispersion that many local administrations do not
66 possess to tailor regulations for their cities. This is why architectural and urban planning
67 processes often fail to incorporate design strategies to enhance urban ventilation (Oke, 1988a).
68 Therefore, the definition of broad design guidelines and urban ventilation estimation strategies
69 that are of wide applicability across many cities would be most useful for an easier
70 implementation of urban ventilation criteria within planning and architectural design processes.

71

72 While urban structures differ among different cities as well as between different neighbourhoods
73 within the same city, arguably one of the most characteristic world-wide urban typology is the
74 urban street canyon. The urban street canyon, is a typological urban configuration in which the
75 dominant sources of pollution, vehicle emissions, concentrate in close proximity to the
76 pedestrians (Britter and Hanna, 2003). Therefore, the urban street canyon has been often studied
77 as an archetypal model in the context of urban air quality, urban ventilation, and urban heat
78 island investigations, with the aim of developing a universal understanding of these problems
79 that is of wide applicability.

80

81 Within an urban street canyon, the presence of dominant circulation patterns and the turbulent
82 momentum and scalar exchanges between the inside and the outside region of the canyon are
83 very important aspects to take into account for dispersion calculations. For high building height
84 (H) to street width (W) ratios, a particularly adverse flow regime could occur where the flow
85 above the canyon skims across with minimal exchanges with the air inside the canyon (skimming
86 flow regime, (Oke, 1988b)). That is, for street canyons with a wind angle nearly perpendicular to
87 the main axis of the canyon, when the building spacing is reduced beyond a certain threshold, a
88 decoupling of the flows above and below the canyon occurs. One way to quantify these
89 exchanges is via a street canyon transfer velocity U_e , induced by mean (including dispersive) and
90 turbulent fluxes; this transfer velocity has been extensively studied both experimentally and
91 numerically (Vardoulakis et al., 2003). For air quality applications (or urban heat), the exchange
92 velocity is best defined through the average rate of mass (or heat) transfer in or out of the urban

93 canopy layer at a horizontal plane of interface between the in-canopy and above-canopy flows.
94 Britter and Hanna (2003) introduced the concept of exchange velocity for the first time and
95 studied the spatial temperature distribution and scalar exchanges at the plane of interface, to
96 conclude that U_e was approximately 1% of the characteristic wind velocity U_{ref} above the street
97 canyon. U_e is also frequently used in numerical simulations (e.g. Hamlyn and Britter, 2005;
98 Solazzo and Britter, 2007). Di Sabatino et al. (2007) and Di Sabatino et al. (2008) used the
99 exchange velocity to compare the performance of the $k-\varepsilon$ turbulence closure model and the
100 advection-diffusion method. Hamlyn and Britter (2005) estimated U_e as a fraction of U_{ref} and
101 found that it ranges from 0.3% to 1% for regular cube arrays with variable packing densities.
102 Solazzo and Britter (2007), through numerical studies, applied the concept of U_e to a street
103 canyon with weak buoyancy effect, and concluded that the temperature inside the street canyon
104 is nearly uniform and that U_e is about 1% of the free-stream wind speed.

105

106 Estimations of exchange velocities were also performed through experimental work. Barlow and
107 Belcher (2002) and Barlow et al. (2004) developed wind tunnel experiments using the
108 Naphthalene sublimation technique. In their analysis, they used the concept of a transfer velocity
109 to relate the flux out of the canyon to the concentration within it and reported that the transfer
110 velocity to wind speed aloft ratio varies with the building aspect ratio, reaching a maximum in
111 the wake interference regime. This regime occurs in street canyons with $0.3 < H/W < 0.65$ (i.e.
112 more widely spaced than the skimming regime) and is characterized by stronger vertical
113 exchanges and interactions of the wakes of distinct buildings. Salizzoni et al. (2009) estimated
114 the exchange velocity between the canyon and the external flow by measuring the cavity wash-
115 out time, that is, the time it takes for the whole air cavity volume of the street canyon to be
116 removed from the street canyon, and addressed the influence of the external turbulence on the
117 transfer process. Salizzoni et al. (2011) developed wind tunnel experiments using the PIV
118 technique and concluded that turbulent transfer is due to the coupling between the instabilities
119 generated in the shear layer above the canyons and the advected turbulent structures in the outer
120 boundary layer (the air above the urban boundary layer), and proposed to estimate the mass
121 exchange between a two-dimensional cavity and the overlying boundary layer by looking at the
122 pollutant wash-out from the cavity.

123

124 The exchange velocity has also been used for the so called “city breathability” concept that was
125 introduced by Neophytou and Britter (2005) to express the potential of a city to remove pollutant
126 and heat entrapment from urban environments. The same urban breathability ventilation
127 indicator was used, among others, by (Buccolieri et al., 2010; Panagiotou et al., 2013; Tominaga,
128 2012). Panagiotou et al. (2013) quantified city breathability using U_e and conducted Reynolds-
129 Averaged Navier Stokes (RANS) simulations for an inhomogeneous urban area to conclude that
130 urban morphologies determine the shape and size of vortical structures that are present in the
131 flow field, and thereby the exchange processes with the flow above. However the studies
132 developed did not systematically study the effect of building morphology. Buccolieri et al.
133 (2015), also through RANS simulation, studied city breathability by combining two ventilation
134 concepts: mean flow rate and age of air. They developed studies of aligned arrays of cubes with
135 variable areal building densities and concluded that the local mean age of air increases
136 substantially by increasing the density. A similar strategy was followed by Ramponi et al. (2015)
137 who looked at the ventilation performance of street canyons by means of the local mean age of
138 air. As described by Ramponi et al. (2015) the local mean age of air (τ_p) is a statistical measure
139 of the time it takes for a parcel of air to reach a given point in the flow field after entering this
140 flow field. That is, for urban wind flow, it can be defined as the average time it takes for the
141 external “fresh” air parcel that enters into the street canyon to then exit that canyon (Hang et al.,
142 2009).

143

144 Another frequently used ventilation indicator is the Air Exchange Rate (ACH), that is, the
145 volumetric air exchange between the street canyon and free atmosphere per unit time (Liu et al.,
146 2005). Liu et al. (2005), Riain et al. (1998), making use of LES, investigated the concept of air
147 exchange rate (ACH), pollutant exchange rate, average pollutant concentration, and pollutant
148 retention time, to quantify the street canyon ventilation and pollutant removal performance. Xie
149 et al. (2006) developed numerical studies to investigate the effect of solar radiation on the ACH
150 of an idealized street canyon and reported that the air exchange rate ACH_w induced by the
151 vertical velocity fluctuation w' is generally larger than ACH_w induced by the mean vertical
152 velocity \bar{w} .

153 Since LES requires high computational resources, Li et al. (2005) estimated ACH using the more
154 cost-effective RANS technique, by assuming isotropic turbulence at the top of the canyon. Their

155 RANS model used a $k-\varepsilon$ closure, and hence this isotropy assumption was needed to infer the
156 vertical velocity variance from the computed turbulent kinetic energy (TKE). The RANS ACH
157 was reported to produce a slight over prediction of the LES ACH, with a deviation within 20% .
158 These studies were followed by Cheng et al. (2009) who also used RANS with a $k-\varepsilon$ turbulence
159 closure to study street canyon ventilation & pollutant removal under various heating
160 configurations & building geometries. A similar approach was followed by Moonen et al. (2011)
161 who introduced the concept of Ventilation Potential (VP) and developed RANS and LES studies
162 of various street canyon and courtyard building geometries with variable angles of attack (angle
163 between the street canyon axis and the wind direction). The ventilation potential in that study
164 was described as a statistical measure to assess the removal of scalars and was defined by using
165 the magnitude of the flux through the plane of interface, normalized by the free-stream wind
166 speed and parameterized as a function of the courtyard's length-to-width ratio and of the angle of
167 attack of the incoming wind flow.

168

169 In these previous studies, various ventilation indicators (one should point out however that all
170 these indicators are correlated) have been utilized to assess the influence of parameters such as
171 building aspect ratios, incoming inflow turbulence characteristics, or angles of attack on the
172 street canyon urban ventilation. In cases when computationally less demanding approaches for
173 the computation of street ventilation have been sought, a RANS approach was selected. Some of
174 these prior studies that have used RANS models for the computation of street ventilation have
175 reported results to be within a reasonable uncertainty range in comparison to experimental or
176 LES results. However, given the inherent limitations of RANS models where all turbulent fluxes
177 (the full spectrum) need to be parameterized, the general validity of RANS to estimate the
178 ventilation potential of urban street canyons remains in question. RANS in general is particularly
179 challenged by complex geometries, similar to the ones we simulate here as presented later, where
180 intricate flow separation behaviour might occur (Slotnick et al., 2014). Given these limitations
181 and the fact that RANS models do not account for turbulent transport in a direct manner, they are
182 not ideal to calculate the air ventilation and pollutant dilution rates. LES on the other hand
183 captures the transport produced from a broader spectrum of scales, namely the large eddies that
184 in fact are the most important for canyon exchanges. LES explicitly calculates the resolved-scale

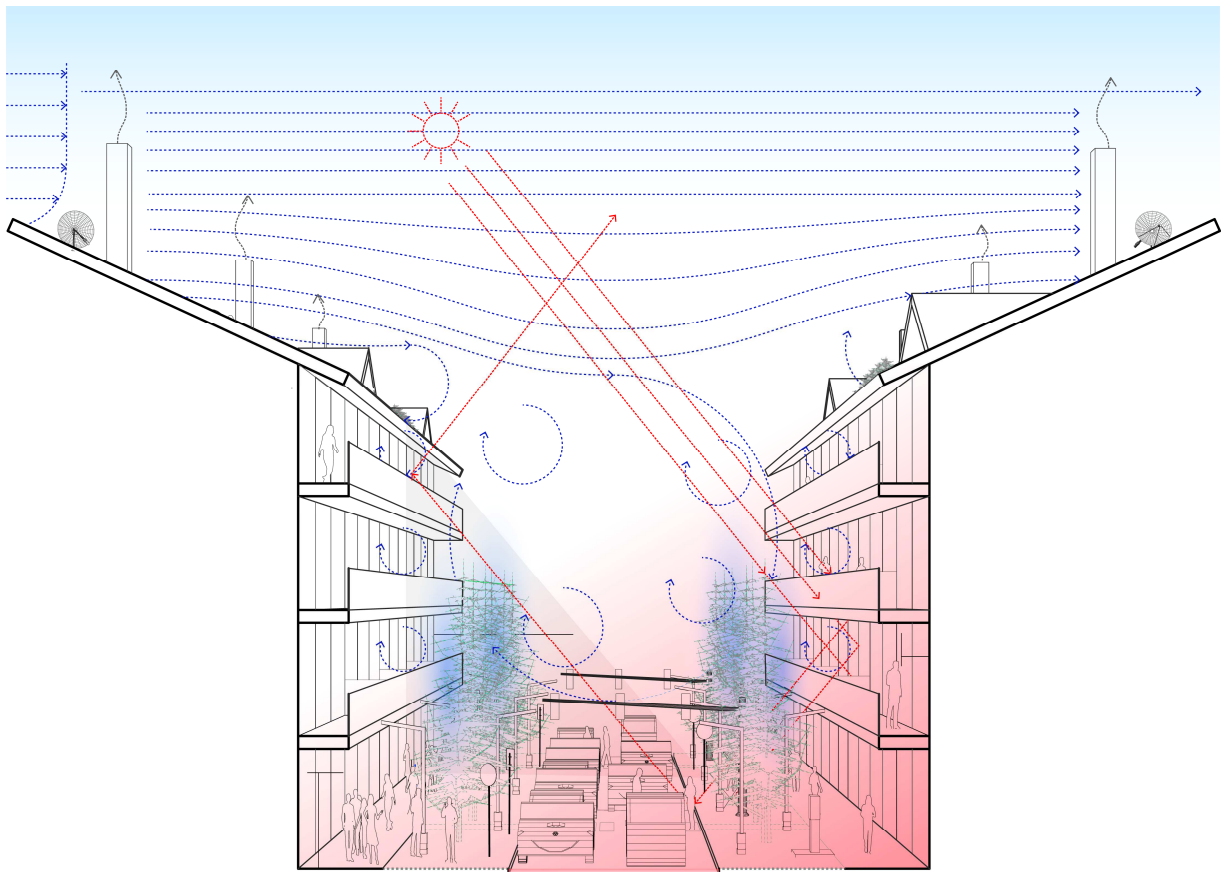
185 turbulent transport and models only small subgrid-scale processes. Therefore, LES is the tool of
186 choice for determining ventilation rates. Thus, for the street ventilation studies presented in this
187 paper, the LES technique has been utilized.

188 Another important aspect to take into account is that prior literature has mainly focused on the
189 study of ‘box like’ idealized building geometries disregarding the influence of further
190 architectural scale geometrical variations in street ventilation. That is, the morphological
191 parameters of urban street canyons have been generally reduced to the plan area λ_T and frontal
192 area λ_F densities. The total building plan area, A_P , and the total building frontal area, A_F , in a
193 total built lot of area, A_T , can be used to define the “lambda parameters”: the areal or planar
194 density being $\lambda_P = A_P / A_T$ and the frontal area density $\lambda_F = A_F / A_T$ (Britter and Hanna, 2003). To
195 a lesser extent, the influence of the building streamwise length (W) to height ratio, as well as the
196 influence of the angle of attack of the wind flow relative to the main street axis, have also been
197 researched. However, the majority of this literature investigated cuboid building shapes, i.e. flat
198 roofs. Only a limited number of prior studies have looked at more complex street canyon
199 building geometries, such as pitched roof configurations. Notably, these investigations have
200 found architectural geometrical variations to have a strong influence on the street canyon air flow
201 dynamics. Rafailidis (1997) and Rafailidis and Schatzmann (1996) developed wind tunnel
202 studies to investigate the influence of pitched roof building arrays on street flow and pollutant
203 dispersion and concluded that altering the roof geometry can have bigger impact on urban air
204 quality than modifying canyon aspect ratios. These investigations were followed by (Dezső-
205 Weidinger et al., 2003; Huang et al., 2009; Kastner-Klein et al., 2004; Kastner-Klein and Plate,
206 1999; Kellnerova et al., 2012; Takano and Moonen, 2013; Theodoridis and Moussiopoulos,
207 2000; Xie et al., 2005; Yassin, 2011) who through wind tunnel and numerical studies,
208 highlighted the role of roof geometry on street canyon air flow and turbulence statistics.

209 However, the main focus of these papers was not the estimation of urban ventilation. Therefore,
210 the effect of architectural considerations such as variable roof designs on urban ventilation
211 remains poorly understood. Furthermore, the impact of further architectural and street level
212 features, such as those depicted in (Fig. 1), on street ventilation is yet to be researched. These
213 knowledge gaps motivate this study, which aims to advance our understanding of urban
214 ventilation by considering the ACH of various street canyon geometries with variable façade and
215 roof geometries. A suite of LES cases is modelled to compute the air exchange rate for street

216 canyon morphologies with variable roof and façade configurations. The research complements
217 the experimental and LES results presented by Llaguno-Munitxa et al. (2017), where the focus
218 was on validating the LES and investigating the mean and turbulence statistics of the different
219 geometries. Further LES cases have been performed for this paper to compute the ACH of five
220 variations on building geometry, as detailed in the next section.

221



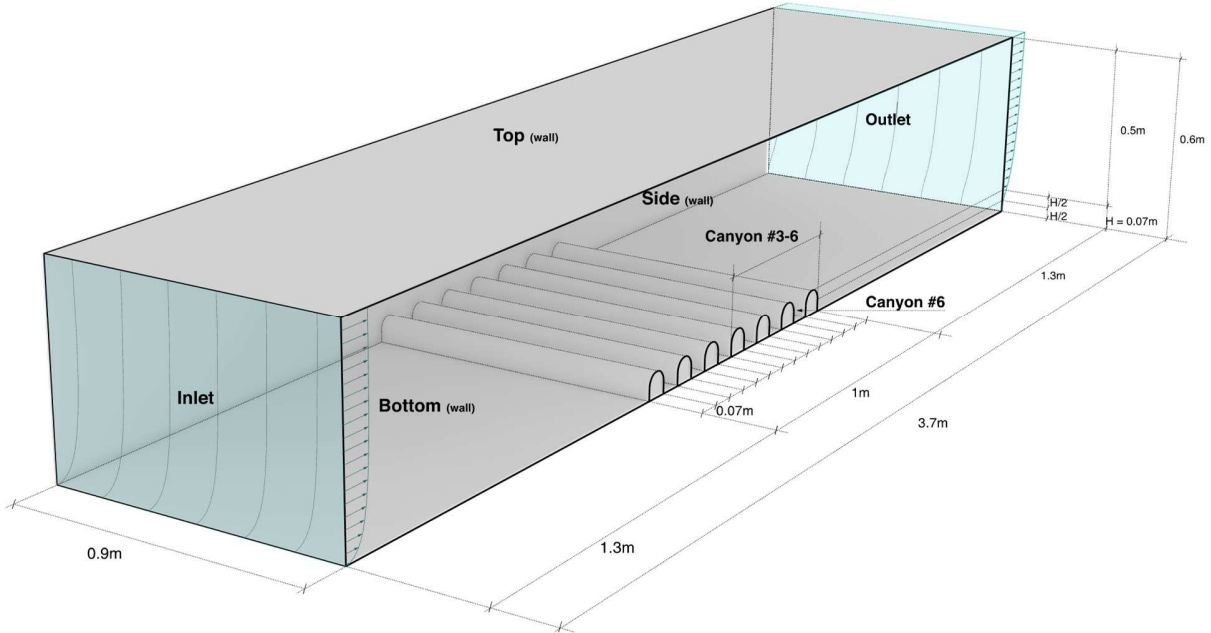
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223 **Fig. 1** Illustrative figure to show a typical urban canyon scenario. Pollutants emitted by vehicles
224 and chimneys, and the entrapment of thermal pollution are illustrated to show their dependence
225 on urban furniture and local architecture.

226

227 Specifically, the driving questions of this paper are: 1) How does roof and façade geometry
228 influence air exchange between a canyon and the air aloft? 2) How can this exchange rate be
229 accurately parameterized in the absence of the direct measurements allowed by LES (from the
230 mean velocity and TKE available through RANS for example)? How does the street level
231 concentration of a pollutant depend on the emission rate of that pollutant, its concentration above

232 the street canyon, and urban geometry? The details of the simulations are presented in the
233 following two sections, and the results are analysed and reported in section 4. A summary and
234 conclusions are included in section 5.



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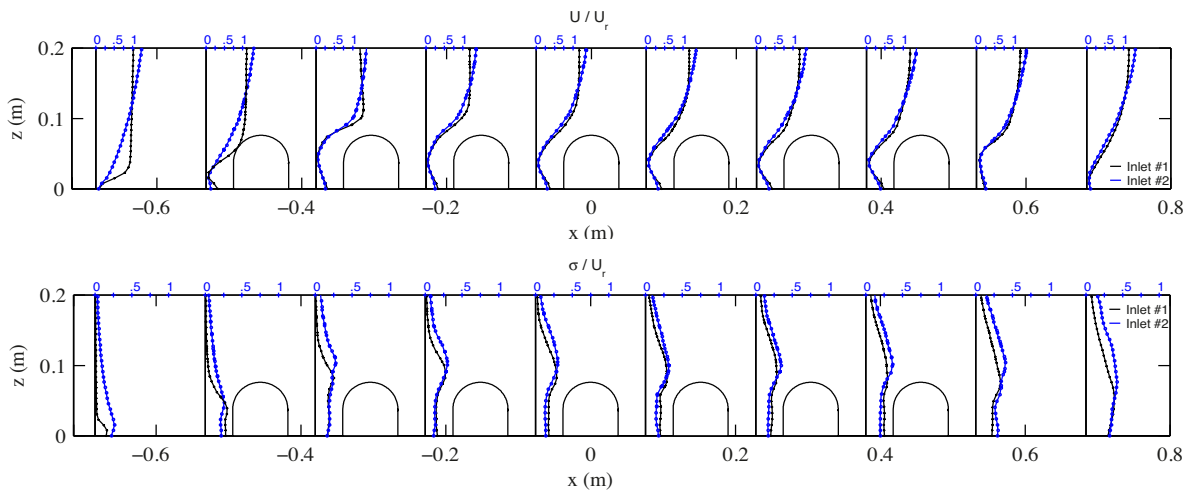
Fig. 2 A schematic of the LES computational domain.

238 **2 Building Geometries**

239 The computational domain is nominally 3.724 m long, 0.912 m wide and 0.608 m tall, and the
240 top, bottom, and side walls have been specified as hydrodynamically smooth wall boundaries
241 mimicking the cross section of the wind tunnel that was used to validate the LES code (Llaguno-
242 Munitxa et al., 2017). An underlying assumption is that the Reynolds number (Re) is sufficiently
243 elevated such that the results are not strongly dependent on the length scales used in the problem.
244 This assumption was investigated in Llaguno-Munitxa et al. (2017) and found to be acceptable,
245 though continued dependence on Re was noted since the code used (Fluent) does not discard the
246 viscous term as many codes used for atmospheric simulations do. Seven building arrays have
247 been positioned perpendicular to the approach flow and thus the resulting six street canyons are
248 aligned in the span wise direction (see Fig 2). In order to guarantee a fully developed wind
249 profile, the measurements and simulation data analysis have been conducted in Canyon#06, the
250 last downstream canyon. Figure (3) shows the vertical profiles of mean velocity for the central

251 axis for one of the tested geometries, the round roof, obtained with two different inflows (that we
 252 will detail shortly) to confirm that the results from the last one are indeed representative of a
 253 fully developed (i.e. infinite) array and not strongly dependent on the inflow. These results
 254 coincide with those obtained by Brown et al. (2000) who developed wind tunnel studies
 255 composed of a similar seven-building array configuration, and who reported that only after
 256 canyon #3 or #4 can the flow be considered “in equilibrium” or fully developed.

257



258

259 **Fig 3** The top figure displays the normalized mean velocity magnitude for the round roof
 260 geometry for the central axis of all 6 canyons (flow is from left to right). The bottom figure
 261 displays the total root mean square (rms) velocity σ_t for the central axis of all 6 canyons. Two
 262 inlet conditions are displayed (inlet #1 and inlet #2) as will be described in Section #3.

263

264 An aspect ratio of $S/H = 1$ has been defined for the street canyons (where S is the spacing
 265 between the buildings and H is their maximum height (the vertex for non-flat roofs). In the
 266 simulations, we use $S = H = 0.07$ m. The vortex circulation that is created in street canyons
 267 oriented perpendicular to the approach flow has been described in prior publications (e.g.
 268 Hunter et al., 1990). The angle of attack has been constrained to 90° in the present simulations,
 269 representing canyons that are perpendicular to the mean wind. The frontal area density λ_F and
 270 the plan area density λ_P (Britter and Hanna, 2003) have been kept constant and the atmospheric
 271 stability is neutral in all simulations since we aim to strictly focus on the influence of the
 272 architectural scale geometrical features. The building geometries that have been studied are: i)

273 the flat roof ii) the pitched roof, iii) the round roof, iv) the terraced building and v) building with
 274 façade balconies.

275

276 3 Numerical setup

277 Large-eddy simulations have been performed for the 5 studied building geometries. As opposed
 278 to RANS models, LES directly calculates the large-scale turbulent structures (larger than the grid
 279 or filter scale) and only requires modelling of the smaller scales. This is one of the main reasons
 280 why LES is at present the most appropriate tool for determining ventilation rates (at realistic Re)
 281 and has become widely used for turbulent flow simulation in engineering and environmental
 282 applications, including for urban flows (Anderson et al., 2015; Bou-Zeid et al., 2009; Giometto
 283 et al., 2016; Inagaki et al., 2012; Li et al., 2016; Nazarian et al., 2017; Xie and Castro, 2009;
 284 Yaghoobian et al., 2014). Here we use the LES solver of Ansys Fluent 14.5. The filtered LES
 285 continuity and momentum equations solved by Fluent LES reduce for incompressible neutral
 286 flow to:

$$287 \quad \frac{\partial \tilde{u}_i}{\partial x_i} = 0, \quad (1)$$

$$288 \quad \frac{\partial \tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_j} (\tilde{u}_i \tilde{u}_j) = -\frac{1}{\rho} \frac{\partial \tilde{p}}{\partial x_i} + 2\nu \frac{\partial \tilde{S}_{ij}}{\partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j}. \quad (2)$$

289 The tilde ($\tilde{\cdot}$) here denotes filtering; p is the pressure; u_i the velocity vector; x_i the position vector;
 290 S_{ij} is the strain rate tensor; τ_{ij} is the subgrid scale (SGS) stress tensor; ν is molecular viscosity;
 291 and ρ is the fluid density. The deviatoric part of τ_{ij} is modelled in Fluent via an eddy viscosity
 292 closure ($\tau_{ij}^D = -2\nu_t S_{ij}$), while the isotropic part is added to the pressure as is common in many
 293 LES codes (see for example Bou-Zeid (2005)) . The Algebraic Wall-Modelled LES (WMLES)
 294 SGS model has been used in the numerical experiments. WMLES is a hybrid RANS/LES
 295 method (RANS is used in the regions where the turbulence is in equilibrium and LES is used
 296 where non-equilibrium occurs). Through this approach, the need to resolve the viscous sublayer
 297 is relaxed (wall-resolved LES, see Pope (2000)) and the computational cost of the simulations is
 298 substantially reduced. The SGS eddy viscosity ν_t in WMLES is calculated through the

299 formulation of Shur et al., (2008). This formulation combines a mixing length model for the
 300 RANS region, a modified Smagorinsky model (Smagorinsky, 1963) for the LES region, and the
 301 wall damping function of (Piomelli et al., 1988). The resulting expression of ν_t hence features a
 302 hybrid mixing length scale (ANSYS 2013):

$$303 \quad \nu_t = \min \left[(\kappa d_w)^2, (C_{smag} \Delta)^2 \right] S \left[1 - \exp - \left| - \left(\frac{y^+}{25} \right)^3 \right| \right]. \quad (3)$$

304 Here, d_w is the distance to the wall; S is the strain rate magnitude; $\kappa = 0.41$ is the von Kármán
 305 constant; $C_{Smag} = 0.2$ is the Smagorinsky model constant; and y^+ is the distance normal to the
 306 wall in viscous units. This LES model uses a modified grid filter scale to account for the grid
 307 anisotropies in wall-modelled flows:

$$308 \quad \Delta = \min \left(\max \left(C_w d_w; C_w h_{max}; h_{wn} \right); h_{max} \right), \quad (4)$$

309 where, h_{max} is the maximum length of the cell's edge, h_{wn} the wall-normal grid spacing, and
 310 $C_w = 0.15$ a constant.

311
 312 The SIMPLEC scheme is used for the pressure-velocity coupling. The spatial discretization for
 313 the momentum equation uses the Least Squares Cell based method for the gradient, standard
 314 method for the pressure, and bounded central differencing for the momentum. An implicit
 315 second-order scheme is used for the time advancement. The dimensional time step size has been
 316 set to $dt = 0.00025$ s. The cases have been run for 60,000 time-steps. The eddy turnover time is \sim
 317 0.0422 s due to the small spatial scale of the model (see table 2); therefore, each simulation
 318 includes about 355 eddy turnovers, which is sufficient for the statistics to converge. The time-
 319 step ensures that the Courant–Friedrichs–Levy (CFL) number is always smaller than 1 (≈ 0.06)
 320 at all grid points. The initial 40,000 time-steps were not considered in the calculations to remove
 321 the influence of the initial conditions, hence the results shown are averaged over the last 20,000
 322 time steps, equivalent to about 120 eddy turnovers (about 5 seconds in physical time).

323
 324 The simulation has been set so that it provides a sufficient degree of similarity with a typical
 325 urban-like street canyon environment, though the length scale of the model building was reduced
 326 to $L_m = 0.07$ m for the validations against wind tunnel experiments reported in (Llaguno-Munitxa

327 et al., 2017). An equivalent real world prototype would have a characteristic length scale of $L_{\text{ref}} =$
 328 15 m (typical street canyon building height), and a typical urban characteristic velocity of $U_{\text{ref}} =$
 329 2 ms^{-1} . Therefore, the studied length scale ratio L_m/L_p between the model and the real building is
 330 $\approx 1/200$. The LES simulations have been conducted at $U_r = 1.8 \text{ m s}^{-1}$, the upstream incoming air
 331 velocity at $2H$, corresponding to a Reynolds number $Re_M = 9.12 \times 10^3$, based on the 0.07m length
 332 scale of the buildings and an air viscosity of $1.5 \times 10^{-5} \text{ m}^2 \text{ s}^{-1}$. Given the scale differences between
 333 the model and the prototype, the required velocities to be achieved to meet dynamic similarity
 334 (match Re) were not reproducible in the wind tunnel as described in (Llaguno-Munitxa et al.,
 335 2017), and subsequently they were not reproduced in all numerical simulations. Re will have
 336 some quantitative impacts on the results, especially so for the round roof geometry case, that
 337 were assessed by conducting simulations at an $Re \approx 2 \times 10^6$ that is closer to typical real-world
 338 values (see Llaguno-Munitxa et al., (2017)). The broad conclusion from that study is that the
 339 impact of geometry on urban ventilation will not be drastically influenced by the Re (Llaguno-
 340 Munitxa et al., 2017), and thus geometries can be compared for their ventilation potential using
 341 the smaller domain simulation we already conducted (although quantitative results will be
 342 sensitive to Re). Given these findings, and given the variability of Re in various real-world
 343 applications, we focus here on the larger number of simulations performed at the same Re as, and
 344 validated against, our previous wind tunnel studies.

345

346 A grid with hexahedral cells is employed in the three-dimensional domains. Grid sensitivity
 347 studies were performed for the computational mesh and a grid cell resolution of
 348 $0.007 \times 0.007 \times 0.007 \text{ m}$ has been adopted. The exact number of grid nodes varied between
 349 geometries, but it was $\approx 4.75 \times 10^6$ nodes with $\approx 80 \times 120 \times 490$ spanning the z , y , and x directions,
 350 respectively. A distance of 1.308 m was left between the first street canyon model and the inlet
 351 of the domain and from the last canyon model to the outlet, mimicking the wind tunnel. The
 352 essential simulation parameters are summarized in Table 1.

353 **Table 1.** Numerical set-up parameters

Front/top area density	$\lambda_p \lambda_t = 0.076 \text{ m}$
Inlet velocity	$U_r = 1.8 \text{ ms}^{-1}$
Local grid scale	$\Delta = 0.0076 \text{ m}$

Flow time across full domain	$T_{FD} = L U_r^{-1} = 2.06 \text{ s}$
Time computed	$T_c = 5 \text{ s}$
Building-scale eddy turnover time	$T_{T0} \approx H U_r^{-1} = 0.0422 \text{ s}$

354

355 The outlet has been specified as a zero-gradient boundary to generate a fully developed flow. For
356 the inlet, a mean logarithmic velocity profile with a fluctuating velocity generated using the so-
357 called “Vortex Method”, which generates a time-dependent inlet condition through the
358 introduction of a random 2D vortex as detailed in Fluent theory guideline (ANSYS 2013), has
359 been used with 190 vortices. The turbulent intensity has been set to 5% and the turbulent to
360 molecular viscosity ratio to 10. The log law mean profile simply follows the classic formulation:

$$361 \quad u_z = \frac{u_*}{k} \left[\ln \left(\frac{z-d}{z_0} \right) \right], \quad (5)$$

362 where the upwind terrain roughness is set to $z_0 = 0.03 \text{ m}$, the friction velocity to $u_* = 0.34 \text{ ms}^{-1}$,
363 and the displacement height to $d = 0.03 \text{ m}$. This results in an inlet profile that has significant
364 shear at the scale of the building, mimicking inflow from other buildings upwind. The same inlet
365 conditions (called *Inlet #2*) have been applied to all studied building geometries. More details on
366 the numerical setup can be found in Llaguno-Munitxa et al. (2017).

367

368 The simulations were also performed with a laminar inlet and a homogeneous flow profile
369 (called *Inlet #1*). Fig. 3 displays the results obtained with the two different inlet conditions. *Inlet*
370 *#1*, that is the laminar inlet, and *Inlet #2*, the turbulent log profile. This comparison aims to
371 display the self-similarity of the mean and turbulence statistics after canyon 3 or 4. Therefore,
372 Fig. 3 confirms that by canyon #6 (the canyon that this paper will be focusing on) the flow
373 characteristics are not as sensitive to the inflow conditions as they are from canyon #1 until
374 canyon #3. This consideration is important given the variability of inflow conditions that can be
375 present in urban environments. The results obtained following the present numerical setup are
376 thus considered to provide a sufficient degree of comparability to general urban like inflow
377 conditions over large neighbourhoods with similar geometries.

378

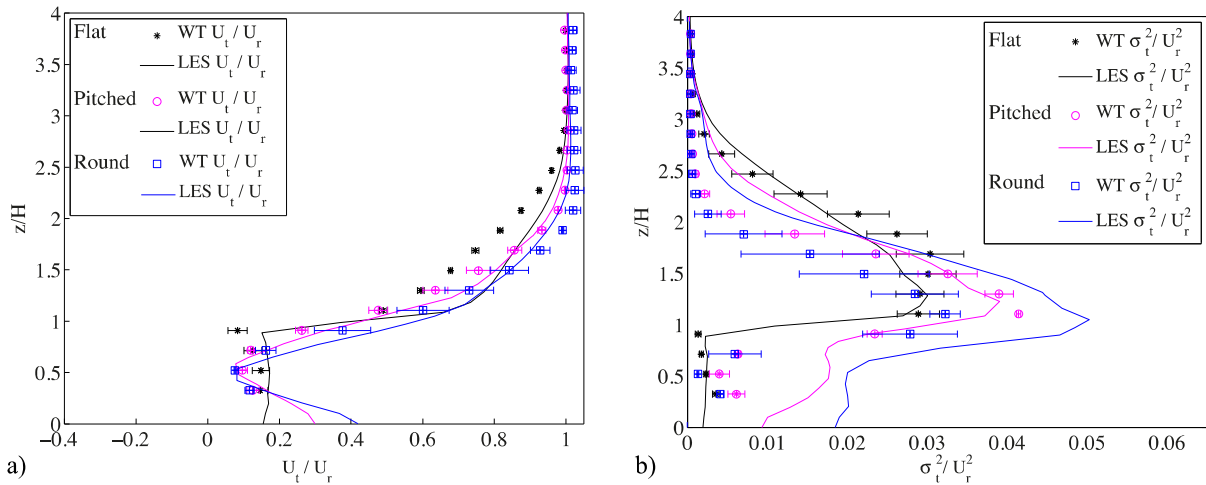
379 4 Validation

380 The code with the same numerical and domain setup was extensively validated in Llaguno-
381 Munitxa et al. (2017). As such, here we will only provide a summary of these validations so the
382 reader can appreciate the strengths and weaknesses of the LES for the flows investigated in this
383 paper.

384 The numerical experiments (using Inlet #1) have been validated against the wind tunnel data
385 collected by Llaguno-Munitxa et al. (2017) for canyon #6 and for three of the tested building
386 geometries, the flat roof, pitched roof and round roof geometries. In figure (4), the LES mean
387 and variance results are compared for canyon #6, and for the flat, pitched, and round roof
388 geometries, against the wind tunnel results. The comparison of the wind tunnel and LES results
389 for the flat roof geometry show a good agreement, with the largest discrepancies at heights
390 between $1H$ and $2H$ for the mean velocities. The σ_t^2 (the sum of the streamwise and vertical
391 variances that the hotwire captures) plots also display a good agreement with differences smaller
392 than 15%. For the pitched roof geometry, the comparison of the mean velocity between the wind
393 tunnel and LES results also shows a very good agreement with differences smaller than 5%; a
394 similarly good agreement is observed for the case of the round roof geometry mean velocity. On
395 the other hand, the σ^2 comparisons between the wind tunnel and LES results show larger
396 discrepancies for both the pitched and round roof geometries in comparison to the σ^2 plots of the
397 flat roofs or to the means. The wind tunnel and LES results agree qualitatively on higher
398 turbulence levels for the pitched and round roofs in comparison to the flat roof; however, LES
399 appears to overpredict the turbulence statistics in comparison to the wind tunnel results,
400 especially so for the round roof geometry. Differences in the inlet velocity or an underestimation
401 by the hot wire of the variance induced by the low velocity in the canyon might be possible
402 causes for this discrepancy; however, it would be expected that such a mismatch would also
403 influence the results of the flat roof and the means. Thus, the more plausible cause is that the
404 LES has more difficulty in capturing the turbulence inside the canopy over non-flat roofs, and
405 subsequently the turbulence levels inside as well as outside the canopy layer are affected. This is
406 related to the fact that, for LES, capturing the separation correctly, particularly over round roofs,
407 is more challenging. Temmerman et al. (2003) provides an in-depth analysis of the challenges of
408 LES to model the flow over a round hill. For the flat roof, the separation occurs at the corner of
409 the building and thus is easy to capture (Aynsley, 1999). However, for the other roofs with more

410 complex shapes, the geometries do not impose a clear separation point, and so the LES might
 411 have more difficulty matching it exactly especially in simulations like ours where LES relies on
 412 wall-modelling. Moreover, the separation will also be sensitive to the effective Re of the
 413 simulation.

414 The results obtained for the flat roof geometry (using Inlet #1) have also been validated against
 415 data from Brown et al (2000) who, for a similar setup with an array of 7 buildings, studied the air
 416 flow and turbulence statistics. These validations have been reported in Llaguno-Munitxa et al.
 417 (2017) and will not be reproduced here. Vertical profiles have been compared for canyon #2,
 418 canyon #6 (the canyon where the LES results have been displayed), and downstream. The mean
 419 velocity profiles were found in very good agreement with differences of about 5%. The turbulent
 420 kinetic energy results display larger discrepancies than the mean velocity results; however the
 421 differences remain acceptable. Overall, the profile trends are captured accurately and the
 422 quantitative errors remain moderate.



423

424

425 **Fig 4** Wind Tunnel and LES result (with imposed Inlet #1 inflow conditions) comparison for
 426 canyon #6 until $4H$. All values are normalized by the reference velocity U_r , which has been taken
 427 at $2.5H$ upstream. The left panel depicts the wind tunnel and LES wind speed, U_t , for the Flat
 428 roof, Pitched roof, and Round roof. U_t is the magnitude of the velocity vector, mainly composed
 429 of the streamwise and vertical components. The right panel depicts the corresponding wind
 430 tunnel and LES total variances σ_t^2 . For more details refer to Llaguno-Munitxa et al. (2017).

431

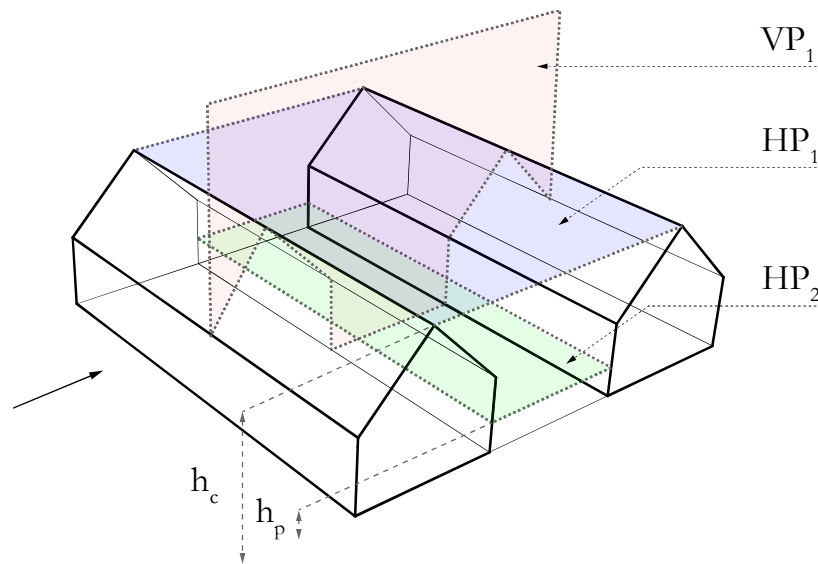
432

433

434 **5 Air Exchange Rate (ACH)**

435 Air exchange from within a canyon generally can take place horizontally (along the street axis)
436 and vertically (across the interface plane aligned with the roof vertices). For the archetypical
437 urban street canyon studied in this paper however, the canyon is assumed to be very long such
438 that the vertical exchanges are the principal source of clean fresh air. The studied building
439 geometries therefore follow an idealized 2-dimensional ‘infinite’ building array configuration,
440 and focus is therefore placed on the analyses of the vertical air exchanges. One must note
441 however that real canyons can have complex 3-dimensional mean flow patterns where this
442 assumption is not applicable.

443 The instantaneous vertical perturbation velocities w' have been saved from the LES runs for
444 directly computing ACH at HP_1 : the exchange at the plane of interface between the urban
445 canopy layer and the free atmosphere, and HP_2 : the exchange across a horizontal plane at the
446 pedestrian level (see Fig. 5) for all studied building geometries. The instantaneous w' velocities
447 for the vertical plane VP_1 as indicated in (Fig. 5) have also been saved to understand the
448 variability of w' in the section plane. For all planes and sections, the same number and sequence
449 of time-steps have been recorded and analyzed over about 120 eddy turnover times as detailed
450 above.



451 **Fig 5** Air Exchange HP_1 and HP_2 and section plane VP_1 locations. The figure illustrates a limited
452 section of the canyons; and VP_1 is in the middle of the domain span, halfway between the side
453 walls.
454
455

456 5.1 Direct LES ACH estimation

457

458 The Air Exchange Rate calculations for the HP_1 and HP_2 planes have been performed by
 459 studying the flow across both planes for 20,000 time-steps (5s computed time) as described in
 460 section #3. The data have been saved at the cell centre for HP_1 , HP_2 , and VP_1 . The number of
 461 cells in the studied HP_1 and HP_2 planes ranged from 1900 for the flat roof to 5520 for the pitched
 462 roof (bear in mind that the top exchange planes for the pitched and round roofs are twice larger
 463 and the terraced building exchange plane is 0.4H larger than the exchange plane for flat roof and
 464 geometry with balconies). For the VP_1 plane, the number of cells for the flat roof case was 800
 465 and for the pitched roof it was 1111.

466

467 The vertical fluxes for HP_1 and HP_2 planes for a given street canyon volume are directly
 468 computed by integrating the mass flux out of the canyon following:

469

$$ACH_{LES}(m^3/s) = \underbrace{\iint_A \left(\underbrace{\frac{1}{T} \int_0^T w^+ dt}_{\text{temporal averaging}} \right) dA}_{\text{spatial integration}} \quad (6)$$

470 where T is the total time averaging period, that is, 5 s. A is the area of HP_1 or HP_2 planes over
 471 which the ACH has been computed. w^+ reflects the recorded instantaneous positive vertical
 472 velocities (while w^- that will be used later are the negative ones). This is essentially the time-
 473 average of the positive vertical velocity (flow exiting the canyon) at each point, integrated or
 474 summed spatially over the whole plane. Normalizing by the street canyon volume V_c (where the
 475 subscript c refers to the canyon, and h_c is the depth of the canyon) yields ACH^* defined as:

476

$$ACH^*(s^{-1}) = \frac{ACH}{V_c} \quad (7)$$

477 From (Eq. 6) and (Eq. 7), for the simple case of a flat roof where $V_c = h_c A$, we obtain:

478

$$ACH^*(s^{-1}) = \frac{1}{h_c} \underbrace{\left(\frac{1}{A} \iint_A \left(\underbrace{\frac{1}{T} \int_0^T w^+ dt}_{\text{temporal averaging}} \right) dA \right)}_{\text{spatial averaging}} = \frac{1}{h_c} \langle \overline{w^+} \rangle. \quad (8)$$

479 The overbar here denotes temporal averaging, while the angled brackets denote spatial
 480 averaging. Distinguishing between these two averaging operators is very important in spatially-
 481 variable flows over complex terrain. For two-dimensional configurations with uniform street
 482 profiles in the longitudinal axis and with an invariant total air mass inside the canyon, continuity
 483 imposes that:

$$484 \quad \langle \overline{w} \rangle = \langle \overline{w^+} \rangle + \langle \overline{w^-} \rangle = 0 \quad \Rightarrow \quad \langle |\overline{w}| \rangle = 2 \langle \overline{w^+} \rangle. \quad (9)$$

485 Where the vertical bars denote the absolute value of w . Therefore, the ACH^* can be estimated
 486 (again for the simple flat roof case for illustration) following:

$$487 \quad ACH^*(s^{-1}) = \frac{ACH}{V_c} = \frac{1}{h_c} \langle \overline{w^+} \rangle = \frac{1}{h_c} \frac{1}{2} \langle |\overline{w}| \rangle. \quad (10)$$

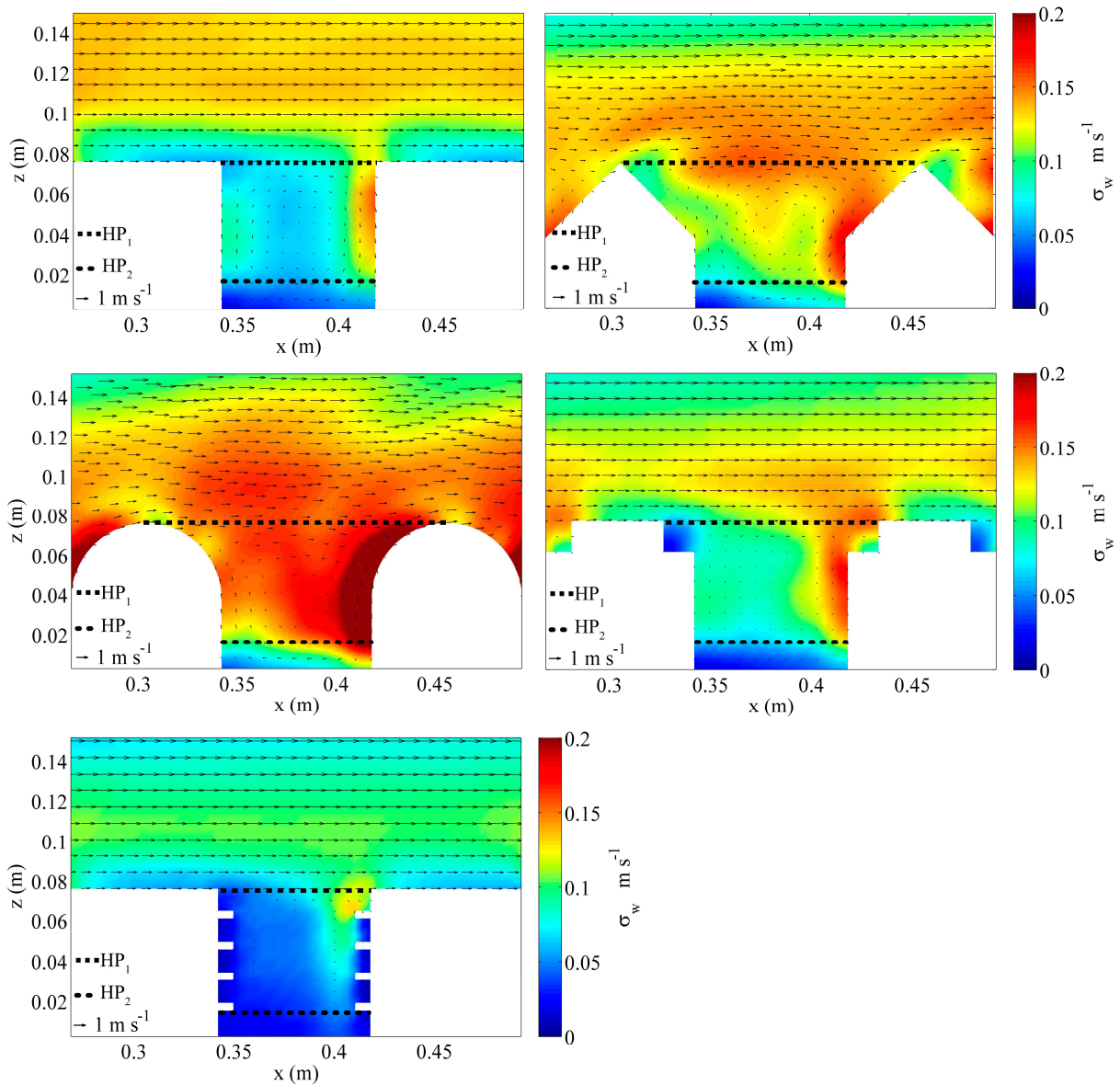
488 If the roof is not flat, h_c in Eqs 8 and 10 should simply be replaced by an effective height
 489 $h_e = V_c/A$. As such, the exchanges are produced by (i) the turbulent perturbations from the
 490 temporal mean that modulate $\overline{w^+}$, as well as by (ii) the coherent patterns of the time-averaged
 491 mean flow that modulate $\langle \overline{w^+} \rangle$ and produce the so-called dispersive fluxes. Note that if Eq. (9)
 492 does not hold and a mean flux $\langle \overline{w} \rangle \neq 0$ exists, Eq. (10) is still a correct expression that accounts
 493 for both turbulent and dispersive fluxes, but the mean flux needs to be added to get the total
 494 ACH. The dispersive and turbulent components are illustrated in figure 6 that depicts the flow
 495 field for the vertical plane VP_I . The pseudocolor plot shows the vertical turbulent rms velocity σ_w
 496 and the vector plot shows the mean (time-averaged) velocity patterns. As reported in the paper
 497 that precedes this research (Llaguno-Munitxa et al., 2017), σ_w substantially increases for the
 498 cases of the pitched and round roof geometries in comparison to the flat roof geometry. The
 499 round roof geometry is the case where the largest turbulence intensities are observed, regardless
 500 of what inflow is imposed. For the flat roof geometry, the stagnation point is located at the
 501 windward vertex of the roof corner, and for the pitched and round roofs it is located in the
 502 middle of the windward roof slopes. The flow separation point on the other hand, occurs at the
 503 leeward vertex for the flat roof, slightly below the crest for the pitched roof, and almost half way
 504 down the leeward roof side for the round geometry. In all cases, the highest turbulence levels are
 505 observed in the shear zone near the roof level, but the depth of this zone varies for the different
 506 cases. For the pitched and round roofs, the roof shape creates a strong downdraft inducing higher

507 turbulent intensities and mean flow. The roof set-back produces a similar, but less intense, effect.
508 Balconies, on the contrary, limit the flow access to the canyon, reducing the air circulation
509 entrance in the windward face and consequently reducing σ_w over and below the shear layer.

510
511 Within the canyon, the round roof geometry generates the largest σ_w , while the flat roof reduces
512 the vertical turbulent exchanges between the urban canopy layer and the free atmosphere. The
513 terraced building, in comparison to the flat roof, increases the mean and turbulence velocities
514 within canyon; however, the effect of terraces appears to be subtle in comparison to the changes
515 produced by the other geometries. In all cases, a flow recirculation is discernible within the street
516 canyon. It is also observable that the presence of balconies promotes the stagnation of air within
517 the canyon, reducing the strength of the standing vortex as well as the turbulence intensity. In a
518 similar way, the balconies seem to be interfering with the smaller eddies substantially reducing
519 σ_w within the canyon.

520
521 Many of the qualitative results observed for the VP_I plots are also observable in Fig .7 that
522 depicts ACH sections. Horizontal transects along the central x -axis of the ACH planes have been
523 gathered to compare \bar{w} and σ_w profiles for the studied building geometries. Figure (7a) displays
524 a comparison of the \bar{w} plots for HP_I (note that the width of the exchange plane is variable for
525 the different geometries). The pitched and rounds roofs show the largest \bar{w} velocities, especially
526 in the ACH area adjacent to the downstream roof slope. This implies that they generate the
527 largest dispersive fluxes. In both cases (and especially for the case of the pitched roof geometry),
528 the flow separation as observed in Fig. 6, creates a strong downdraft which explains the increase
529 in the negative \bar{w} and associated increase in the positive one further downstream. A similar
530 effect is observed for the set back roof, but to a reduced extent. The flat roof and the building
531 with balconies show similar tendencies. The differences observed between the studied
532 geometries are most visible for the σ_w plots in (Fig. 7b). The round roof shows the largest
533 turbulence levels in the HP_I plane followed by the pitched roof. Similarly to the \bar{w} plot,
534 particularly for the case of the round roof geometry, the largest σ_w are observed adjacent to the
535 downstream roof slope. The set back roof shows similar tendencies, but the turbulent intensities
536 are smaller than for the pitched and round roof geometries. The flat roof and building with
537 balconies geometries are the ones with lowest σ_w .

538 While ACH is generally computed in planes analogous to HP_1 where the exchanges are generally
539 largest given the proximity of the plane to the shear layer, it is most likely that ACH planes that
540 are closer to the ground level or pedestrians, such as HP_2 , will be the locations in the Urban
541 Canopy Layer (UCL) where the lowest turbulence intensity and vertical velocities occur.
542 Therefore, given the importance of the lowest layer of the canyon for pedestrian exposure to
543 pollution and heat, this area is probably more critical in terms of urban ventilation than the whole
544 canyon ventilation assessed at HP_1 . The two should be analyzed together to ensure that fresh air
545 not only makes it into the canyon (through HP_1), but also to pedestrian level (through HP_2). Fig.
546 7c shows \bar{w} for HP_2 . The within canyon vortex is most visible for the case of the round roof
547 where a larger velocity gradient is observed between the upstream and downstream faces. The
548 pitched and flat roof geometries display very similar \bar{w} magnitudes. The balconies and set back
549 roof geometry, show the lowest \bar{w} velocities, denoting a weaker within canyon vortex. Fig. 7d
550 shows the σ_w plots for HP_2 . The results show similar trends to those observed in Fig. 7b for HP_1 .
551 The HP_2 of the round roof geometry displays the highest σ_w , followed by the pitched roof and the
552 set back and flat roof geometries. The geometry that generates the lowest σ_w at the HP_2 plane is
553 the geometry with the façade with balconies, as was the case at HP_1 . In general, for both planes,
554 the geometries that produce the strongest dispersive exchanges also produce the strongest
555 turbulent exchanges.

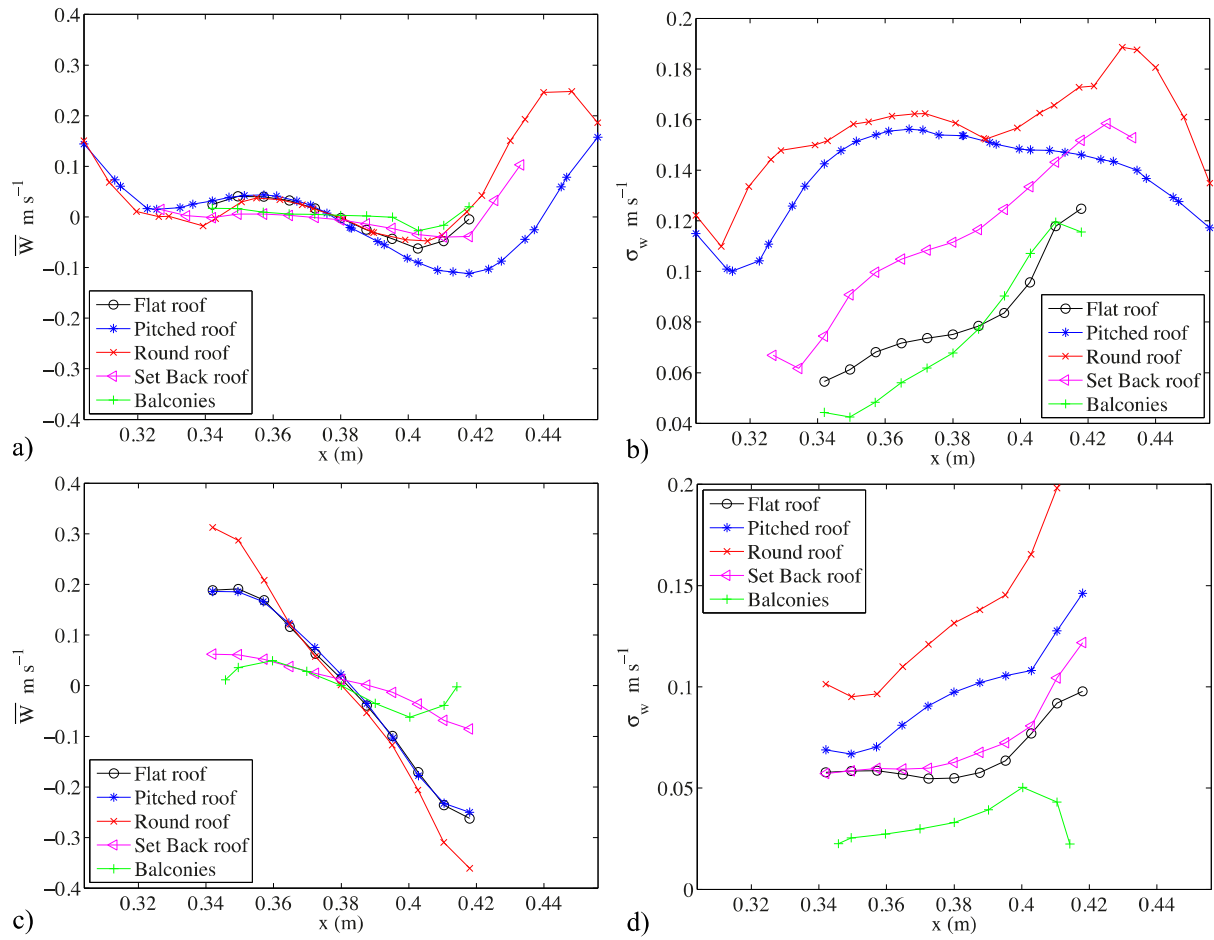


556

557 **Fig 6** LES results for air flow and vertical turbulence intensity for the 5 different building
 558 geometries. The time-averaged velocity is displayed with the vector plot, and σ_w with
 559 pseudocolor plots. The thick dashed lines denote the locations of the exchange planes
 560 considered.

561

562



563

564 **Fig 7** LES results for spatially-averaged (along the street canyon longitudinal axis, y-direction)
 565 exchange planes HP_1 and HP_2 : a) the mean vertical velocity \bar{w} for HP_1 ; b) σ_w for HP_1 ; c) the
 566 mean vertical velocity \bar{w} for HP_2 ; and d) σ_w for HP_2 . Note that the rakes displayed in the figure,
 567 show the data computed for the ACH planes HP_1 and HP_2 , which only cover the central area of
 568 the canyon, thus the portions adjacent to the walls have not been included (which explains why
 569 the mean velocity averages over x would not be exactly 0 for all cases).
 570

571 The formulation described in Eq. (10) has been followed to calculate the direct LES estimation
 572 ACH^*_{LES} (including turbulent and dispersive exchanges) for the HP_1 and HP_2 planes. Table (2)
 573 shows the results for plane HP_1 and Table. (3) shows the results for plane HP_2 . These two tables
 574 also show the extrapolation of the obtained results to *real* building prototype scales. For scaling
 575 to the real world from the LES results, the non-dimensional parameter that can be considered
 576 invariant to scale (if the Re sensitivity effects are ignored) is the exchange velocity to reference
 577 velocity ratio U_e/U_{ref} . This ratio is hence the same for the LES model and real world prototype.
 578 Since $ACH = U_e A_c$, one can then write

579
$$ACH^{real} = U_e^{real} A^{real} = \frac{U_e^{real}}{U_e^{LES}} U_e^{LES} \frac{A^{real}}{A^{LES}} A^{LES} = \frac{U_e^{real}}{U_e^{LES}} \frac{A^{real}}{A^{LES}} ACH^{LES}. \quad (11)$$

580 In agreement with the patterns observed in Fig. 5 and Fig. 6, the round roofs show the largest
 581 ACH_{LES}^* , followed by the pitched roof, the set-back geometry, the flat roof, and the geometry
 582 with balconies, with results over four times smaller for the geometry with balconies in
 583 comparison to the round roof geometry at HP_1 , and over 5 times smaller at HP_2 . The equivalent
 584 real building was assumed to have $U_{ref} = 2 \text{ ms}^{-1}$ and $H = W = 15\text{m}$ for the following calculations
 585 (following a 1/200 scale ratio between the LES and real prototype). In LES the longitudinal
 586 length of the exchange planes is 0.68 m (note that the HP_1 and HP_2 exchange planes do not
 587 extend to the lateral walls) and its equivalent real prototype length (following the same 1/200)
 588 results in 137m. The ACH_{Real} is then computed from Eq. (11) with $U_e^{real} / U_e^{LES} = 2 / 1.8$ and $A^{real} /$
 589 $A^{LES} = 200^2$.

590 **Table 2** HP_1 LES and real prototype scaled based on Eq. 11.

Building Geometries	ACH_{LES}^* (s^{-1})	A_c (m^2)	V_c (m^3)	$ACH_{LES} = V_c ACH_{LES}^*$ ($\text{m}^3 \text{ s}^{-1}$)	ACH_{Real} ($\text{m}^3 \text{ s}^{-1}$)
Flat Roof	0.3973	0.0519	0.00395	0.00156	69.332
Pitched Roof	1.0619	0.1039	0.00493	0.00524	232.886
Round Roof	1.6504	0.1039	0.00437	0.00721	320.441
Façade Set-back	0.6096	0.0727	0.00426	0.00259	115.109
Façade Balconies	0.3333	0.0519	0.00395	0.00131	58.221

591

592 **Table 3** HP_2 LES and real prototype scaled based on Eq. 11.

Building Geometries	ACH_{LES}^* (s^{-1})	A_c (m^2)	V_p (m^3)	$ACH_{LES} = V_p ACH_{LES}^*$ ($\text{m}^3 \text{ s}^{-1}$)	ACH_{Real} ($\text{m}^3 \text{ s}^{-1}$)
Flat Roof	1.3657	0.0519	0.00197	0.00268	119.109
Pitched Roof	2.1067	0.0519	0.00197	0.00415	184.442
Round Roof	2.1747	0.0519	0.00197	0.00428	190.220
Façade Set-back	0.7945	0.0519	0.00197	0.00156	69.332
Façade Balconies	0.4357	0.0519	0.00197	0.00085	37.777

593

594

595 5.2 ACH^* estimation from RANS

596

597 As addressed by Cheng et al. (2009) and Li et al. (2005), the difference between the computation
 598 time of RANS and LES models is very large. Urban planning and architectural design processes
 599 require fast decision-making and therefore the time and expertise required to perform LES
 600 calculations are generally not available. Therefore, it is worth looking into alternative estimates
 601 of ACH that require less computationally demanding simulations such as RANS.

602

603 With this ambition, Li et al. (2005) described a formulation as an alternative to their previously
 604 published LES based ACH computation (Liu et al., 2005). Their formulation based on the results
 605 obtained from a RANS k - ε model related the ACH to the perturbation velocity at the exchange
 606 plan of interest following:

$$607 \quad ACH_{\sigma_w} = \frac{1}{2} \iint_A \overline{w'w'}^{1/2} dA = \frac{1}{2} A \langle \sigma_w \rangle, \quad (12)$$

608 where the primes denote the perturbation velocity relative to its ensemble mean, which could be
 609 surrogated by the time average (but not the spatial average). This formulation makes some
 610 simplifications that we will revisit later in the paper. Furthermore, isotropic turbulence was
 611 assumed in the street canyon in previous studies to relate the standard deviation of vertical
 612 velocity to the turbulent kinetic energy (k) that is available from RANS with a closure such as k -
 613 ε :

$$614 \quad k = \frac{(\overline{u'u'} + \overline{v'v'} + \overline{w'w'})}{2} \approx \frac{3\overline{w'w'}}{2} \Rightarrow \sigma_w = \overline{w'w'}^{1/2} \approx \left(\frac{2}{3}k\right)^{1/2}. \quad (13)$$

615 By combining (eq. 12) and (eq. 13), this ACH estimate leads to the following equation:

$$616 \quad ACH_{\sigma_w} = \frac{1}{\sqrt{6}} \iint_A \sqrt{k} dA = \frac{1}{\sqrt{6}} A \langle \sqrt{k} \rangle. \quad (14)$$

617 However, as observed in Figs. 6 and 7, \overline{w} , \overline{u} , σ_w and σ_u are substantially different for the various
 618 geometries. Therefore, assuming that the turbulence is isotropic might not be an adequate
 619 simplification. For such assumption to be more accurate, a degree of isotropy should be defined
 620 for the different building geometries as well as for the different ACH planes. Perhaps the more

621 important point to underline is that the estimation proposed by (Li et al., 2005) does not take into
 622 account the mean and dispersive fluxes. In spatially-variable flows such as the one we study
 623 here, even if the spatially and temporally averaged (mean) velocity at the plane of interface is
 624 zero, the spatial variability of the time-averaged velocity field results in a dispersive flux (Poggi
 625 and Katul, 2008; Raupach and Shaw, 1982), as we noted earlier. Moreover, in realistic 3D
 626 canopies, even the spatially and temporally averaged mean vertical velocity might not be zero.
 627 Another approach for ACH estimation proposed by Cheng et al. (2008) followed the formulation
 628 of Li et al. (2005) and proposed an alternative based on the eddy covariance method; it
 629 confirmed the point we underline here that the mean dispersive component was important and
 630 therefore has to be considered.

631
 632 Moonen et al. (2011) proposed an alternative formulation for RANS simulations when the
 633 turbulence statistics are not known; this ACH estimation is based on the vertical velocity
 634 component:

$$635 \quad ACH_w = \iint_A \frac{\bar{w} + |\bar{w}|}{2} dA, \quad (15)$$

636 This formulation also only requires RANS. It accounts for the mean fluxes (via the spatial
 637 integration of \bar{w}) and the dispersive fluxes (via the spatial integration of the absolute value of
 638 the time averaged velocity $|\bar{w}|$), but it ignores the turbulent fluxes. The authors indeed conclude
 639 that the impact of the turbulent contribution is significant and should be accounted for.

640 In tables 4 and 5 the results obtained following a σ_w -based $ACH^*_{\sigma_w}$ estimation as given in Eq.
 641 (12) following Cheng et al. (2008), Li et al. (2005) and a time-averaged vertical velocity \bar{w}
 642 based formulation ACH^*_w following Eq. (15) by Moonen et al. (2011) are provided. ACH^*_w
 643 significantly underestimates the ACH specially for the top plane compared to the LES direct
 644 calculations. This is despite the fact that ACH^*_w includes the (mostly positive but small) mean
 645 exchanges that are non-zero as shown in the tables and that are excluded from the ACH_{LES} based
 646 on Eq. (10) (the small mean flux is due to the fact that we exclude the regions adjacent to the
 647 sidewalls and thus the flow is not perfectly homogeneous in the cross-stream direction). $ACH^*_{\sigma_w}$
 648 performs well for the top plane (where the time averaged velocities are small as shown in Fig. 7),
 649 but large errors occur for HP_2 where the contribution of the dispersive transport is more

650 significant due to larger $|\overline{w}|$. The estimate that assumes isotropy to infer σ_w based on k (eq. 14) is
651 not included, but it will necessarily be inferior to the ones based directly on σ_w since it involves
652 further simplifications.

653

654 Since these two formulations are both not satisfactory, we propose here a new formulation based
655 on the folded normal distribution as an alternative for estimating the *ACH* from RANS. This
656 formulation uses the mean vertical velocities $\langle \overline{w} \rangle$ and vertical turbulence statistics σ_w , which can
657 be obtained through CFD simulations based on RANS with closures that provide this variance
658 (e.g. second-order closures), or alternatively by assuming isotropy if only k is available such as
659 in models with a k - ϵ closure (these are the most common codes in practice).

660

661 Fluent provides us with the time averaged \overline{w} and σ_w ; recall that the time averaged velocity \overline{w} at
662 a given location is not zero. Therefore, at every point in space we can define $w = \overline{w} + w'$. Two
663 challenges arise when trying to compute the *ACH*. The first is that summation and taking the
664 absolute value are not commutative operations and therefore, referring to Eq. (10),

665 $|\overline{w}| = |\overline{\overline{w} + w'}| \neq |\overline{\overline{w}}| + |\overline{w'}| = |\overline{\overline{w}}| + |\overline{w'}|$ and by extension $|\overline{w'}| \neq |\overline{w'}|$ (note however that for the mean

666 we can write $|\overline{\overline{w}}| = |\overline{\overline{w}}| = |\overline{\overline{w}}|$). The second challenge arises since time averaging and squaring are

667 also not commutative operations and hence the variance σ_w^2 , which can be computed directly

668 from LES or from RANS (assuming isotropy if needed), cannot be used to inform us on $|\overline{w'}|$

669 since $\sigma_w^2 = \overline{w'^2} = \overline{|w'|^2} = \overline{|w'|^2} \neq \overline{|w'|^2}$ (note that this inequality is ignored in the model of Li et al.

670 (2005) presented in Eq. (12), resulting in the cancellation of the dispersive flux contributions).

671 These challenges imply that the actual exchange, which is related to $|\overline{w}|$ cannot, in general, be

672 exactly related to the mean and the standard deviation of w .

673 To overcome this hurdle, we will assume that w has a normal (Gaussian) distribution. Figure 8

674 shows the probability distributions of w' for all studied building geometries and the two studied

675 exchange planes HP_1 and HP_2 , and compares them to the Gaussian distribution curve. The plots

676 show that the distribution of w' for all different building geometries is very well approximated by

677 the Gaussian. There are discrepancies at the tails but these tails are very infrequent (notice the

678 log-scale of the y axis) Therefore, this implies that $|w|$ can be assumed a folded normal

679 distribution (Leone et al., 1961) and its mean (time average) $\overline{|w|}$ can be related to \overline{w} and σ_w at
 680 each spatial point, and then averaged in space to get the ACH following Eq. (10). The folded
 681 normal distribution of a Gaussian variable w is the distribution of its absolute value $|w|$, which
 682 will have the following mean:

$$683 \quad \overline{|w|} = \sqrt{\frac{2}{\pi}} \sigma_w \exp\left(-\frac{\overline{w}^2}{2\sigma_w^2}\right) - \overline{w} \operatorname{erf}\left(-\frac{\overline{w}}{\sqrt{2}\sigma_w}\right), \quad (16)$$

684 where erf is the error function. Therefore the ACH equation (following from Eq. (10) becomes:

$$685 \quad ACH_{FND} = \frac{A_c}{2} \left\langle \sqrt{\frac{2}{\pi}} \sigma_w \exp\left(-\frac{\overline{w}^2}{2\sigma_w^2}\right) - \overline{w} \operatorname{erf}\left(-\frac{\overline{w}}{\sqrt{2}\sigma_w}\right) \right\rangle. \quad (17)$$

686 In Tables 4 & 5, a comparison of the ACH calculation methodologies ACH^*_{LES} , ACH^*_{FND} ,
 687 $ACH^*_{\sigma_w}$, and ACH^*_w are included in columns 1, 2, 3, and 4, respectively, for the different
 688 building geometries. Note that the * here denotes that the provided ACH_{LES} , ACH_{FND} , ACH_{σ_w} and
 689 ACH_w results have been normalized based on their respective canyon volumes, V_c and V_p
 690 reported in tables 2 and 3, for the top and bottom exchange planes HP_1 and HP_2 , respectively.
 691 The mean $\langle \overline{w} \rangle$, dispersive $\langle \overline{|w|} \rangle$, and the turbulent σ_w exchange velocity have also been included
 692 in columns 5, 6 and 7 respectively. It is important to remember that the formulations for ACH^*_{LES}
 693 and ACH^*_{FND} include the combined effect of the dispersive and the turbulent fluxes, while
 694 $ACH^*_{\sigma_w}$ only accounts for the turbulent fluxes and ACH^*_w only takes into account the mean and
 695 dispersive fluxes (these formulations can be directly recovered from the corresponding exchange
 696 velocities upon dividing by $2 \times h_c$ (recall h_c is the effective canyon depth)).

697

698 For the case of HP_1 , as shown in in Column 3 of Table 4, the ACH^*_{FND} model is the one that
 699 produces the closest results to ACH^*_{LES} , with deviations below 2%. The second best performing
 700 model for HP_1 is $ACH^*_{\sigma_w}$. This is not surprising given that at the interface of the urban canopy
 701 layer is where the highest turbulent fluxes are observed. Thus for HP_1 , larger discrepancies are
 702 observed between ACH^*_w and ACH^*_{LES} .

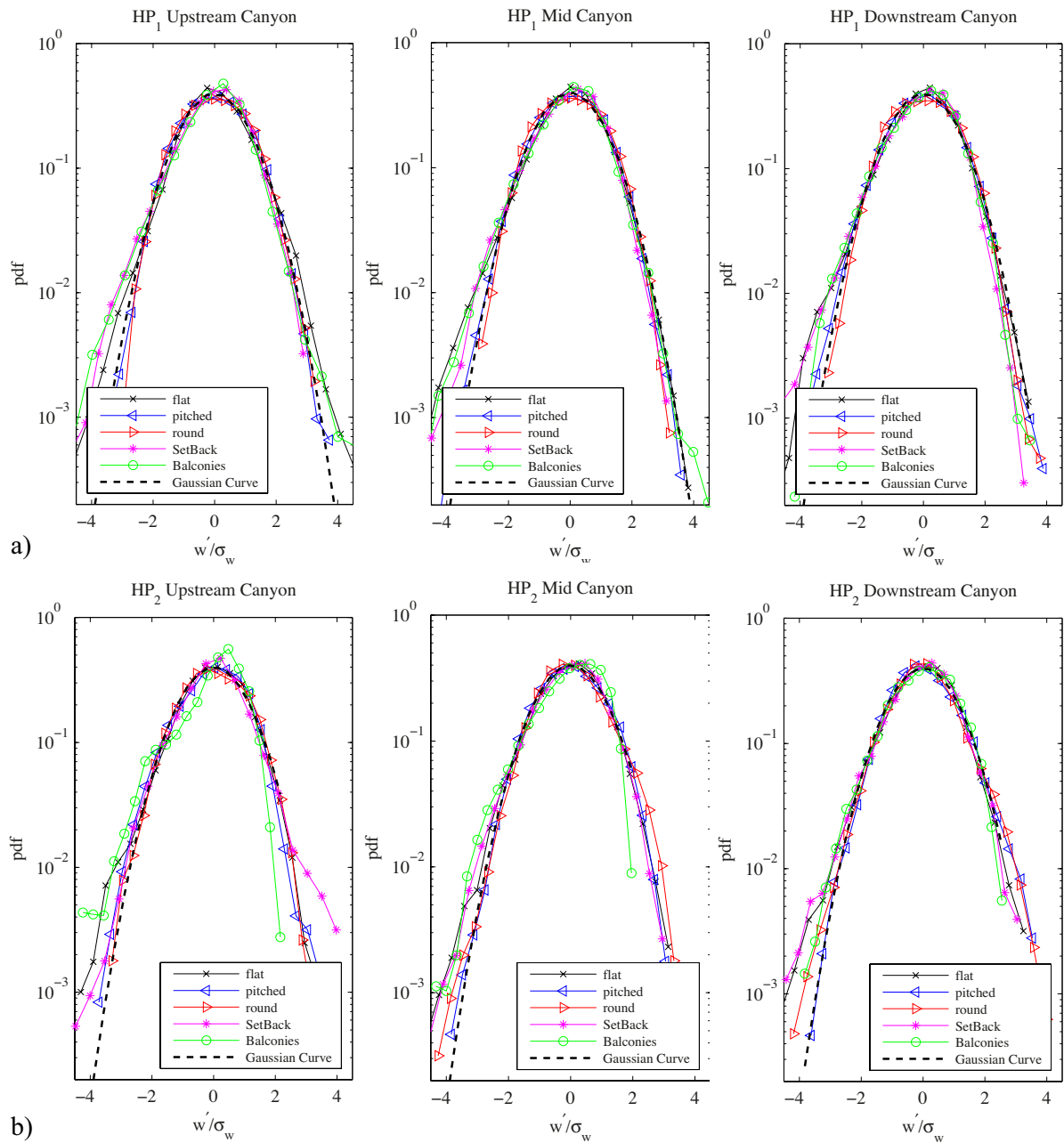
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704 In Column 2 of Table 5, the folded estimate ACH^*_{FND} is shown for HP_2 . As for HP_1 , the results
705 obtained following the folded estimate show a very good agreement with deviations smaller than
706 2%. As for HP_1 , the round roof geometry shows the largest direct LES estimate followed by the
707 pitched roof, the set-back geometry, the flat roof, and the geometry with balconies. The
708 exchanges are 5 times larger for the round geometry than for the geometry with balconies. But
709 for the case of HP_2 , the contribution of $\langle \bar{w} \rangle$ and σ_w becomes more geometry dependent, thus the
710 $ACH^*_{\sigma_w}$ results show larger disagreements with ACH^*_{LES} results than those observed for HP_1 .
711 ACH^*_w on the other hand shows closer results to ACH^*_{LES} , given that at HP_2 the dispersive fluxes
712 are more dominant (compare the corresponding exchange velocities at the two planes).

713 Overall, the results obtained following the folded estimate method ACH^*_{FND} show excellent
714 agreement with the direct LES estimates. Thus based on the studies included in this paper, the
715 model ACH^*_{FND} produces the estimates that best match the results obtained through the direct
716 LES computations, revealing the importance to account for both the dispersive and turbulence
717 fluxes in the ACH estimation methodologies. The skill of the FND method is not surprising
718 since, following Eq. (17), the results obtained by ACH^*_{FND} should exactly match the ACH^*_{LES} if
719 the obtained velocity measurements were exactly Gaussian. Since figure 8 illustrates, the
720 deviation from the Gaussian is only observed at the tails of the plot (again note the log-scale of
721 the y axis). At the peaks that are more frequent, the results display a Gaussian distribution,
722 resulting in the good match between the ACH^*_{LES} and ACH^*_{FND} .

723

724 The exchange velocities listed in Tables 4 and 5 further illustrate that both turbulent and
725 dispersive fluxes are important, though turbulent exchanges dominate near the canyon top, while
726 dispersive ones dominate near street level. The mean fluxes in our 2-dimensional configuration
727 are negligible, but again not exactly zero since the configuration is not truly infinite and
728 homogeneous in the cross-stream direction and since we exclude regions near the walls.



729

730 **Fig 8** Probability distributions for the perturbation velocity w' for cross-stream lines at various
 731 streamwise locations for all studied building geometries. Upper panel a) shows the results
 732 obtained for the top plane HP_1 . The figure to the left shows the mid canyon (in the x -direction)
 733 distribution plot followed by the leeward (upstream when looking at a canyon, middle panel) and
 734 downstream (downstream when looking at a canyon, right panel) canyon facades. Lower panel
 735 b) shows the results obtained for the bottom plane HP_2 . The figure to the left shows the mid
 736 canyon plot, again followed by the leeward and windward distributions. All results can be
 737 reasonably approximated by the Gaussian distribution depicted by the dashed black line, despite
 738 discrepancies at the tails that are significant for exchanges.

739 **Table 4** HP_1 air exchange rates

Building Geometries	ACH^*_{LES} (s^{-1})	ACH^*_{FND} (s^{-1})	$ACH^*_{\sigma_w}$ (s^{-1})	ACH^*_w (s^{-1})	$\langle \overline{w} \rangle$ ($m \times s^{-1}$) (mean exchange velocity)	$\langle \overline{w} \rangle$ ($m \times s^{-1}$) (dispersive exchange velocity)	σ_w ($m \times s^{-1}$) (turbulent exchange velocity)
Flat roof	0.3973	0.4006	0.3113	0.4044	0.0134	0.0481	0.0474
Pitched roof	1.0619	1.0609	1.1273	0.5249	-0.0004	0.0502	0.1070
Round roof	1.6504	1.6311	1.5655	1.2175	0.0277	0.0747	0.1317
Set back roof	0.6096	0.6141	0.7196	0.2867	0.0075	0.0261	0.0843
Façade balconies	0.3333	0.3303	0.3635	0.2312	0.0146	0.0206	0.0553

740

741 **Table 5** HP_2 air exchange rates

Building Geometries	ACH^*_{LES} (s^{-1})	ACH^*_{FND} (s^{-1})	$ACH^*_{\sigma_w}$ (s^{-1})	ACH^*_w (s^{-1})	$\langle \overline{w} \rangle$ ($m \times s^{-1}$) (mean exchange velocity)	$\langle \overline{w} \rangle$ ($m \times s^{-1}$) (dispersive exchange velocity)	σ_w ($m \times s^{-1}$) (turbulent exchange velocity)
Flat roof	1.3657	1.3668	0.5642	1.3739	0.0055	0.0988	0.0428
Pitched roof	2.1067	2.1070	1.2169	2.0064	0.0090	0.1434	0.0924
Round roof	2.1747	2.1792	1.3311	1.9795	0.0052	0.1451	0.1011
Set back roof	0.7945	0.8087	0.6443	0.6933	0.0044	0.0482	0.0489
Façade balconies	0.4357	0.4390	0.2790	0.3659	-0.0011	0.0289	0.0212

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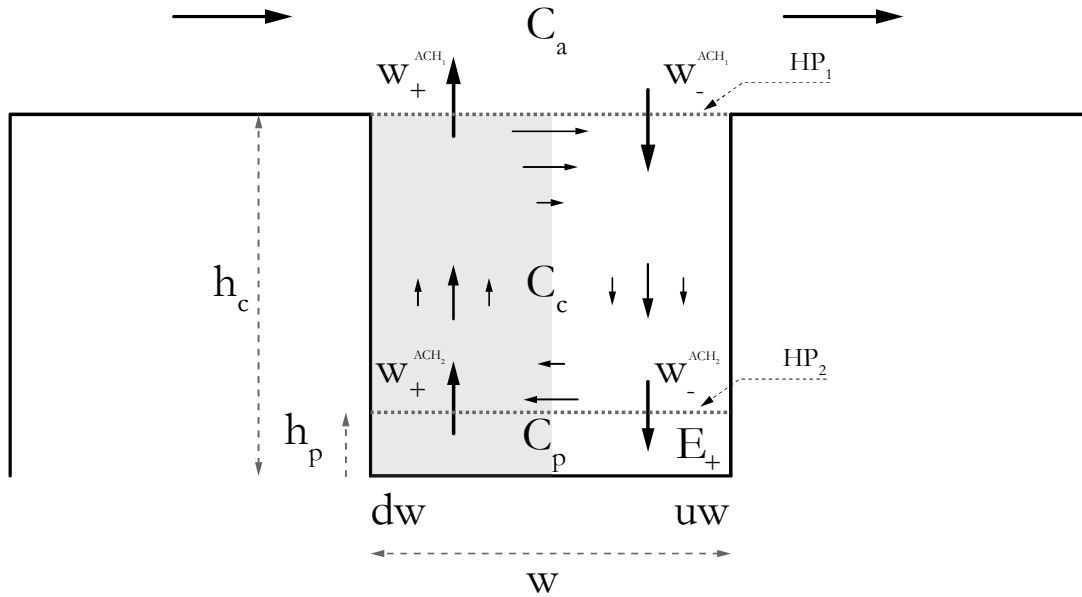
743

744 **5.3 Pollutant Concentration (PC) estimation**

745

746 To infer pollutant concentration from LES or RANS for a given case, the most direct and
 747 accurate way is to solve the budget equation of a tracer (that could be reactive). If one then aims
 748 to estimate pollutant concentration at pedestrian level, the influence of geometry, as well as
 749 location of the pollutant emission and reactivity of that chemical, can be captured. Since
 750 pollutant emissions and transport were not directly simulated in our LES, a pollutant
 751 concentration estimation formulation is proposed to compare the impacts on the pollutant
 752 concentration levels of the studied building geometries. This method is not as accurate as the
 753 direct simulation of a tracer, but it has the advantages of (i) not focusing on a specific pollutant

754 emission location, and (ii) being applicable to wind tunnel data (where a pollutant concentration
 755 is difficult to measure) or other CFD results that cannot capture tracer budgets (either existing
 756 data or for codes where passive tracers are not included). As such, it is generally useful to be able
 757 to estimate, albeit approximately, pollutant concentrations and how they are influenced by
 758 geometry from air exchange considerations alone.



759
 760 **Fig 9** Street canyon pollutant exchange diagram.

761
 762 The pollutant exchange between the canyon and the free atmosphere, that is through plane HP_1 is
 763 determined by the vertical exchanges w^+ and w^- as depicted in (Fig. 9). C_a is the free atmosphere
 764 concentration. If the canyon is assumed to consist of one well-mixed reservoir, C_c would be the
 765 average canyon concentration below HP_1 in this one-reservoir model. A_c refers to the area of the
 766 HP_1 plane. E_+ stands for the pollutant source emission rate (in kg s^{-1}).

767
 768 Therefore, the variability in the concentration C_c will depend on the time t it takes to exchange
 769 the volume of air contained within the canyon. Using a simple mass balance model that assumes
 770 that air leaving the canyon is at C_c and air entering is at C_a (we will revisit this assumption later):

771

$$V_c \frac{dC_c}{dt} = \left(-\langle \overline{w^+} \rangle C_c + \langle \overline{-w^-} \rangle C_a \right) A_c + E_+ \quad (18)$$

772 All terms have dimensions of mass over time. As described in the prior section, we can replace
 773 w^+ and $-w^-$ with the absolute mean velocity statistics $\langle |\bar{w}| \rangle / 2$:

$$774 \quad V_c \frac{dC_c}{dt} = \frac{\langle |\bar{w}| \rangle}{2} (-C_c + C_a) A_c + E. \quad (19)$$

775 Under steady state, this yields:

$$776 \quad C_c - C_a = \frac{2}{\langle |\bar{w}| \rangle} \times \frac{E}{A_c}. \quad (20)$$

777 Using eq. (10) we can then write

$$778 \quad C_c - C_a = PC = \frac{E}{ACH^* h_c A_c} = \frac{E}{ACH}. \quad (21)$$

779 Following Eq. (21), and knowing the pollutant emission rates and the computed ACH as per (Eq.
 780 10), the concentration within the street canyon can be estimated. CO is used here as an example,
 781 and an estimation of the emission rate is performed following the guidance of (EPA, 2008, 2014)
 782 where the average gasoline vehicle emission rate is estimated to be 5.8 g CO km^{-1} (for an
 783 approximate velocity of 30 km h^{-1}). From this reference, we obtain that each vehicle emits 0.048
 784 g CO s^{-1} . A density of about 145 vehicles per km of road (Ingram and Liu, 1999; NYSDOT,
 785 2011) is assumed; therefore, for a road section with a length of 0.137 km, the emission of 19 cars
 786 has been presumed, which would yield a CO emission rate of 912 mg CO s^{-1} .

787

788 According to the EPA National record on CO Air Quality trends, a reasonable estimate for the
 789 average CO concentration in the atmosphere C_a is 3 mg CO m^{-3} . Based on the ACH estimations
 790 obtained for the real scale buildings (as shown in Table. 2 & 3) and following the emission rate
 791 of 912 mg CO s^{-1} , and the above described concentration in the atmosphere C_a , the pollutant
 792 concentration estimations can be computed. However, since the concentration at ground level,
 793 i.e. below HP_2 , can be significantly higher than the canyon-average, this approach can be
 794 extended to a two-reservoir model to estimate the pollutant concentration to which pedestrians
 795 are exposed.

796

797 Assuming that the emissions are released below HP_2 , they first have to get to the upper part of
 798 the canyon through HP_2 , and then leave the canyon through HP_1 . We can then write under steady
 799 state

$$800 \quad (\eta_p C_p - C_c) ACH_2 = E, \quad (22)$$

801 where C_p is concentration at pedestrian level, C_c is concentration between planes HP_1 and HP_2 .
 802 η_p is the ventilation efficiency at the pedestrian introduced to account for the fact that the air
 803 below and above HP_2 are not truly perfectly mixed. Polluted air lofted upwards in the canyon
 804 might be re-entrained down below HP_2 . This then yields:

$$805 \quad C_c = \eta_p C_p - \frac{E}{ACH_2}, \quad (23)$$

806 The mass balance for the air space between HP_1 and HP_2 , under steady state, then reflects the
 807 fact that pollutant flux through HP_1 and HP_2 must be equal, which when combined with Eq 23
 808 yields

$$809 \quad \begin{aligned} E &= (\eta_p C_p - C_c) ACH_2 = (\eta_c C_c - C_a) ACH_1 \\ &= \left(\eta_c \left(\eta_p C_p - \frac{E}{ACH_2} \right) - C_a \right) ACH_1 = \left((\eta_c \eta_p C_p - C_a) ACH_1 - \frac{\eta_c ACH_1 E}{ACH_2} \right) \end{aligned} \quad (24)$$

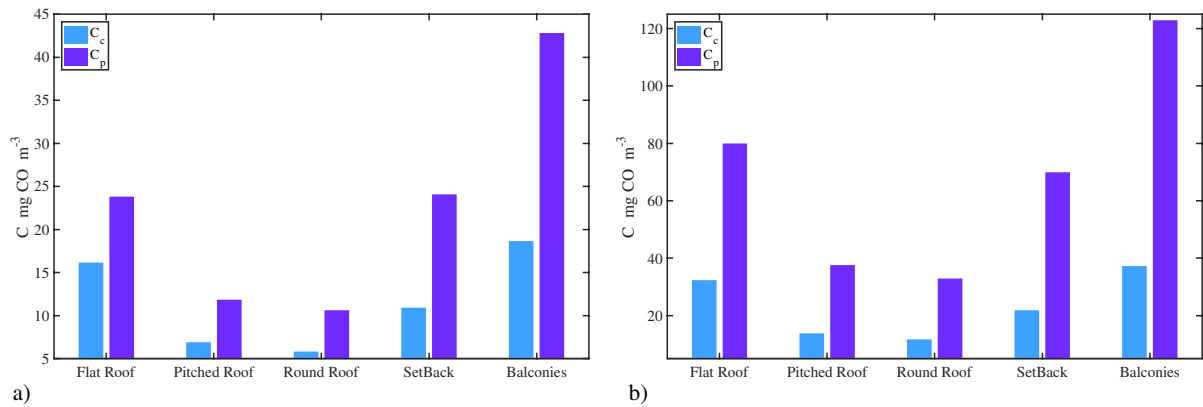
810 Where η_c is the ventilation efficiency at the street canyon top, again introduced to account for re-
 811 entrainment of polluted air into the canyon. From this formulation, we can therefore obtain the
 812 value for C_p as a function of E

$$813 \quad C_p = \frac{C_a}{\eta_c \eta_p} + \left(\frac{1}{\eta_c \eta_p ACH_1} + \frac{1}{\eta_p ACH_2} \right) E \quad (25)$$

814 HP_1 and HP_2 , thus act like resistances in series to the ventilation of pollutant from the street
 815 level. One should note here that the ventilation efficiencies can only be exactly estimated from
 816 simulations where the pollutant is actively represented as a tracer. Their values will depend on
 817 many factors such as emitter locations and geometry. As such, the influence of geometry can
 818 exceed what is inferred from differences in ACH if it turns out it has a big impact on ventilation
 819 efficiency. This however would require another study that delves into such analyses and cannot
 820 be adequately addressed in this paper. Therefore, here we will restrict the scope to investigating
 821 the influence of variations in the values of η_c and η_p on the concentrations.

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This concentration, denoted as C_p (following Eq. 25), accounts for the concentration of air contained below HP_2 , while C_c in this two-reservoir model (following Eq. 23) denotes the pollutant concentration contained between HP_1 and HP_2 (see Fig. 9). The emitter has been assumed to be located fully below HP_2 , representing the CO emissions released from the circulating passenger vehicles.



829 **Fig 10** Street canyon pollutant exchange: the blue colour bars display the C_c results (the PC contained between HP_1 and HP_2) while the purple colour displays the C_p results (the PC contained below HP_2) a) shows the results obtained for a ventilation efficiency of $\eta_p = \eta_c = 1$, while b) shows the results obtained for a ventilation efficiency of $\eta_p = \eta_c = 0.5$.

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Figure (10) displays the concentrations computed following Eqs. (23) and (25). Two cases have been studied (i) with a ventilation efficiency of $\eta_p = \eta_c = 1$ (an overly optimistic scenario where the full volume of air within the canyon would be exchanged in one event), and (ii) with a ventilation efficiency of $\eta_p = \eta_c = 0.5$ (where exchanges occur in smaller volumes allowing some emitted pollutants to remain in the canyon following the exchange of a full volume; this results from the effect of re-entrainment for example and the shortcomings of the fully-mixed reservoir assumption. Taking into account that the current NAAQS for CO establish an environmental limit of 9 mg m^{-3} of carbon monoxide (EPA, 2010), the computed concentrations included in (Fig. 10a) following $\eta_p = \eta_c = 1$ remain within tolerable limits for the pitched and round roof geometries; however, the remaining geometries exceed the EPA limit. Figure 10.b, where $\eta_p = \eta_c = 0.5$ is used, shows that the pollutant concentrations both for C_p and C_c exceed the tolerable limits for all studied building geometries. This in fact underlines the limitations of air

847 exchange studies if not coupled with analyses of ventilation efficiency. As shown in (Fig. 10.b),
848 C_p ranges from 32.97 mg m⁻³ (for the round roof building geometry) to 122.94 mg m⁻³ (for the
849 building geometry with balconies). Overall it is clear that, as discussed for the *ACH* results, the
850 pollutant concentrations both at the pedestrian level and across *HP*₂ as well as across *HP*₁, are
851 substantially higher for the geometry with balconies than for the round roof or pitched roof
852 geometries.

853

854 In the methodology used here for PC calculations, it is important to reiterate that only passenger
855 vehicle emissions have been considered. Heavy duty transport has not been taken into account.
856 Also emissions from households have not been considered. Therefore, for a comprehensive study
857 of CO emissions, a more detailed emission source estimation would need to be performed, and
858 ventilation efficiencies need to be quantified more accurately.

859 **6 Conclusions**

860 Mean flow and turbulence in an urban street canyon have been studied to understand the effect of
861 variations in building geometries on street ventilation. The Air Exchange Rate (*ACH*) has been
862 computed for two planes within the urban street canyon, one located at the building-top level and
863 the second just above the pedestrian level. Direct LES estimations ACH_{LES} have been performed
864 and the differences between the studied geometries analyzed. The results show that the round
865 geometry is the one that most favourably promotes urban ventilation, while on the contrary the
866 geometry with the façade with balconies is the one that most severely compromises urban
867 ventilation. The building geometry with the round roof creates over two times larger exchanges
868 than the one with balconies below *HP*₁ (the plane passing through the vertices of the buildings)
869 and 5 times larger below *HP*₂ (the pedestrian level air exchange plane at 0.2 times the building
870 height). Therefore, the study has shown that roof and façade geometries strongly influence the air
871 exchanges between the street canyon and the free stream flows. Based on the ACH_{LES} estimate,
872 the Pollutant Concentration (PC) within the canyon can be computed for the different building
873 geometries. A two-reservoir model was developed and applied to compute these pollutant
874 concentrations at the pedestrian level C_p (Below *HP*₂) and in the the canyon core C_c (between
875 *HP*₁ and *HP*₂) for an illustrative example of carbon monoxide vehicular emissions; it shows
876 similar trends with building geometry as those observed for the ACH_{LES} estimates, with rounder

877 and smoother walls promoting more exchanges. The ventilation efficiency of a given geometry
878 however plays a role in the actual ventilation; this requires further analysis using simulations that
879 resolve the budget of the pollutant mass.

880

881 A novel formulation to compute the ACH has been proposed using data of mean vertical velocity
882 and σ_w . This method, based on a folded normal distribution model of the vertical velocity, seeks
883 to reduce the computational requirements so that ACH calculations can be performed with results
884 obtained from RANS models with closures that provide σ_w . The comparisons between the direct
885 LES results ACH_{LES} and the folded normal distribution estimates ACH_{FND} show a very good
886 agreement with mean errors of less 2%, and maximum errors of around 4%. This is a significant
887 improvement over two alternatively previous formulations that were tested here. Therefore, the
888 results obtained from the folded normal distribution model provide a good approximation to the
889 direct LES results, and can be used as a computationally less-demanding alternative that can use
890 σ_w and the temporal and spatial mean of the vertical velocity $\langle \bar{w} \rangle$ obtained through RANS
891 simulations.

892

893 Some of the limitations of the study are related to the assumed idealized deep street canyon
894 building configurations with extruded 2-dimensional section profiles (with uniform building
895 heights and aligned facades). In real urban configurations, building profiles generally vary along
896 the longitudinal axis of the street canyon, and the later has a finite length. Furthermore, the
897 approach flow angle of attack has been constrained to perpendicular to the street canyon axis.
898 Isothermal conditions have also been imposed and thus surface heating or cooling was not
899 considered, but it will have appreciable impact on the results. Therefore, while the results
900 obtained can help us develop an understanding of the role that street canyon geometry plays in
901 street ventilation, a complete picture of how flow and ventilation behave in realistic
902 heterogeneous urban configurations, where 3-dimensional flow dynamics are significant,
903 remains to be developed.

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909
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915
916 **References**

- 917 Anderson, W., Li, Q., Bou-Zeid, E., 2015. Numerical simulation of flow over urban-like topographies and
918 evaluation of turbulence temporal attributes. *Journal of Turbulence* 16, 809-831.
- 919 ANSYS, 2013. ANSYS Fluent Theory Guide. Release 15.0. Ansys, Inc., Canonsburg, PA.
- 920 Aynsley, R.M., 1999. Shape and Flow: The Essence of Architectural Aerodynamics. *Architecture Science*
921 *Review* 42, 69-74.
- 922 Barlow, J.F., Belcher, S.E., 2002. A Wind Tunnel Model for Quantifying Fluxes in the Urban Boundary
923 Layer. *Boundary-Layer Meteorology* 104, 131-150.
- 924 Barlow, J.F., Harman, I.N., Belcher, S.E., 2004. Scalar Fluxes from Urban Street Canyons Part I:
925 Laboratory Simulation. *Boundary-Layer Meteorology* 88, 279-306.
- 926 Bou-Zeid, E., 2005. Large Eddy Simulation of Atmospheric Boundary Layer Flow over Heterogeneous
927 Surfaces. Johns Hopkins University, Baltimore, Maryland.
- 928 Bou-Zeid, E., Overney, J., Rogers, B.D., Parlange, M.B., 2009. The Effects of Building Representation
929 and Clustering in Large-Eddy Simulations of Flows in Urban Canopies. *Boundary-Layer Meteorology*
930 132, 415-436.
- 931 Britter, R.E., Hanna, S.R., 2003. Flow and Dispersion in Urban Areas. *Annual Review of Fluid*
932 *Mechanics* 35, 469-496.
- 933 Brown, M.J., Lawson, R.E., DeCroix, D.S., Lee, R.L., 2000. Mean Flow and Turbulence Measurements
934 around a 2-D Array of Buildings in a Wind Tunnel, *Conf. Appl. of Air Pollut. Meteorol.*, 11th.
935 *Am.Meteorol.Soc.*, Long Beach, Calif.
- 936 Buccolieri, R., Salizzoni, P., Soulhac, L., Garbero, V., Di Sabatino, S., 2015. The Breathability of
937 Compact Cities. *Urban Climate* 13, 73-93.
- 938 Buccolieri, R., Sandberg, M., Di Sabatino, S., 2010. City Breathability and Its Link to Pollutant
939 Concentration Distribution within Urban-Like Geometries. *Atmospheric Environment* 44, 1894-1903.
- 940 Cheng, W.C., Liu, C.H., Leung, D.Y.C., 2008. Computational Formulation for the Evaluation of Street
941 Canyon Ventilation and Pollutant Removal Performance. *Atmospheric Environment* 42, 9041-9051.
- 942 Cheng, W.C., Liu, C.H., Leung, D.Y.C., 2009. On the Correlation of Air and Pollutant Exchange for
943 Street Canyons in Combined Wind-Buoyancy-Driven Flow. *Atmospheric Environment* 43, 3682-3690.
- 944 Dezső-Weidinger, G., Stitou, A., Van Beeck, J., Riethmuller, M.L., 2003. Measurement of the Turbulent
945 Mass Flux with PTV in a Street Canyon. *Journal of Wind Engineering and Industrial Aerodynamics* 91,
946 1117-1131.
- 947 Di Sabatino, S., Buccolieri, R., Pulvirenti, B., Britter, R.E., 2008. Flow and Pollutant Dispersion in Street
948 Canyons Using FLUENT and ADMS-Urban. *Environmental Modeling & Assessment* 13, 369-381.
- 949 Di Sabatino, S., Solazzo, E., Paradisi, P., Britter, R., 2007. A Simple Model for Spatially-Averaged Wind
950 Profiles Within and Above an Urban Canopy. *Boundary-Layer Meteorology* 127, 131-151.

951 EPA, 2008. Average Annual Emissions and Fuel Consumption for Gasoline-Fueled Passenger Cars and
 952 Light Trucks. Office of Transportation and Air Quality. Environmental Protection Agency, Washington.
 953 EPA, 2010. Quantitative Risk and Exposure Assessment for Carbon Monoxide - Amended U.S.
 954 Environmental Protection Agency Office of Air Quality Planning and Standards Health and
 955 Environmental Impacts Division North Carolina.
 956 EPA, 2014. Greenhouse Gas Emissions from a Typical Passenger Vehicle. Office of Transportation and
 957 Air Quality. Environmental Protection Agency, EPA.
 958 Giometto, M., Christen, A., Meneveau, C., Fang, J., Krafczyk, M., Parlange, M., 2016. Spatial
 959 Characteristics of Roughness Sublayer Mean Flow and Turbulence Over a Realistic Urban Surface.
 960 *Boundary-Layer Meteorol* 160, 425-452.
 961 Hamlyn, B., Britter, R.E., 2005. A Numerical Study of the Flow Field and Exchange Processes within a
 962 Canopy of Urban-Type Roughness. *Atmospheric Environment* 39, 3243-3254.
 963 Hang, J., Sandberg, M., Li, Y., 2009. Age of Air and Air Exchange Efficiency in Idealized City Models.
 964 *Building and Environment* 44, 1714-1723.
 965 Howard, L., 1838. *The Climate of London, Deduced from Meteorological Observations Made at Different*
 966 *Places in the Neighbourhood of the Metropolis.* C.Baldwin Printer, London.
 967 Huang, Y., Hu, X., Zeng, N., 2009. Impact of Wedge-Shaped Roofs on Airflow and Pollutant Dispersion
 968 Inside Urban Street Canyons. *Building and Environment* 44, 2335-2347.
 969 Hunter, L.J., Watson, I.D., Johnson, G.T., 1990. Modelling Air Flow Regimes in Urban Canyons. *Energy*
 970 *and Buildings* 15-16, 315-324.
 971 Inagaki, A., Castillo, M.C.L., Yamashita, Y., Kanda, M., Takimoto, H., 2012. Large-Eddy Simulation of
 972 Coherent Flow Structures within a Cubical Canopy. *Boundary-Layer Meteorology* 142, 207-222.
 973 Ingram, G.K., Liu, Z., 1999. Determinants of Motorization and Road Provision. Policy Research Working
 974 Papers, World Bank Group.
 975 Kastner-Klein, P., Berkowicz, R., Britter, R., 2004. The Influence of Street Architecture on Flow and
 976 Dispersion in Street Canyons. *Meteorology and Atmospheric Physics* 87, 121-131.
 977 Kastner-Klein, P., Plate, E.J., 1999. Wind-Tunnel Study of Concentration Fields in Street Canyons.
 978 *Atmospheric Environment* 33, 3973-3979.
 979 Kellnerova, R., Kukacka, L., Jurcakova, K., Uruba, V., Janour, Z., 2012. PIV Measurement of Turbulent
 980 Flow Within a Street Canyon: Detection of Coherent Motion. *Journal of Wind Engineering and Industrial*
 981 *Aerodynamics* 104-106, 302-313.
 982 Landsberg, H.E., 1981. *The Urban Climate.* Academic Press, New York.
 983 Leone, F.C., Nelson, L.S., Nottingham, R.B., 1961. The Folded Normal Distribution. *Technometrics* 3,
 984 543-550.
 985 Li, Q., Bou-Zeid, E., Anderson, W., Grimmond, S., Hultmark, M., 2016. Quality and Reliability of LES
 986 of Convective Scalar Transfer at High Reynolds Numbers. *International Journal of Heat and Mass*
 987 *Transfer* 102, 959-970.
 988 Li, X.X., Liu, C.H., Leung, D.Y.C., 2005. Development of a K-epsilon Model for the Determination of
 989 Air Exchange Rates for Street Canyons. *Atmospheric Environment* 39, 7285-7296.
 990 Liu, C., Leung, D., Barth, M., 2005. On the Prediction of Air and Pollutant Exchange Rates in Street
 991 Canyons of Different Aspect Ratios Using Large-Eddy Simulation. *Atmospheric Environment* 39, 1567-
 992 1574.
 993 Llaguno-Munitxa, M., Bou-Zeid, E., Hultmark, M., 2017. The influence of building geometry on street
 994 canyon air flow: Validation of large eddy simulations against wind tunnel experiments. *Journal of Wind*
 995 *Engineering and Industrial Aerodynamics* 165, 115-130.
 996 Moonen, P., Dorer, V., Carmeliet, J., 2011. Evaluation of the Ventilation Potential of Courtyards and
 997 Urban Street Canyons using RANS and LES. *Journal of Wind Engineering and Industrial Aerodynamics*
 998 99, 414-423.
 999 Nazarian, N., Martilli, A., Kleissl, J., 2017. Impacts of Realistic Urban Heating, Part I: Spatial Variability
 1000 of Mean Flow, Turbulent Exchange and Pollutant Dispersion. *Boundary-Layer Meteorology*, 1-27.

1001 Neophytou, M.K.A., Britter, R.E., 2005. Modelling the Wind Flow in Complex Urban Topographies: a
1002 Computational-Fluid-Dynamics Simulation of the Central London Area, Fifth GRACM International
1003 Congress on Computational Mechanics, Limassol, Cyprus.

1004 Ng, E., 2009. Policies and technical guidelines for urban planning of high-density cities – air ventilation
1005 assessment (AVA) of Hong Kong. *Building and Environment* 44, 1478-1488.

1006 Ng, E., 2012. Towards planning and practical understanding of the need for meteorological and climatic
1007 information in the design of high-density cities: A case-based study of Hong Kong. *International Journal*
1008 *of Climatology* 32, 582-598.

1009 NYSDOT, 2011. New York State Department of Transportation. 2011 Traffic Data Report for New York
1010 State, New York.

1011 Oke, T.R., 1987. *Boundary Layer Climates*. Methuen & Co. Ltd, York, UK.

1012 Oke, T.R., 1988a. Street Design and Urban Canopy Layer Climate. *Energy and Buildings* 11, 103-113.

1013 Oke, T.R., 1988b. The Urban Energy Balance. *Progress in Physical Geography* 12, 471-508.

1014 Panagiotou, I., Nophytou, M.K.A., Hamlyn, B., Britter, R.E., 2013. City breathability as quantified by the
1015 exchange velocity and its spatial variation in real inhomogeneous urban geometries: An example from
1016 central London urban area. *Science of the Total Environment* 442, 466–477.

1017 Piomelli, U., Moin, P., Ferziger, J.H., 1988. Model Consistency in Large Eddy Simulation of Turbulent
1018 Channel Flows. *Physics of Fluids* 31, 1884-1891.

1019 Poggi, D., Katul, G.G., 2008. Micro and macro dispersive fluxes in canopy flows. *Acta Geophys* 56, 778-
1020 799.

1021 Pope, S.B., 2000. *Turbulent flows*. Cambridge University Press, New York.

1022 Rafailidis, S., 1997. Influence of Building Areal Density and Roof Shape on the Wind Characteristics
1023 Above a Town. *Boundary-Layer Meteorology* 85, 255-271.

1024 Rafailidis, S., Schatzmann, M., 1996. Physical Modeling of Car Exhaust Dispersion in Urban Street
1025 Canyons. The Effect of Slanted Roofs. *Air Pollution Modelling and its Application XI*.

1026 Ramponi, R., Blocken, B., de Coo, L.B., Janssen, W.D., 2015. CFD Simulation of Outdoor Ventilation of
1027 Generic Urban Configurations with Different Urban Densities and Equal and Unequal Street Widths.
1028 *Building and Environment* 92, 152-166.

1029 Raupach, M.R., Shaw, R.H., 1982. Averaging Procedures for Flow Within Vegetation Canopies. .
1030 *Boundary-Layer Meteorology* 22, 79-90.

1031 Riain, C.M.N., Fisher, B., Martin, C.J., Littler, J., 1998. Flow Field and Pollution Dispersion in a Central
1032 London Street. *Environment Monitoring and Assessment* 52, 299-314.

1033 Salizzoni, P., Marro, M., Soulhac, L., Grosjean, N., Perkins, R.J., 2011. Turbulent Transfer Between
1034 Street Canyons and the Overlying Atmospheric Boundary Layer. *Boundary-Layer Meteorology* 141, 393-
1035 414.

1036 Salizzoni, P., Soulhac, L., Mejean, P., 2009. Street Canyon Ventilation and Atmospheric Turbulence.
1037 *Atmospheric Environment* 43, 5056-5067.

1038 Shur, M.L., Spalart, P.R., Strelets, M.K., Travin, A.K., 2008. A hybrid RANS-LES approach with
1039 delayed-DES and wall-modelled LES capabilities. *International Journal of Heat and Fluid Flow* 29, 1638-
1040 1649.

1041 Slotnick, J., A. Khodadoust, J. Alonso, D. Darmofal, W. Gropp, E. Lurie, Mavriplis, D., 2014. CFD
1042 Vision 2030 Study. NASA, Langley Research Center, Hampton, Virginia

1043 Smagorinsky, J., 1963. General Circulation Experiments with the Primitive Equations, in: James
1044 E.Caskey, J. (Ed.), *Montly Weather Review*. Weather Bureau, Washington D.C.

1045 Solazzo, E., Britter, R.E., 2007. Transfer Processes in a Simulated Urban Street Canyon. *Boundary-Layer*
1046 *Meteorology* 124, 43-60.

1047 Takano, Y., Moonen, P., 2013. On the Influence of Roof Shape on Flow and Dispersion in an Urban
1048 Street Canyon. *Journal of Wind Engineering and Industrial Aerodynamics* 123, 107-120.

1049 Temmerman, L., Leschziner, M.A., Mellen, C., Fröhlich, J., 2003. Investigation of Subgrid-Scale Models
1050 and Wall-Function Approximations in Large Eddy Simulation of Separated flow in a Channel with
1051 Streamwise Periodic Constrictions. *International Journal of Heat and Fluid Flow* 24, 157-180.

1052 Theodoridis, G., Moussiopoulos, N., 2000. Influence of Building Density and Roof Shape on the Wind
1053 and Dispersion Characteristics in an Urban Area. A numerical study. *Environmental Monitoring and*
1054 *Assessment* 65, 407–415.
1055 Tominaga, Y., 2012. Visualization of city breathability based on CFD technique: case study for urban
1056 blocks in Niigata City. *Journal of Visualization* 15, 269-276.
1057 Transport of London, 2015. Low Emission Zone. <https://tfl.gov.uk/modes/driving/low-emission-zone>.
1058 Accessed 15th of June 2016.
1059 UNFPA, 2014. Population and Sustainable Development in the Post-2015 Agenda, p. 56.
1060 Vardoulakis, S., Fisher, B.E.A., Pericleous, K., Gonzalez-Flesca Hernandez, N., 2003. Modelling air
1061 quality in street canyons: a review. *Atmospheric Environment* 37, 155-182.
1062 WHO, 2014. World Urbanization Prospects 2014. United Nations.
1063 Xie, X., Huang, Z., Wang, J., Xie, Z., 2005. The Impact of Solar Radiation and Street Layout on Pollutant
1064 Dispersion in Street Canyon. *Building and Environment* 40, 201-212.
1065 Xie, X., Liu, C.H., Leung, D.Y.C., Leung, M.K.H., 2006. Characteristics of Air Exchange in a Street
1066 Canyon with Ground Heating. *Atmospheric Environment* 40, 6396-6409.
1067 Xie, Z.T., Castro, I.P., 2009. Large-Eddy Simulation for Flow and Dispersion in Urban Streets.
1068 *Atmospheric Environment* 43, 2174-2185.
1069 Yaghoobian, N., Kleissl, J., Paw, U.K.T., 2014. An Improved Three-Dimensional Simulation of the
1070 Diurnally Varying Street-Canyon Flow. *Boundary-Layer Meteorology* 153, 251-276.
1071 Yassin, M.F., 2011. Impact of Height and Shape of Building Roof on Air Quality in Urban Street
1072 Canyons. *Atmospheric Environment* 45, 5220-5229.

1073