

Evaluation of pollutant exposure using virtual walkers and large-eddy simulation: application to an idealised urban neighbourhood

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Abstract

Urban air quality studies have primarily focused on pollutant dispersion; however, **spatial or temporal concentrations collected at discretely distributed grid points (or fixed receptors) do not reflect the actual pollutant exposure of pedestrians. Using large-eddy simulation (LES) with virtual walkers implemented, this study investigates pollutant exposure of walking agents (or moving receptors) in an urban turbulent boundary-layer flow** developed over an aligned building array under the influence of different wind directions. **The spatial variability of the exposure risks are found to be better captured by the moving receptors than the fixed receptors along the same agent walking tracks. We demonstrate that the actual exposure can differ significantly from results interpreted from data recorded by the fixed receptors (corresponding to Eulerian estimates) and show that large discrepancies occur in avenues near the source,** wherein dispersion of the point release has not occurred on larger spatiotemporal scales. In most scenarios, optimal evacuation routes are shown to be ones that deviate as much as possible from the dominant wind direction; **however, one needs to decide the priority of moving to further avenues first or immediately adjusting the walking direction.** The results should serve as a useful baseline reference for environmental health impact assessment and evacuation route planning against hazardous releases of air pollutants in more complex urban environments.

Keywords: Pollutant exposure, virtual walker, moving receptor, urban street canyon

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1. Introduction

Rapid urbanization has significantly accelerated anthropogenic and industrial activities in and around urban areas. Emissions of gaseous pollutants are imposing increasingly growing risks to urban air quality (Wong et al., 2019; Zheng and Yang, 2022; Wang et al., 2022). In the case of accidental releases of hazardous pollutants, accurate prediction of the exposure risk to the polluted air is vital for effective emergency response and evacuation route planning.

In the pollutant dispersion literature, researcher are more concerned about the time-mean concentration. Numerical modelling (e.g. Lo and Ngan, 2020; Masoumi-Verki et al., 2021), measurements (e.g. Jiang and Yoshie, 2018; Mo and Liu, 2018; Xing and Brimblecombe, 2018; Marucci and Carpentieri, 2020) and analytical (e.g. Belcher et al., 2015; Tzella and Vanneste, 2016) studies have highlighted scalar statistics, such as concentration fields in urban districts (Blocken et al., 2016), flux exchanges across the canopy (Chung and Liu, 2013; Panagiotou et al., 2013) and mixing with the clean air (Duan et al., 2019). Assessments of exposure have **typically been made for fixed receptors, namely based on data recorded at the grid points discretely distributed over the computational domain (Scungio et al., 2018; Wang et al., 2019; Cui et al., 2021; Zhang et al., 2023). Subsequent results are interpreted from Eulerian calculations** of the pollutant fields—associated diagnostics essentially rely on spatiotemporal averages (e.g. Tiwary et al., 2011; Ng and Chau, 2014; He et al., 2017). **Although this approach simplifies the calculation, it neglects outliers and assumes homogeneity, which can be of critical impact during emergency response.**

The risk of exposure may vary greatly as a receptor moves from one position to another. Using LES and a Lagrangian stochastic model (LSM) (Weil et al., 2004), Lo and Ngan (2017) quantified the exposure in terms of the total time spent by a pollutant particle in the region of concern. Although the residence time (a measure of exposure) was calculated by integration along particle trajectories, the ‘clock’ was spatially fixed in the region of concern, which is equivalent to setting a fixed receptor. **Therefore, the method cannot extend to simulating the pedestrian walking behaviour, and hence the spatial variability of exposure along the walking route cannot be captured.** Recent attention on exposure in the urban air quality literature has been directed towards vehicle-induced emissions (Zhao et al., 2021; Zheng and Yang, 2022);

however, they represent moving sources rather than moving receptors. Accurate prediction of the exposure risk of walking agents in urban districts has remained a concern challenging urban environmental health and sustainability (Vardoulakis et al., 2016).

The exposure of moving agents to air pollution depends on the meteorological forcing such as wind, which directly affects the pattern of the scalar field, specifically the center-of-mass translation downstream and the crosswind spread by turbulent diffusion (Davidson et al., 1995). The combined effects essentially define the size of a polluted area and, by extension, the spatially varying exposure risks. Obviously, influence of urban topography can be important as well. For example, for an aligned grid of building obstacles, the windward building facades are by definition perpendicular to the dominant wind; however, the arrangement of the array can be viewed as staggered when the wind direction is rotated. For the former, advection by the mean flow along the street (i.e. channelling) is non-negligible; for the latter, the channel flow is diminished—a pollutant scalar undergoes a more winding path as in a staggered array and the obstruction of building facades can be important (Blunn et al., 2022). Therefore, wind direction can be of qualitatively impact on pollutant exposure.

Multiple timescales are involved in the quantification of exposure. This can be of particular importance during emergency response against environmental incidents of toxic chemicals. It is well known that the mean concentration within a unit-aspect-ratio street canyon decays exponentially fast for an instantaneous pollutant source (DePaul and Sheih, 1985); however, safety is not necessarily ensured even if an agent’s walking speed is on a timescale shorter than that for the decay. One needs to compete with the timescale associated with ventilation (that is how quickly pollutants are removed from the control domain) and mixing (namely how rapidly a pollutant scalar mixes with the clean air). As pollutants disperse downwind, it is unknown if a walking agent can have sufficient time to be evacuated before the ambient air gets highly contaminated.

To understand pollutant exposure of moving receptors, the paper is organized as below. Sec. 2.1 describes the geometry of an idealised urban district represented by a grid of aligned building cuboids. Sec. 2.2 provides further details of the model setups with the focus on the moving agents and the forcing. The LES model is described in Sec. 2.3 with the model validation given in Appendix A. Sec. 3.1 presents the decay of the mean concentrations and the scalar variances, wherein the associated decay timescales

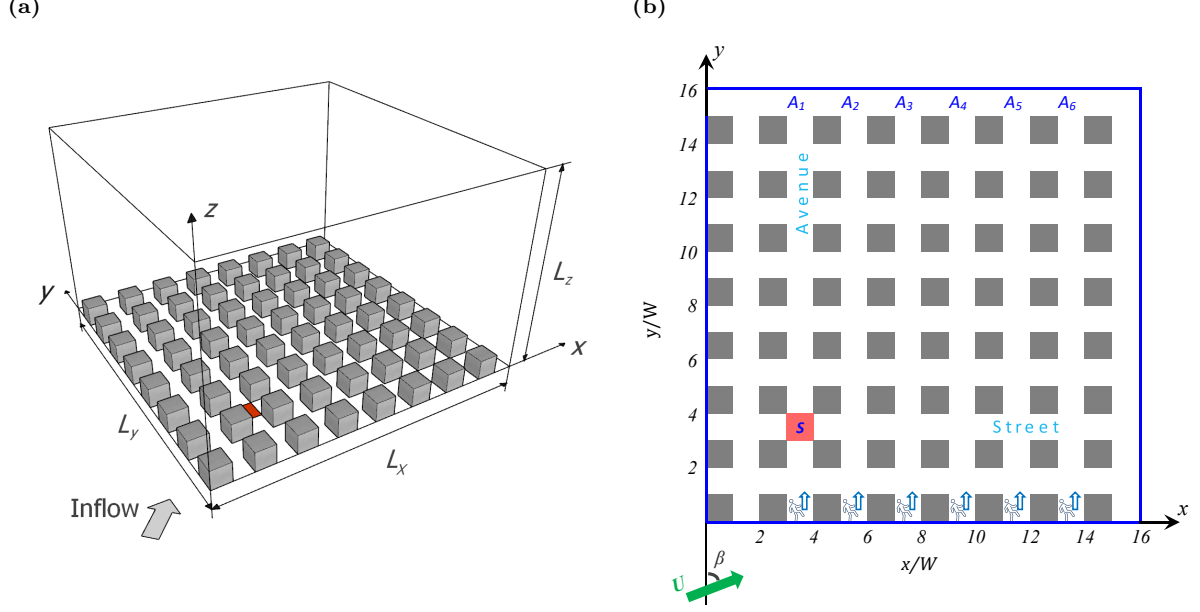


Figure 1: Schematic diagram of virtual agents walking along the avenues of an aligned building array. (a) 3D view of the computational domain; (b) plan view with the walking agents indicated. The blob highlighted in red in avenue A_1 denotes an instantaneous ground-level pollutant release (see Eq. 1). The virtual walkers move along the avenues in the spanwise direction, y , and β denotes the angle between the agent walking direction with respect to the dominant wind direction. $L_x = L_y = 16H$ and $L_z = 6.5H$ denote the domain dimensions, where H is the height of the building cuboid.

are quantified. The PDFs and CDFs of pollutant exposure are analysed in Sec. 3.2, wherein exposure risks are compared for moving and fixed receptors, and evacuation routes planning for four scenarios discussed in Sec. 3.3. Discussion and summary are given in Sec. 4 and Sec. 5, respectively.

2. Methodology

2.1. Urban geometry

As in many previous studies of urban pollutant dispersion (e.g. Davidson et al., 1995; Marucci and Carpentieri, 2020), we consider an idealised urban district represented by an array of regularly aligned building cuboids (see Fig. 1 for a schematic diagram). The building array consists of 8 building rows $\times$ 8 building columns. As in Duan and Ngan (2019), unblocked rows and columns are referred to as “streets” and “avenues”, respectively.

The domain dimensions are $L_x = 320 \times \Delta x = 320 \text{ m}$ ($= 16H$) in the east-west (or

x) direction, $L_y = 320 \times \Delta y = 320 \text{ m}$ ($= 16H$) in the north-south (i.e spanwise or y direction) **and** $L_z = 130 \times \Delta z = 130 \text{ m}$ ($= 6.5H$) **in the vertical (z), comparable with Wang and Ngan (2021) and Ma and Cheng (2023). The spatial resolution is isotropic, i.e. $\Delta x = \Delta y = \Delta z = 1 \text{ m}$ ($= H/20$), which meets the suggested best practices for urban computational fluid dynamics that the canyon walls be separated by at least 10 grid points (Franke et al., 2011). The building widths (W), avenue widths and street widths are equal to the building height $H = 20 \text{ m}$, **which implies a homogeneous urban topography, i.e. the canyon aspect ratios in x and y directions are unity ($AR_x = AR_y = H/W = 1$), and reduced ventilation in the turbulent flow of the skimming flow regime (Hunter et al., 1992).****

2.2. Forcing and moving agents

An impulse area source is prescribed at the ground level of a street-avenue intersection from the leading corner of the array. After the flow has reached statistical stationarity, pollutant is released at time t_0 , implying a source flux,

$$S = S_0 \delta(x - \vec{x}_0, t - t_0), \quad (1)$$

where S_0 denotes a source emission strength, which is specified arbitrarily as a constant, and $\vec{x}_0$ denotes a source location. **As opposed to a continuously released source (e.g. Marucci and Carpentieri, 2020; Wang and Ngan, 2021), the construction of the initial-value problem herein allows the quantification of pollutant decay rates and associated decay timescales (DePaul and Sheih, 1985).**

The flow is forced by a prescribed pressure gradient, ΔP . Following Wang and Ngan (2021) and Blunn et al. (2022), an approaching wind of $\theta \in [0^\circ, 45^\circ]$ with regard to the x -axis is considered, which is equivalent to a $\beta \in [45^\circ, 90^\circ]$ wind with respect to the agent walking direction (along the y - axis). Because the current work is focused on the exposure of moving agents, the latter notation, β , is used (see Fig. 1). For $\beta = 90^\circ$, $\Delta P = 0.6 \times 10^{-3} \text{ Pa m}^{-1}$, which generates the familiar canyon circulations within the building rows and channel flows along the streets. For a 45° wind, the building obstacles form a staggered array (Coceal et al., 2014). **For completeness, the flow patterns are presented in Fig. 2. It can be seen the counter-rotating wake vortices are altered as the dominant wind is rotated and the symmetry of the vortex pair is retained for the $\beta = 45^\circ$ diagonal wind. The streamline geometries agree**

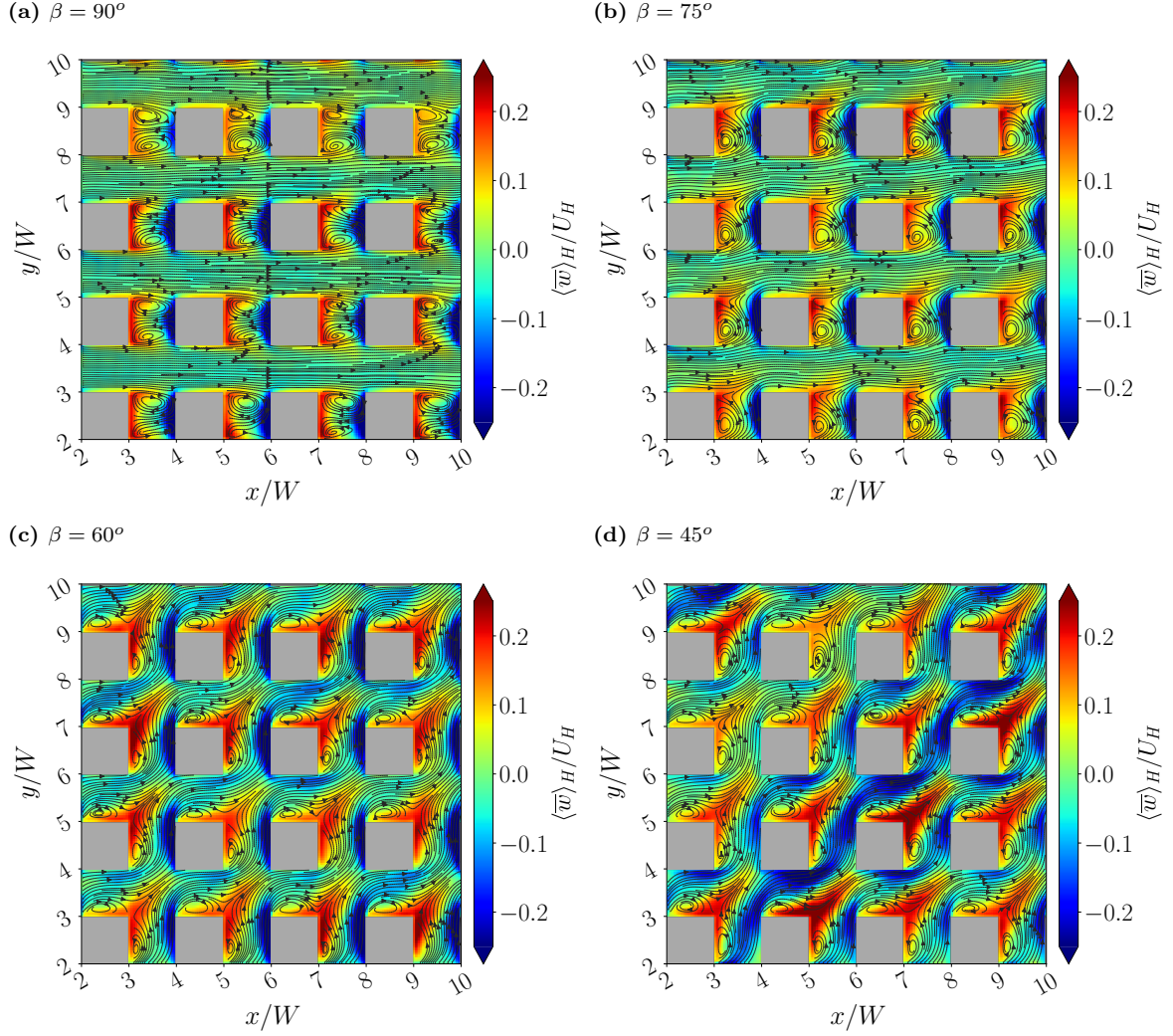


Figure 2: Streamline geometries for different β . The flows are shaded by the nondimensionalized mean vertical velocity component, wherein $\langle \vec{\cdot} \rangle_H$ denotes temporal and vertical averaging for $z/H = [0, 1]$. U_H corresponds to the absolute velocity slightly above the roof level.

well with previous studies of turbulent flow around building cuboids of an aligned array (e.g. Claus et al., 2012; Coceal et al., 2014; Wang and Ngan, 2021).

The Reynolds number based on the building height (H) and the freestream wind speed (U_{ref}) is $Re \equiv U_{\text{ref}} H / \nu \sim \mathcal{O}(10^6)$, which is comparable with the LES study of Wang and Anderson (2019) and Blunn et al. (2022), but is a few orders of magnitude greater than Inagaki and Kanda (2008) and Cheng and Castro (2002) because they considered scaled urban topographies, and is smaller than Liu et al. (2022) by two orders of magnitude because the maximum building height (180 m) of a real urban district was used as the

characteristic length scale. **The Re implies that the turbulent flow is in the fully rough regime (Castro and Robins, 1977).**

Virtual agents (i.e. moving receptors) initially set near the south boundary of the building array (see Fig. 1) start walking along the avenues at the instant of the tracer release (at t_0 , see Eq. 1). Once the north boundary is reached, the walkers reenter the domain from the south boundary and walk north once more. This prescription is maintained from the source release till the end of the simulation, whereby pollutant concentrations (C) experienced during the periodic walking along the avenues are recorded. **It is noteworthy that the moving agents essentially emulate the pedestrian walking behaviour in real urban environments.**

Implementation of the virtual walkers in LES essentially follows the virtual flight measurements of Schröter et al. (2000) and Sühling and Raasch (2013). The agent walking speed, $V_{\text{agent}} = 1.34 \text{ m s}^{-1}$, specified herein lies in the range of average walking speeds of $1.0 \text{ m s}^{-1} - 1.5 \text{ m s}^{-1}$ for adults (Mansfield et al., 2018; Mohamed and Appling, 2020). **For a moderate wind considered in the current study, $V_{\text{agent}}/\langle \bar{u} \rangle > 1$ in the pedestrian region, where $\langle \bar{u} \rangle$ is the mean streamwise velocity component (see Fig. 3).**

Data recorded by the moving receptors will be compared with that for fixed receptors (y_n), namely the grid points discretely distributed along the agent walking tracks in the y -direction. Therefore, the subscript n indicates the spanwise grid index.

2.3. Large-eddy simulation

The boundary-layer flow and scalar dispersion are simulated using PALM 6.0 (Maronga et al., 2020), which is a LES model developed specifically for atmospheric and oceanic boundary layer studies. The model is based on the implicitly filtered non-hydrostatic and incompressible Boussinesq equations. **Subgrid-scale (SGS) fluxes are parameterised using a dynamic SGS model according to Germano et al. (1991) and Heinz (2008), which allows the occurrence of backscatter (namely negative values of SGS eddy viscosity) while ensuring stability. The SGS eddy viscosity and diffusivity are obtained from additional prognostic equations for the SGS turbulent kinetic energy based on the assumption that energy transport by SGS eddies is proportional to the local gradients of the mean quantities.** Detailed descriptions of the governing equations of the LES model can be found in Lau

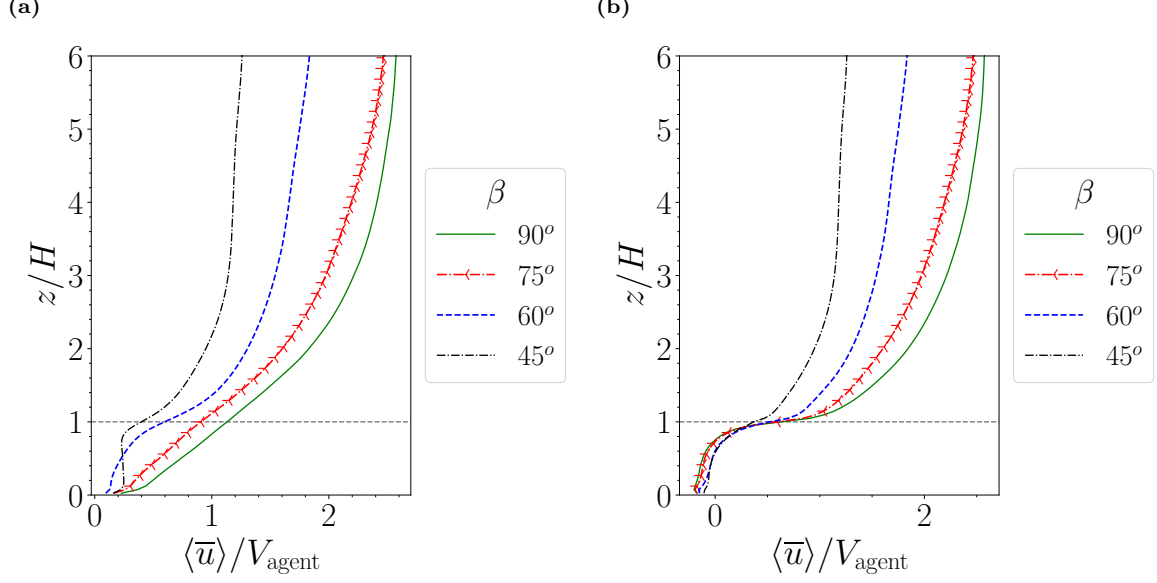


Figure 3: Vertical profiles of the streamwise velocity component, u , normalised by the agent walking speed, V_{agent} . (a) Ensemble average along the middle of the repeating streets, $y/W = 2N + 1.5$; (b) ensemble average along the middle of the repeating building rows, $y/W = 2N + 0.5$, where $N = 0, 1, \dots, 6$. Dashed horizontal line indicates $z/H = 1$. $\langle \bar{u} \rangle$ denotes temporal and horizontal averaging.

and Ngan (2018) and Maronga et al. (2020). Therefore, they are not repeated here.

As in Liu et al. (2005), periodic boundary conditions are applied in the lateral directions, whereby an infinitely spread urban region is assumed. To prevent nonphysical accumulation of pollutants within the domain, concentrations at the lateral edges are set to zero after Wang et al. (2021). At solid surfaces, there is no-slip for the velocity components and Neumann (zero-gradient) for scalars. A Neumann boundary condition is also applied at the domain top. Unresolved Reynolds shear stresses near walls are parameterised by assuming a constant-flux layer between the roughness height, z_0 , and the first grid layer following the Monin-Obukhov similarity theory (MOST) (Monin and Obukhov, 1954). As in previous studies (Park et al., 2015; Yoshida et al., 2018; Duan and Ngan, 2020), the roughness lengths for momentum and passive scalar are identical, with $z_0 = 0.1\text{m}$, which is representative of very rough walls (Letzel et al., 2012).

A third-order Runge-Kutta time-stepping scheme (Williamson, 1980) combined with an upwind-biased fifth-order finite differencing scheme is applied in solving the advection

terms for momentum and scalar. This combination has proven effective for ensuring accuracy and algorithmic simplicity (Wicker and Skamarock, 2002). The Courant-Friedrichs-Lewy (CFL) criterion was set to 0.9 with variable integration timesteps (~ 0.2 s) to guarantee numerical stability. The Poisson equation for pressure is solved with the multigrid method, which is highly optimised for Intel processors used for running the current model.

The 3-D model was initialised with a stationary-state wind profile obtained from a 10-hour run of a 1-D model with a Reynolds-average based turbulence parametrisation (Maronga et al., 2020). A 6-hour spin up, $\sim 200t^*$ (where $t^* \equiv H/u_*$ denotes the eddy turnover timescale and $u_* \sim 0.2 \text{ m s}^{-1}$ is the friction velocity), ensures that the turbulent boundary layer has become fully developed and the flow has reached statistical stationarity. Data are subsequently collected at time intervals of $\Delta t = 10 \text{ s}$ ($\sim 0.1t^*$, about four times higher than the temporal resolution of Blunn et al. (2022)) for a duration of 3600 s ($\sim 36t^*$), which are sufficient for the initial-value problem considered herein (Bernardini et al., 2014).

Validation of the LES model is presented in Appendix A.

3. Results and analyses

3.1. Scalar decay and mixing

3.1.1. Decay of volume-averaged concentrations

The removal of pollutants from the control domain (the region for $z/H \leq 1$, hereafter $\mathcal{D}$), i.e. ventilation, directly affects the scalar concentration inside the canyons and hence the exposure of walking agents to the polluted air at different locations. For a release of pollutants at an initial instant (Eq. 1), ventilation can be quantified by the decay rate of $\langle C \rangle(t)/C_0$, the normalised concentration spatially averaged over $\mathcal{D}$. Herein, C_0 denotes the bulk average of the concentration at initial time t_0 .

Physically, the change of β should not alter the exponentially decaying nature of $\langle C \rangle(t)/C_0$ (Davidson et al., 1996). The familiar exponential decay function (DePaul and Sheih, 1985), viz.

$$\langle C \rangle(t)/C_0 \sim \exp\left(-\frac{t}{\tau_r}\right), \quad (2)$$

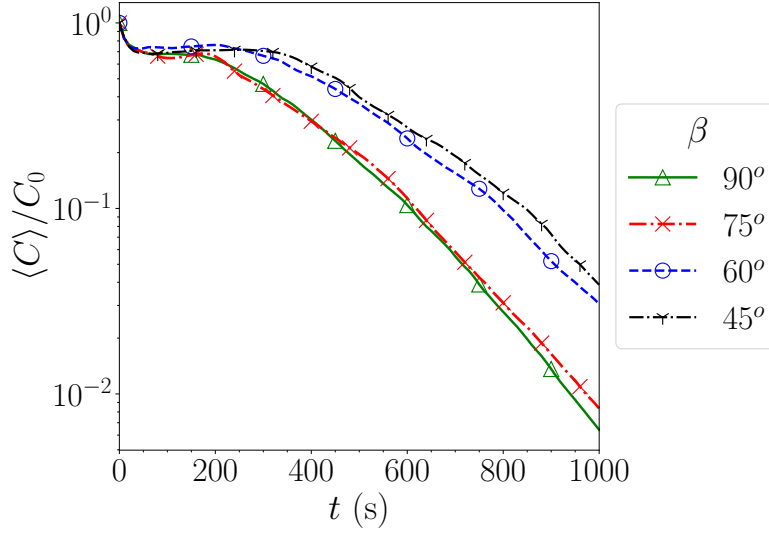


Figure 4: Decay of the normalised concentrations, $\langle C \rangle(t)/C_0$, for different β . As in Duan and Ngan (2020), the initial-stage spin up is excluded in the fitting. For clarity, the time axis is clipped at 1000 s.

where τ_r is known as the retention time (the time required for $\langle C \rangle(t)/C_0$ to reach e^{-1}), should always hold for a unit-aspect-ratio 2D street canyon (Duan et al., 2019) and a cubic 3D building array (Duan and Ngan, 2020). Fig. 4 plots the history of $\langle C \rangle(t)/C_0$. It can be seen that the exponentially decaying behaviour persists when β varies: the minimum R^2 is 0.98. The slight change of the slope reflects the sensitivity to the wind direction.

Longer retention of pollutants within the domain implies high risk of exposure. Fig. 5 shows that the removal of pollutants from $\mathcal{D}$ accelerates as the wind rotates towards the canyon axis (i.e. increased β). This is presumably because ventilation routes below $z/H < 1$ are altered when β is changed. For $\beta = 90^\circ$, ventilation is enhanced by the channel flow along the streets (Blunn et al., 2022). By contrast, for $\beta = 45^\circ$, the wind blows diagonally and ventilation is similar to that in a staggered array (Claus et al., 2012), where the pollutant scalar undergoes a more winding trajectory (Coceal et al., 2014).

3.1.2. Variance decay

The decay of the mean concentration analysed in the above section measures how quickly pollutants are removed and the volume averaging tacitly assumes homogeneity of concentrations in the control domain. An obvious limitation is that it does not quantify inhomogeneity and little can be said about how rapidly air inside the canopy bulk gets

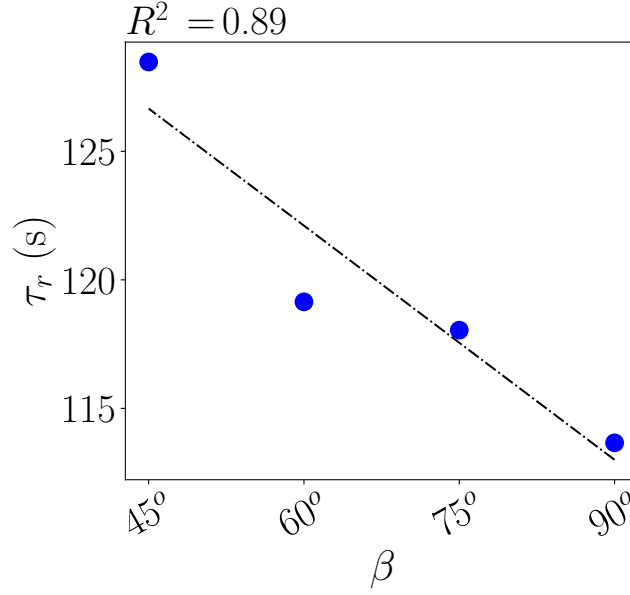


Figure 5: Retention time, τ_r (Eq. 2), associated with the decay of the mean concentrations for different β . The timescale is obtained from least squares regression of the decay of $\langle C \rangle(t)/C_0$ plotted in Fig. 4.

polluted; however, this can be of particular importance for emergency response because it gives a sense of the effectiveness of evacuation to avoid exposure to the air that is highly mixed with the pollutants.

The scalar variance, $\sigma_C^2(t) \equiv (C - \langle C \rangle)^2$, has proven an effective probe to the inhomogeneity and was successfully applied to the quantification of scalar mixing (Duan et al., 2019). The variance-decay rate characterises the rapidity of mixing (Pierrehumbert, 1994), which provides a useful timescale for emergency response reference.

It can be seen in Fig. 6 that the decay stages of the nondimensionalized scalar variance, $\langle \sigma_C^2 \rangle(t)/C_0^2$, differ slightly between early and late times, similarly to the decay of the mean concentrations (Fig. 4 in Sec. 3.1.1). However, unlike that for a 2D canyon (Duan et al., 2019), the initial-stage decay is established almost immediately after the source release and the transition to the late stage occurs much smoother. This is likely due to the fact that for a 2D canyon the variance decay (at long times) is dominantly driven by ventilation across the roof-level open boundary, whilst for a 3D array, pollutants also escape through the sides (Kastner-Klein and Plate, 1999; Jiang and Yoshie, 2018).

Given that the late-time change of scalar variances is primarily driven by the removal of pollutants from the control domain (Duan and Ngan, 2020), the timescale associated with the variance decay, τ_σ , can be defined in a similar manner as that for the decay of

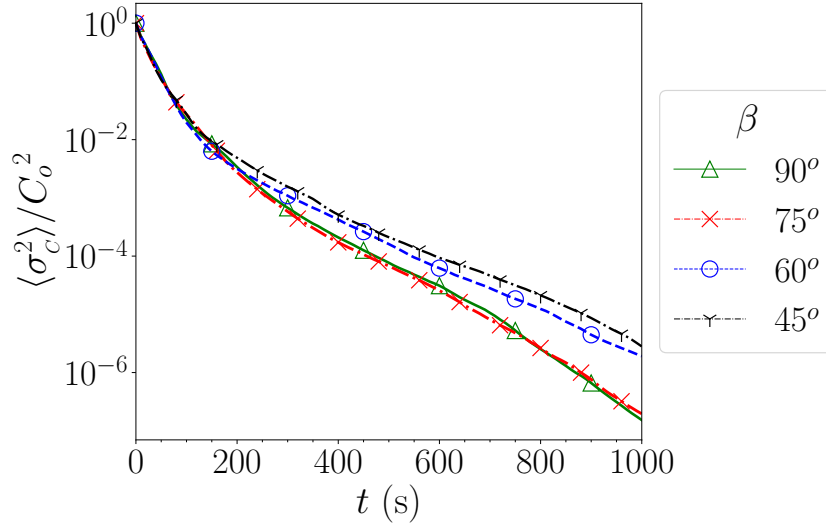


Figure 6: Decay of the normalised scalar variances, $\langle \sigma_c^2 \rangle(t)/C_0^2$. For clarity, the time axis is clipped at 1000 s.

the mean (Eq. 2), viz.

$$\langle \sigma_c^2 \rangle(t)/C_0^2 \sim \exp\left(-\frac{t}{\tau_\sigma}\right). \quad (3)$$

Fig. 7 plots τ_σ for different β . Although the amplitudes do not differ much, τ_σ exhibits a clear linear scaling with β ($R^2 = 0.89$, as τ_r does, cf. Fig. 5), implying that a well planned β , namely evacuation direction with respect to the dominant wind, could reduce the risk of exposure to the air before it is highly mixed with the pollutants.

It is noteworthy that even a small difference in the variance decay timescale can be non-negligible during emergency response when this time difference is translated into a spatial difference. For example, a 10 s difference in time can lead to around 15 m difference in space (even under the current normal walking speed, $1.34 \text{ m s}^{-1} \times 10 \text{ s} \approx 13.4 \text{ m}$), which measures the distance from one avenue to another for densely-packed urban regions.

3.1.3. Avoidance of air mixed with pollutants

A practical concern is if a normal agent walking speed specified in the current study ensures a safe avoidance of the contaminated air. While an accurate calculation needs to account for time-varying meteorological forcing, the geometrical complexity of the urban topography and the uncertainty of the pedestrian walking behaviour in realistic scenarios, a rough estimate follows.

The calculation of the timescale associated with the virtual walker, $\tau_{\text{agent}} \equiv$

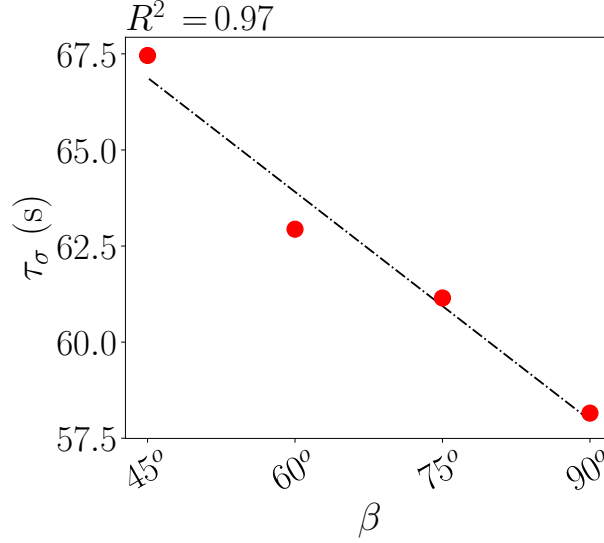


Figure 7: Scalar variance-decay timescales, τ_σ , for different β . Similarly to Fig. 4, the initial transition is excluded in the least squares regression of the exponentially decaying function, Eq. (3).

L/V_{agent} , is straightforward; however, the characteristic length scale, L , is not unique. Taking the domain dimension as the characteristic length scale ($L_y = 320$ m, see Sec. 2.2) and given $V_{\text{agent}} = 1.34 \text{ m s}^{-1}$, $\tau_{\text{agent}} = 238$ s; taking the avenue width as the characteristic length scale ($W = 20$ m), $\tau_{\text{agent}} = 15$ s. The former τ_{agent} is larger than the timescale associated with the scalar mixing (evaluated for the entire domain, cf. Fig. 7), implying an insufficient time at the current walking speed to escape out of the control domain to completely avoid exposure to the polluted air, whilst the latter is smaller than τ_{agent} , indicating that if a walker is near the source (on a spatial scale of one avenue width), there is still adequate time for an effective evacuation to be made.

3.2. Exposure risks

3.2.1. Exposure to $\max C/C_0$

The spatial variability of exposure, which cannot be captured by the mean and variance, is now examined. While the decay of the mean (Sec. 3.1.1) and variance (Sec. 3.1.2) cannot be applied directly to walking agents, because they correspond to an Eulerian calculation, one can quantify the maximum pollutant concentration, $\max C/C_0$, to which a virtual walker is exposed. Letting C_{walker} denote the concentrations recorded by a walker (i.e. C_{walker} are a subset of the Eulerian concentrations, C), $\max C/C_0$ reads

$$\max C/C_0(A_i, \beta) \equiv \max(C_{\text{walker}})(A_i, \beta). \quad (4)$$

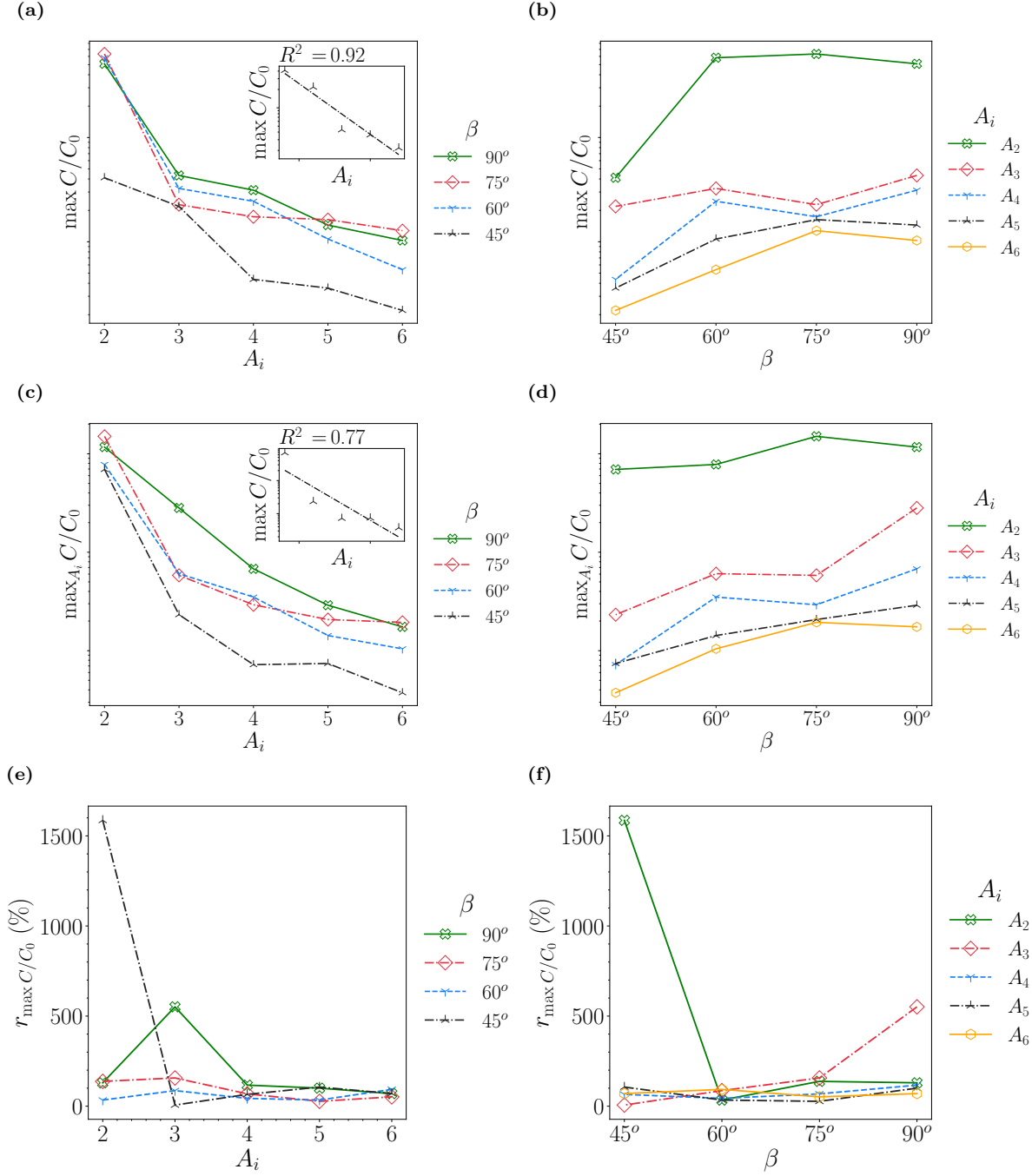


Figure 8: Sensitivity of (a,b) $\max C/C_0$ (Eq. 4) recorded by the walking agents and (c,d) $\max_{A_i} C/C_0$ (Eq. 5) recorded by the fixed receptors discretely distributed along the agent walking tracks to A_i and β ; (e,f) relative differences between $\max C/C_0$ and $\max_{A_i} C/C_0$ (Eq. 6). For reference, the dash-dotted lines in the insets of panels a and c plots the least-squares regression of $\max C/C_0$ versus A_i for $\beta = 45^\circ$. Note the logarithmic scale of the ordinates for panels a-d.

Obviously, $\max C/C_0$ depends on which avenue (A_i) the agent walks along and the wind direction, β .

Figs. 8a,b summarise the $\max C/C_0$ recorded by the agents walking along different

avenues (A_i , panel a) and for different β (panel b). Fig. 8a shows that $\max C/C_0$ decreases rapidly away from the source, particularly for large β in the first few avenues (note the logarithmic scale of the ordinates and the least-squares regression plotted in the inset for reference). The $\max C/C_0$ for $\beta = 45^\circ$ remains smaller than that for other β across all A_i . **This is because the building blockage, which protects pedestrians from immediate exposure to peak concentrations (Wang and Ngan, 2021; Melo et al., 2023), is more prominent for the $\beta = 45^\circ$ diagonal wind (for which the building arrangement is effectively staggered, see Fig. 2). It will be seen in the latter section (Sec. 3.2.2) that this result is also supported by the PDFs.** Fig. 8b shows that the $\max C/C_0$ exhibits an increasing trend with β (when the dominant wind direction deviates more from the agent walking direction), and the amplitude of $\max C/C_0$ is particularly high for A_2 , the avenue close to the source. If an agent is walking in the avenue near the pollutant source (e.g. in A_2), the results suggest evacuation routes towards farther avenues so as to quickly reduce the exposure to $\max C/C_0$, and to decrease β so as to keep $\max C/C_0$ at a relatively lower level.

The $\max C/C_0$ recorded by the walking agents, Eq.(4), may be compared with the maximum concentration recorded by the fixed receptors (y_n) discretely distributed along the same walking track (A_i) of concern (see Sec. 2.2), $\max_{A_i} C/C_0$,

$$\max_{A_i} C/C_0(A_i, \beta) \equiv \max(C)(y_n \in A_i, \beta), \quad (5)$$

Although the patterns of $\max C/C_0$ versus A_i and β (Figs. 8a,b, respectively) and $\max_{A_i} C/C_0$ versus A_i and β (Figs. 8c,d, respectively) appear quite similar, it can be seen that the relative differences (Figs. 8e,f, respectively), viz.

$$r_{\max C/C_0} = \frac{\max_{A_i} C/C_0 - \max C/C_0}{\max C/C_0} (\%), \quad (6)$$

are markedly high. **While it may seem unsurprising that the concentrations collected for fixed locations can differ from that recorded in a moving frame, the difference is surprisingly large for the initial-value problem considered herein, especially for the avenue adjacent to the pollutant source (i.e. A_2) and under the forcing of $\beta = 45^\circ$.** The results indicate that the exposure of a walker to the maximum concentration interpreted from data recorded by the fixed receptors can be significantly overestimated and the actual maximum concentration experienced by the walker can be much smaller.

3.2.2. PDFs and CDFs for moving receptors

The maximum concentrations, $\max C/C_0$, analysed in the above section do not provide a complete picture of exposure. Furthermore, decreasing the exposure to $\max C/C_0$ does not necessarily ensure safety and there could be non-negligible risk (or probability) of exposure to high concentrations (though smaller compared to $\max C/C_0$). This section examines the probability density functions (PDFs) and the cumulative density functions (CDFs) associated with the exposure to pollutants.

The PDFs of concentrations recorded by the virtual walkers (Fig. 9a, c, e, g) show a much fatter tail for A_2 , indicating high probability of exposure to peak concentrations for agents walking in this avenue **due to its immediate vicinity to the source. As dispersion occurs on larger spatiotemporal scales**, the tail becomes progressively thinner for increasing A_i and a few local peaks are seen, e.g. around $C/C_0 = 0.5 \times 10^{-3}$ for A_3 and A_4 in panel a ($\beta = 90^\circ$), **which reflect the spatial variability of the exposure risk during pedestrian walking. Emergence of the local peak concentrations is presumably attributed to the atmospheric turbulence, which occurs in very short-time intervals and is more sensitive to the spatial location than to the wind direction (Roth et al., 2015). As an agent moves along the avenue, perturbations of the atmospheric turbulence from the canyon circulations and the channel flows set in alternately.**

As β is decreased, influence of the channel flow is gradually diminished and pollutants disperse more evenly in the crosswind direction, which agrees with the numerical results of Branford et al. (2011) and Coceal et al. (2014). For $\beta = 45^\circ$ (panel g), the PDF looks relatively smoother (evidently for A_2) and the flow is statistically symmetric about the dominant wind direction. The results imply that staggered arrangement of the building array may help avoid early exposure to high concentrations for agents walking in the avenue near the pollutant source due to the immediate blockage of the building obstacles.

The CDFs help quantify the cumulative risks of exposure to different ranges of concentrations. It can be seen the CDF curves (Fig. 9b, d, f, h) start to diverge for increased C/C_0 . The curve associated with downwind A_i (more notably for small β , e.g. panel h) spans relatively narrower range of C/C_0 , indicating that agents walking in avenues far from the pollutant source are less likely exposed to extremely high concentrations (hereafter C_{extreme} , herein $C/C_0 \gtrsim 1 \times 10^{-3}$ for example), in contrast to agents in the av-

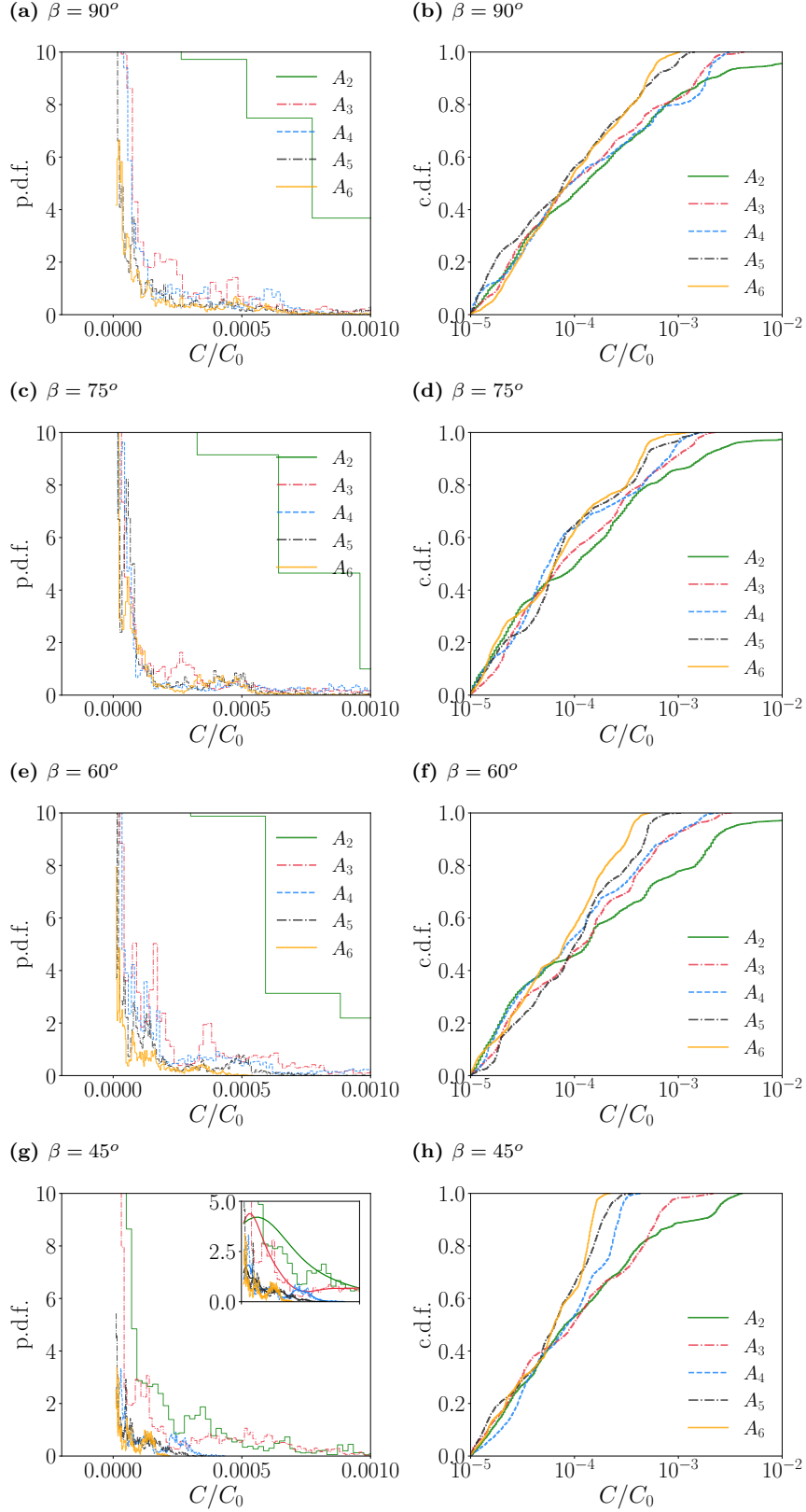


Figure 9: Probability statistics of the normalised scalar concentrations (C/C_0) recorded by the walking agents. (left panels) PDFs (shown as step functions). For clarity, statistics in each bin are normalised such that the bar heights sum to 100, x -axis is clipped at $C/C_0 = 0.001$, and y -axis capped at 10. The smoother curves in the inset of panel g plot the kernel density estimates of the step functions. (right panels) CDFs.

enues near the pollutant source. However, the CDF curves become increasingly steeper at the high-concentration end when A_i is increased, implying the growing cumulative risk, F_{C/C_0} , of exposure to highly polluted air (hereafter C_{high} , though smaller than the extremes, C_{extreme}).

3.2.3. PDFs and CDFs for fixed receptors

Fig. 10 plots the PDFs and CDFs for fixed receptors distributed along the agent walking tracks (cf. Eq. 5). Although they exhibit quite similar patterns compared to the results recorded by the moving agents (see Fig. 9 analysed in Sec. 3.2.2), the curves herein are obviously more smoother. **The difference implies that the spatial variability of the exposure risk during pedestrian walking cannot be sufficiently captured using data recorded by fixed receptors, which corresponds to an Eulerian type of analysis.**

Another notable difference is the behaviour of the PDF tail for the near-source avenue, i.e. A_2 (the step functions plotted in green in left panels). For the fixed receptors herein, the fat PDF tail persists across all β . By contrast, the sensitivity to β is well reflected in the data recorded by the walking agents (cf. Fig. 9 left panels). This is because the concentrations collected by the moving receptors along walking track A_2 may not contain a wide range of concentrations before dispersion occurs on larger spatiotemporal scales, irrespective of the wind direction. In other words, data collected by fixed receptors throughout the entire simulation period naturally contain a wider range of concentrations than that recorded by the walking agents during dispersion.

A direct implication of the thicker PDF tail for A_2 under $\beta = 45^\circ$ (see the step function in Fig. 10g) compared to that recorded by the walkers (see Fig. 9g) is that pollutant exposure to the extremes in A_2 interpreted from the data for fixed receptors tends to be overestimated. A similar trend tends to be so for A_3 under $\beta = 90^\circ$ (see Fig. 10a versus Fig. 9a); however, the sensitivity to β is gradually diminished for avenues further downstream, wherein the pollutant cloud has grown substantially in size and dispersion occurs on much larger spatiotemporal scales.

3.3. Route evaluation

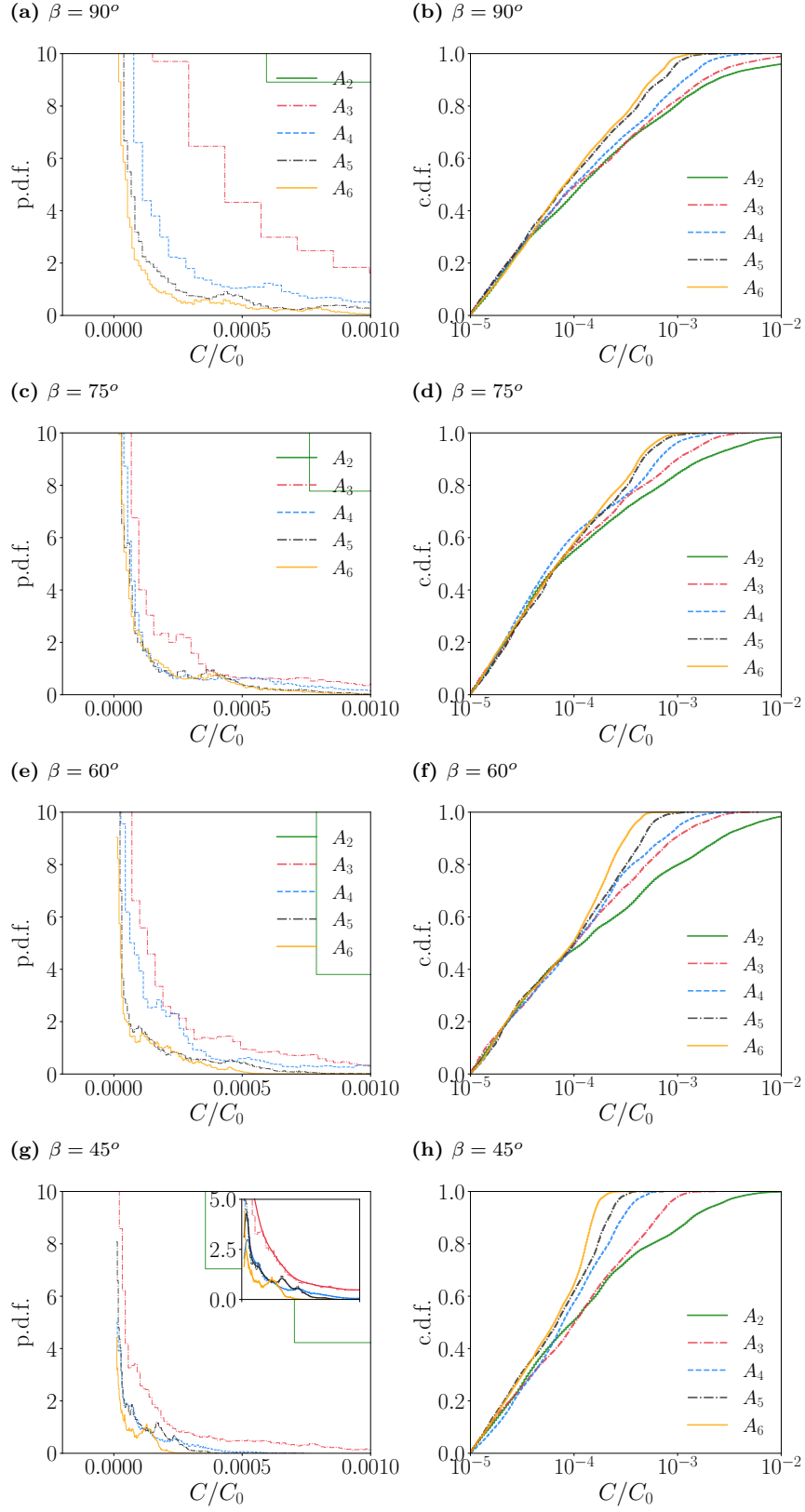


Figure 10: As in Fig. 9, but for fixed receptors, namely the spatial data collected at fixed grid points discretely distributed along the agent walking tracks.

3.3.1. Moving receptors

PDFs and CDFs assess the probability aspects of exposure to the entire spectrum of recorded concentrations; however, it is more important to quantify the exposure risk to the air that is more severely polluted. For a high-concentration range of concern, $C/C_0 \in [a, b]$, the integrated probability of exposure, P (or exposure risk), can be quantified as

$$P_{C_{\text{high}}} \equiv F_{C/C_0}(b) - F_{C/C_0}(a), \quad (7)$$

where F denotes the cumulative probability, and see Fig. 9 for reference of the high-concentration range, $[a, b] \equiv [0.9 \times 10^{-4}, 2.0 \times 10^{-4}]$, which is chosen herein purely for demonstration purpose with no loss of generality. Similarly, the integrated exposure risk to the extremes reads

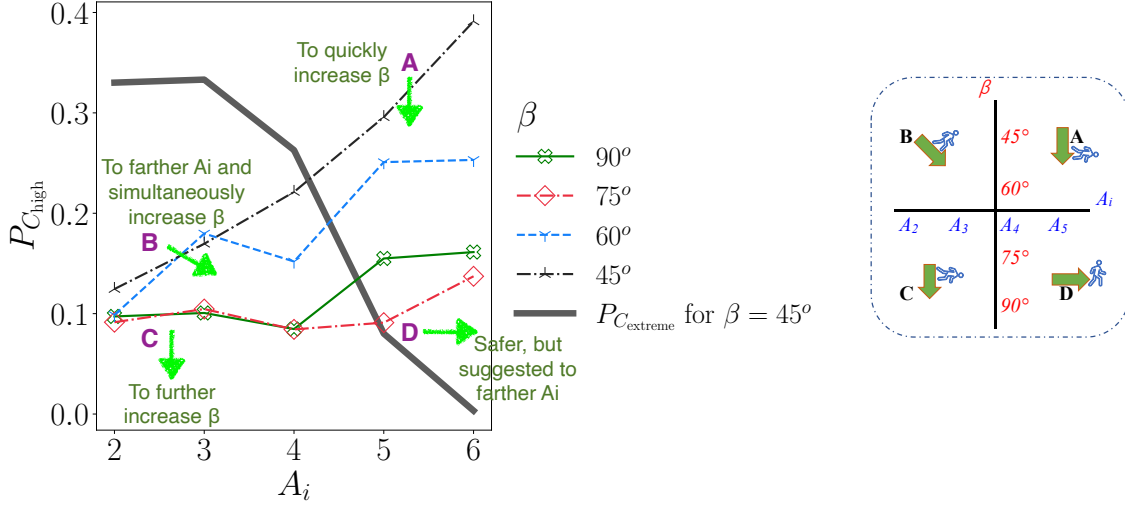
$$P_{C_{\text{extreme}}} \equiv 1 - F_{C/C_0}(b). \quad (8)$$

Fig. 11 plots the exposure risks for different A_i and β . It can be seen that the integrated probability of exposure to the high concentrations, $P_{C_{\text{high}}}$, roughly ranks as $P(A_6) > P(A_5) > P(A_4) > P(A_3) > P(A_2)$ (Fig. 11a). $P_{C_{\text{high}}}$ shows a similar monotonic sensitivity to β (Fig. 11b), and there is $P(\beta_{45^\circ}) > P(\beta_{60^\circ}) > P(\beta_{75^\circ}) > P(\beta_{90^\circ})$. For the integrated probability of exposure to the extremes, $P_{C_{\text{extreme}}}$, an opposite dependence (by definition) is seen on A_i and β , respectively.

The results in Fig. 11 indicate that evacuation routes during pollutant dispersion strongly depend on the meteorological condition (herein β) and the position of the receptor (namely the dynamically changing location of the agents walking along A_i). **During emergency response, the risk of pollutant exposure may be greatly reduced if one could scientifically decide the priority of moving to further avenues first or adjusting the walking direction immediately for given A_i and β .** With no loss of generality, we analyse four scenarios: A, B, C and D (annotated in Fig. 11a left panel and schematically sketched in Fig. 11a right panel), with each scenario corresponding to different values of β and A_i .

It can be seen if agents are located in avenues very close to the pollutant source (as scenarios B and C) and are walking at small β (e.g. 45° , as scenario B) with respect to the dominant wind, it is always safe for agents to move towards farther avenues and simultaneously increase β to reduce $P_{C_{\text{extreme}}}$ meanwhile keeping $P_{C_{\text{high}}}$ low. If agents are in the same avenue, but walking at large β (e.g. 90° , as location C), they are suggested

(a)



(b)

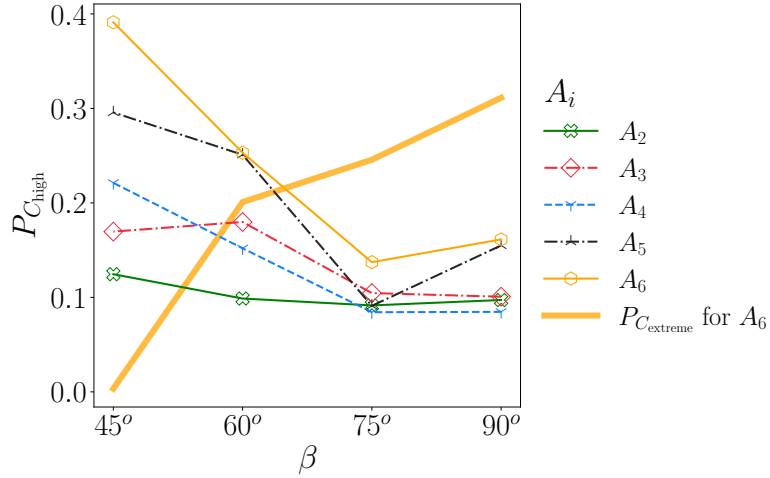


Figure 11: Integrated probability of exposure to high concentrations, $[a, b]$, $P(a < C/C_0 \leq b)$ (i.e. $P_{C_{high}}$, see Eq. 7) for different (a) A_i ; and (b) β . Note that the thicker line (colored in black in panel a and in orange in panel b) plots $P(C/C_0 > b)$ (i.e. $P_{C_{extreme}}$, see Eq. 8) and for clarity, results are only shown for one case: $\beta = 45^\circ$ in panel a and A_6 in panel b. To the right of panel a is a schematic representation of four evacuation scenarios, A, B, C and D. Each scenario corresponds to different values of A_i and β .

to further increase β (i.e. to deviate more from the dominant wind direction). Although spending time moving to farther avenues also reduces $P_{C_{\text{extreme}}}$, it is perhaps not the primary concern during emergency response as $P_{C_{\text{extreme}}}$ is already at a very low level.

If agents are located in remote avenues of a few blocks to the accidental venue (as scenarios A and D) and are walking at small β (e.g. 45° , as scenario A) with respect to the dominant wind, they are suggested to increase β first to quickly decrease $P_{C_{\text{high}}}$ and then direct towards even farther avenues. The evacuation pathway is the same as that for scenario C. If agents are in the same avenue, but walking at large β (e.g. 90° , as scenario D), they are in a relatively much safer condition, but are suggested to stay as far as possible to further decrease $P_{C_{\text{extreme}}}$. The evacuation route planning is similar to that for scenario B.

It is obvious that if agents' locations are in the same avenue with the pollutant source (i.e. in A_1), evacuation routes should be immediately opposite to the dominant wind.

3.3.2. Fixed receptors

Similarly to Fig. 11, Fig. 12 plots the integrated probability of exposure to the high concentration range, C_{high} , but for fixed receptors. Although the general patterns seem quite similar to Fig. 11, a few nontrivial differences in the details of $P_{C_{\text{high}}}$ versus A_i (panel a) and β (panel b) are noteworthy.

For avenues near the source, $P_{C_{\text{high}}}$ appears lower than that experienced by the walkers (cf. Fig. 11a), indicating an underestimation of the exposure risk to the high concentrations actually experienced by a walker. This is particularly so for large β (cf. Fig. 11b). The results imply that although similar evacuation routes as described in the above section (Sec. 3.3.1) may be suggested, **the integrated probability of exposure along the same route cannot be accurately predicted based on the Eulerian estimates.**

4. Discussion

A modified arrangement of the roughness grid may be thought as equivalent to rotating the wind (Branford et al., 2011; Marucci and Carpentieri, 2020; Blunn et al., 2022). The layout of the building obstacles directly affects pollutant exposure. For agents moving along an avenue near the pollutant source, a staggered array (for which the wind perpendicular to the avenue is rotated) is shown to help in the avoidance of early exposure to high concentrations due to the immediate blockage of the near-field building

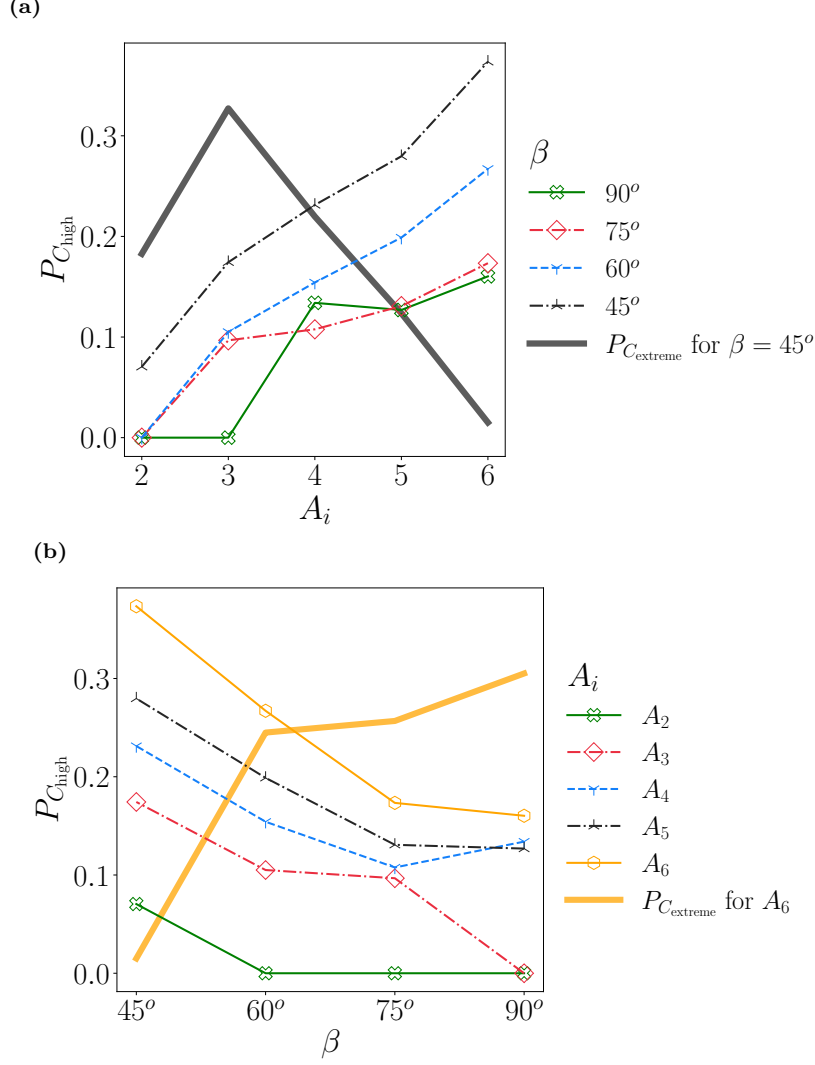


Figure 12: As in Fig. 11, but for fixed receptors, namely the spatial data collected at fixed grid points discretely distributed along the agent walking tracks.

blocks. The simplified urban topography represents a convenient starting point in the literature (e.g. Wang and Ngan, 2021; Li and Katul, 2022); however, spatial characteristics of the mean flow and turbulence in realistic urban districts of high inhomogeneity may vary greatly (Giometto et al., 2016; Hadavi and Pasdarsahri, 2021), wherein the obstruction of solid obstacles could change ventilation and hence exposure qualitatively (Blunn et al., 2022; Liu et al., 2022).

As a typical simplification, neutral stratification, which represents an idealised micro-meteorological condition (cf. Nazarian et al., 2018; Hadavi and Pasdarsahri, 2021; Lee et al., 2023; Li et al., 2023), was assumed in the current work. Under thermal stratification, the center of mass of the pollutant cloud can either descend or be elevated by the buoyancy forcing (Park and

Baik, 2013; Ma and Cheng, 2023). It was shown in Duan and Ngan (2020) that the thermal internal boundary layer for an aligned building array can be four times thicker for a $\Delta T = 12\text{ K}$ ground heating compared to that for a $\Delta T = -2\text{ K}$ ground cooling, where ΔT denotes the temperature increase at the ground level. Ventilation improves for the former and deteriorates for the latter, leading to varying ventilation timescales (the mean tracer age was found to increase by up to 25% for $\Delta T = -4\text{ K}$ and to decrease by up to 80% for $\Delta T = 8\text{ K}$) and hence that the PDFs and CDFs of pollutant concentrations experienced by the virtual walkers would differ significantly compared to that under neutral stratification. However, the exact sensitivity of pollutant exposure for moving agents to the the boundary-layer stability remains unclear.

During accidental releases of hazardous pollutants, both the toxicity and the duration of exposure are important concerns (Greene and Morris, 2006; Scungio et al., 2018). The latter is being investigated in ongoing work using tracer age statistics; however, the former has remained not fully addressed because as in many studies in the literature a tracer gas is oftentimes assumed to be passive and inert for simplicity (e.g. Gao et al., 2022). The toxicity aspect could be worth exploring in future work. Although a continuously-released source (opposed to the impulse source specified in the current study) may preclude the quantification of pollutant decay (this is why it is not used herein), it allows the calculation of exposure for a statistically-steady pollutant field, which is also of great concern in the literature (e.g. Marucci and Carpentieri, 2020; Wang and Ngan, 2021).

A few other simplifications are also enforced to simplify the problem, such as the fixed agent departure location, departure time and the constant walking speed. Although a direct extrapolation of the results to real urban environmental scenarios is not straightforward, they should serve as a useful baseline reference for exposure risk assessment and evacuation route planning for urban regions with well-aligned avenues. Despite the idealised agent walking routes, no assumptions are imposed on the implementation of the methodology presented in the current work, therefore it can be applied to more interesting cases, e.g. for more real origin-destination-based walking trajectories (Tilahun and

Levinson, 2010; Kim and Chung, 2018), which requires further efforts.

5. Conclusions

Pollutant dispersion and exposure have been conventionally quantified based on statistics for fixed receptors, namely fixed grid points discretely distributed in a computational domain. Subsequent spatial or temporal averages may not accurately quantify the exposure of walkers (or moving receptors). The current study investigates pollutant exposure of virtually walking agents (which essentially emulate the pedestrians that walk along the avenues of a real urban district) to an impulse release of gaseous pollutants. The implementation of virtual walkers in LES for pollutant exposure represents the main novelty of this study.

The dispersion of pollutants is driven by a turbulent flow developed over an idealised urban district, an aligned array of unit-aspect-ratio canyons, which implies a skimming flow regime. Impacts of the angle (β) between the agent walking direction (which is fixed to simplify the problem) and the dominant wind direction is examined. Timescales associated with the decay of the scalar mean and variance both exhibit a monotonic dependence on β (Sec. 3.1), indicating temporally variable exposure risks. It is shown that timely evacuation is still possible even if agents are in an avenue adjacent to the release point; however, the results suggest that higher walking speeds must be considered as a walker moves towards avenues further downwind of the domain to ensure an adequate time for evacuation.

For the initial-value problem considered herein, we demonstrate that the actual exposure can differ from simple Eulerian estimates: the maximum concentration exposed by a walker interpreted from data recorded by the fixed receptors along the same walking track is found to be overestimated by a few orders of magnitude. The exposure risks for moving receptors along different avenues, A_i , are quantified using the PDFs and CDFs of the recorded concentrations for different β (Sec. 3.2), and evacuation route planning for minimised exposure risks to the polluted air analysed.

Intuitively, one would expect the exposure risk to be lower along an evacuation route that deviates more from the dominant wind direction and be

farther from the release point. The former is based on the fact that lateral spread of pollutants is much slower than dispersion downwind; for the latter, far-field pollutant concentrations generally have decayed to a substantially low level. In most of the scenarios that differ in β and A_i , the results suggest evacuation routes towards a direction that deviates as much as possible from the dominant wind direction (Sec. 3.3) and, under certain circumstances, walkers are recommended to be contemporarily evacuated towards avenues further downstream; however, this does not always ensure reduced exposure (further demonstrated in Appendix B). The results imply that decision of the priority of moving to further avenues downstream first or deviating immediately from the dominant wind direction for given A_i and β can be important during emergency response.

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Appendix A. Model validation

The current LES model has been extensively validated for urban-scale turbulent boundary-layer flows (Gronemeier et al., 2020) and pollutant dispersion (Resler et al., 2020). We have previously validated this model for a single street canyon (Duan et al., 2019) and an idealised building array (Duan and Ngan, 2020). Following Belcher et al. (2015), the model herein is validated against the experimental data obtained from the EnFlo wind tunnel at the University of Surrey and the DNS data of Branford et al. (2011). We consider a grid of aligned cubic building blocks and a 45° wind with respect to the frontal building facades, identical in setup to that in the DNS (see Fig. A.13).

In both the DNS and the wind-tunnel experiments, a continuous pollutant source was applied, whereby a statistically-steady state scalar field was obtained. By contrast, the current work is focused on an instantaneous source (Eq. 1). To better align with the initial-value problem investigated in the current study, we attempt to expand the validation in a harder way that differs from the conventional ones (e.g. Cheng et al., 2008; Duan et al., 2019), namely a steady scalar field is reconstructed via integration of the results for an instantaneous release. A formal description of the integration can be found in Lo and Ngan (2015) and is therefore not elaborated here.

Fig. A.14 compares the normalised centreline concentrations. While the decay downwind of the source is well captured, the overprediction of the concentration in the first sampling cell is notable. The discrepancy may be attributed to the differences between the source setups: the source was discretised as a Gaussian bell over a few grid points and was prescribed at $z = 0.0625H$ in the DNS, while the LES applied a purely areal source. Far from the source ($x/H > 6$), the LES shows excellent agreement with the measurements and the DNS.

Fig. A.15 plots the lateral concentration profiles at different distances ($2\sqrt{2}H$, $3\sqrt{2}H$, $6\sqrt{2}H$ and $8\sqrt{2}H$) from the source cell measured along the diagonal. There are a few large discrepancies near the plume centre, e.g. in panels a and b. Similar discrepancies are also seen in the DNS of Branford et al. (2011). Despite that, the lateral distributions are reasonably well estimated for various downwind distances and the current LES actually shows improved agreement with the experiments compared to the DNS at some locations (e.g. $x/H = 4$ and 10 in panel b). It is noteworthy that excellent agreement with the wind-tunnel measurements and the DNS data is obtained for the profile tails, suggesting that the plume width is well predicted.

Appendix B. Exposure risks along a diagonal route

In real urban districts, pedestrians may either walk along an avenue or cross a street. While it is difficult to specify a walking trajectory that satisfies personal preferences, we estimate the integrated probabilities of exposure to highly and extremely polluted air (i.e. $P_{C_{\text{high}}}$ (Eq. 7) and $P_{C_{\text{extreme}}}$ (Eq. 8), see Sec. 3.3) along the diagonal of the domain. This specification represents a scenario that includes both pedestrian walking and crossing behaviours in a

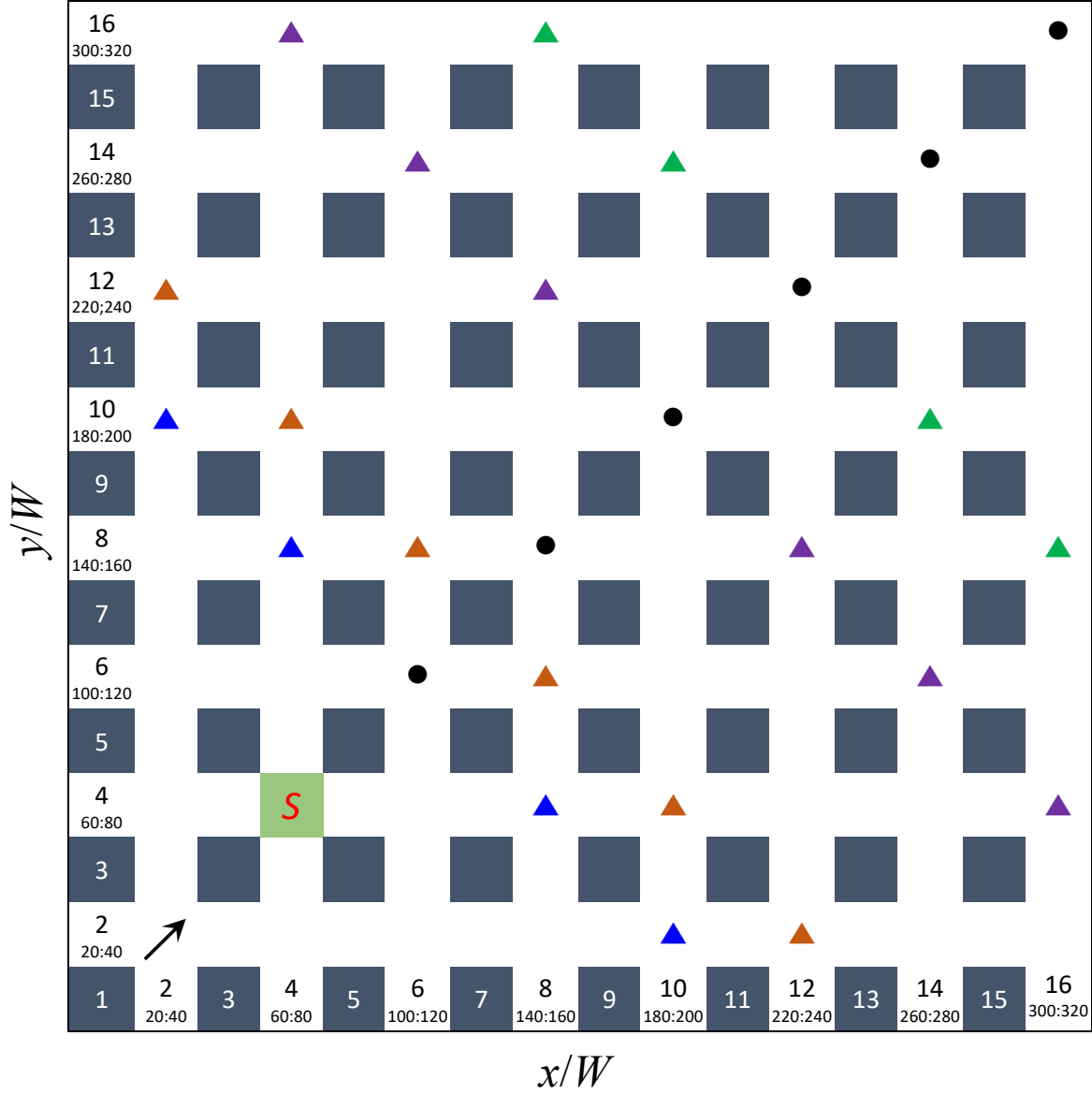


Figure A.13: Schematic diagram of an aligned building array considered in the DNS of [Branford et al. \(2011\)](#) and used for the validation of the current LES model. The arrow denotes the 45° wind. The numbers annotate the rows (y/W) and columns (x/W), as well as the associated grid points. Filled triangles and circles indicate sampling positions for the lateral (crosswind) and centreline (diagonal) profiles, respectively. A delta-function ground-level source (Eq. 1) covers the grid points of 60 – 80 (highlighted in green).

real pedestrian network.

While one would intuitively expect the exposure risk to be lower along an evacuation route that deviates more from the dominant wind direction and be farther from the release point (the diagonal route accounts for the impact of both), a monotonic dependence is not guaranteed. Fig. B.16 shows that

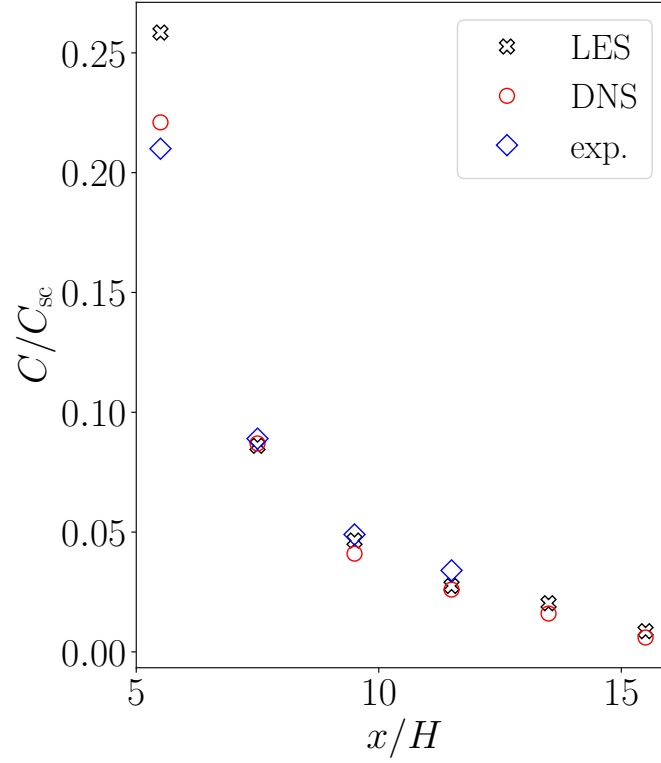


Figure A.14: Comparison of the centreline concentrations normalised by the concentration in the source cell, C_{sc} . Crosses: the current LES model; Circles: DNS of [Branford et al. \(2011\)](#); Squares: wind-tunnel data from the EnFlo wind tunnel at the University of Surrey ([Belcher et al., 2015](#)).

$P_{C_{high}}$ and $P_{C_{extreme}}$ do not change monotonically with β .

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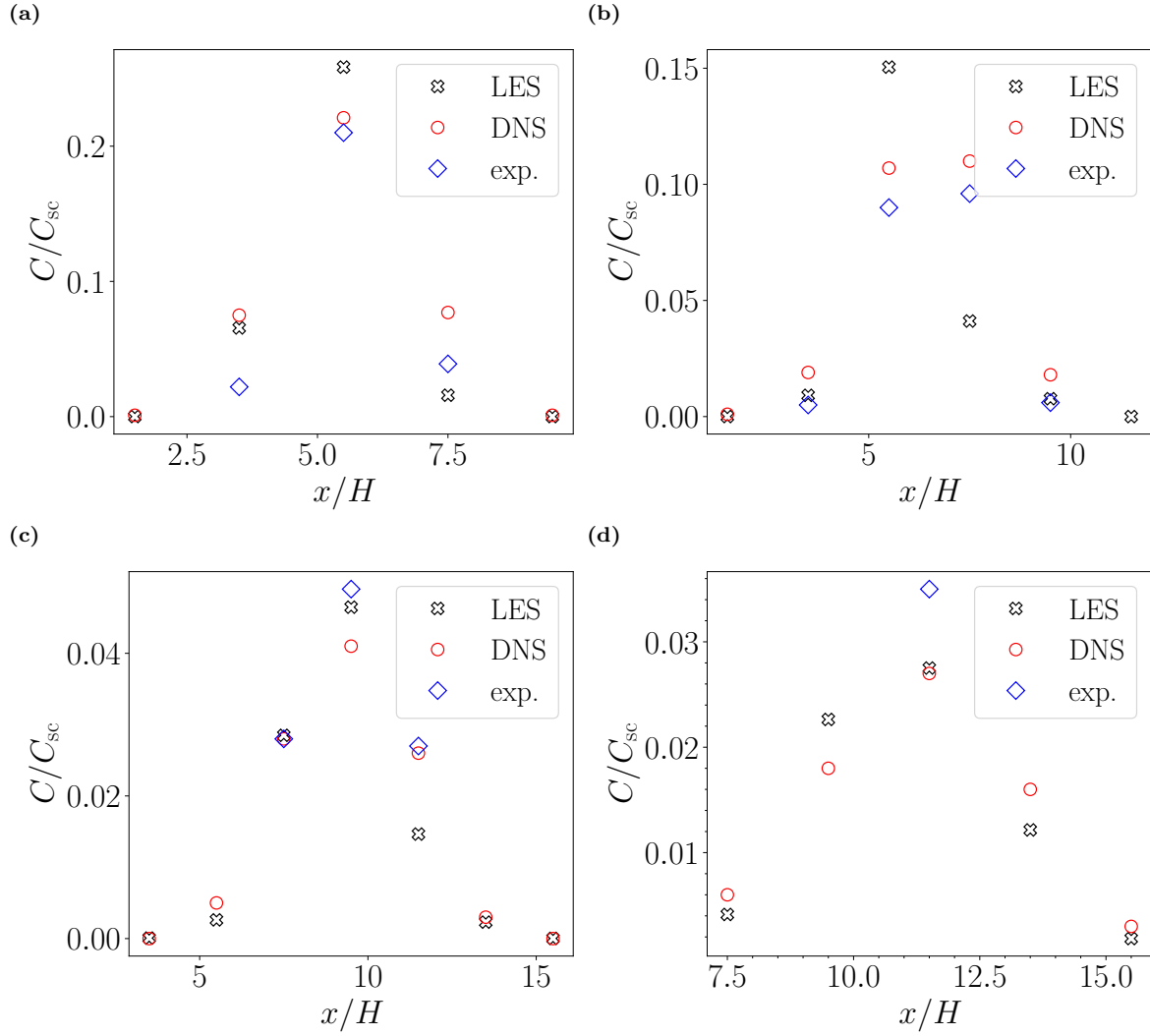


Figure A.15: Lateral profiles of the normalised concentrations at different perpendicular distances from the source: (a) $2\sqrt{2}h$; (b) $3\sqrt{2}h$; (c) $6\sqrt{2}h$; (d) $8\sqrt{2}h$. Crosses: the current LES model; Circles: DNS of Branford et al. (2011); Squares: wind-tunnel data from the EnFlo wind tunnel at the University of Surrey (Belcher et al., 2015).

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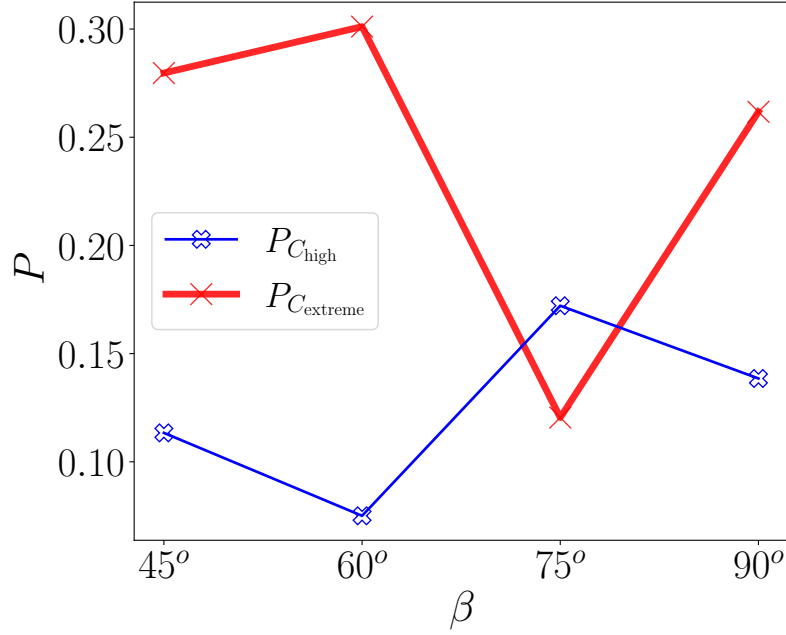


Figure B.16: $P_{C_{\text{high}}}$ and $P_{C_{\text{extreme}}}$ for a diagonal walking route for different β .

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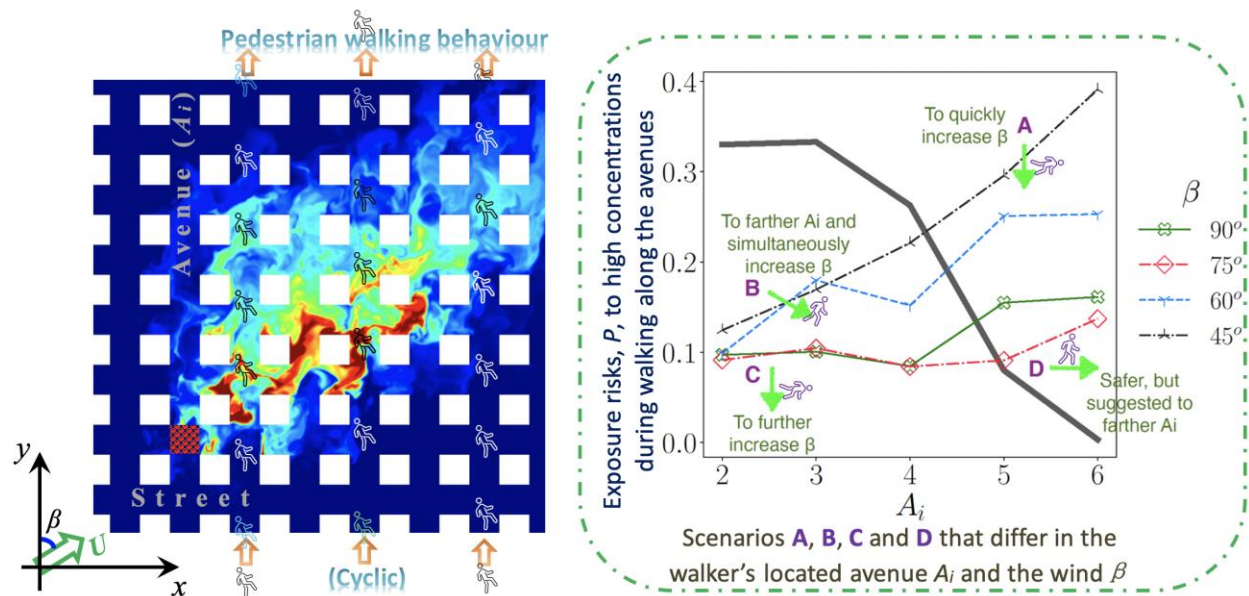
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- Exposure to an impulse release are quantified for virtual walkers using LES.
- Spatial variability of the exposure risk is well captured by moving receptors.
- Actual exposure of pedestrians can differ from simple Eulerian estimates.
- Evacuation routes are discussed for different walker locations and winds.

Evaluation of pollutant exposure using virtual walkers and large-eddy simulation: application to an idealised urban neighbourhood

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Abstract

Urban air quality studies have primarily focused on pollutant dispersion; however, spatial or temporal concentrations collected at discretely distributed grid points (or fixed receptors) do not reflect the actual pollutant exposure of pedestrians. Using large-eddy simulation (LES) with virtual walkers implemented, this study investigates pollutant exposure of walking agents (or moving receptors) in an urban turbulent boundary-layer flow developed over an aligned building array under the influence of different wind directions. The spatial variability of the exposure risks are found to be better captured by the moving receptors than the fixed receptors along the same agent walking tracks. We demonstrate that the actual exposure can differ significantly from results interpreted from data recorded by the fixed receptors (corresponding to Eulerian estimates) and show that large discrepancies occur in avenues near the source, wherein dispersion of the point release has not occurred on larger spatiotemporal scales. In most scenarios, optimal evacuation routes are shown to be ones that deviate as much as possible from the dominant wind direction; however, one needs to decide the priority of moving to further avenues first or immediately adjusting the walking direction. The results should serve as a useful baseline reference for environmental health impact assessment and evacuation route planning against hazardous releases of air pollutants in more complex urban environments.

Keywords: Pollutant exposure, virtual walker, moving receptor, urban street canyon

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1. Introduction

Rapid urbanization has significantly accelerated anthropogenic and industrial activities in and around urban areas. Emissions of gaseous pollutants are imposing increasingly growing risks to urban air quality (Wong et al., 2019; Zheng and Yang, 2022; Wang et al., 2022). In the case of accidental releases of hazardous pollutants, accurate prediction of the exposure risk to the polluted air is vital for effective emergency response and evacuation route planning.

In the pollutant dispersion literature, researcher are more concerned about the time-mean concentration. Numerical modelling (e.g. Lo and Ngan, 2020; Masoumi-Verki et al., 2021), measurements (e.g. Jiang and Yoshie, 2018; Mo and Liu, 2018; Xing and Brimblecombe, 2018; Marucci and Carpentieri, 2020) and analytical (e.g. Belcher et al., 2015; Tzella and Vanneste, 2016) studies have highlighted scalar statistics, such as concentration fields in urban districts (Blocken et al., 2016), flux exchanges across the canopy (Chung and Liu, 2013; Panagiotou et al., 2013) and mixing with the clean air (Duan et al., 2019). Assessments of exposure have typically been made for fixed receptors, namely based on data recorded at the grid points discretely distributed over the computational domain (Scungio et al., 2018; Wang et al., 2019; Cui et al., 2021; Zhang et al., 2023). Subsequent results are interpreted from Eulerian calculations of the pollutant fields—associated diagnostics essentially rely on spatiotemporal averages (e.g. Tiwary et al., 2011; Ng and Chau, 2014; He et al., 2017). Although this approach simplifies the calculation, it neglects outliers and assumes homogeneity, which can be of critical impact during emergency response.

The risk of exposure may vary greatly as a receptor moves from one position to another. Using LES and a Lagrangian stochastic model (LSM) (Weil et al., 2004), Lo and Ngan (2017) quantified the exposure in terms of the total time spent by a pollutant particle in the region of concern. Although the residence time (a measure of exposure) was calculated by integration along particle trajectories, the ‘clock’ was spatially fixed in the region of concern, which is equivalent to setting a fixed receptor. Therefore, the method cannot extend to simulating the pedestrian walking behaviour, and hence the spatial variability of exposure along the walking route cannot be captured. Recent attention on exposure in the urban air quality literature has been directed towards vehicle-induced emissions (Zhao et al., 2021; Zheng and Yang, 2022); however, they represent moving

sources rather than moving receptors. Accurate prediction of the exposure risk of walking agents in urban districts has remained a concern challenging urban environmental health and sustainability (Vardoulakis et al., 2016).

The exposure of moving agents to air pollution depends on the meteorological forcing such as wind, which directly affects the pattern of the scalar field, specifically the center-of-mass translation downstream and the crosswind spread by turbulent diffusion (Davidson et al., 1995). The combined effects essentially define the size of a polluted area and, by extension, the spatially varying exposure risks. Obviously, influence of urban topography can be important as well. For example, for an aligned grid of building obstacles, the windward building facades are by definition perpendicular to the dominant wind; however, the arrangement of the array can be viewed as staggered when the wind direction is rotated. For the former, advection by the mean flow along the street (i.e. channelling) is non-negligible; for the latter, the channel flow is diminished—a pollutant scalar undergoes a more winding path as in a staggered array and the obstruction of building facades can be important (Blunn et al., 2022). Therefore, wind direction can be of qualitatively impact on pollutant exposure.

Multiple timescales are involved in the quantification of exposure. This can be of particular importance during emergency response against environmental incidents of toxic chemicals. It is well known that the mean concentration within a unit-aspect-ratio street canyon decays exponentially fast for an instantaneous pollutant source (DePaul and Sheih, 1985); however, safety is not necessarily ensured even if an agent’s walking speed is on a timescale shorter than that for the decay. One needs to compete with the timescale associated with ventilation (that is how quickly pollutants are removed from the control domain) and mixing (namely how rapidly a pollutant scalar mixes with the clean air). As pollutants disperse downwind, it is unknown if a walking agent can have sufficient time to be evacuated before the ambient air gets highly contaminated.

To understand pollutant exposure of moving receptors, the paper is organized as below. Sec. 2.1 describes the geometry of an idealised urban district represented by a grid of aligned building cuboids. Sec. 2.2 provides further details of the model setups with the focus on the moving agents and the forcing. The LES model is described in Sec. 2.3 with the model validation given in Appendix A. Sec. 3.1 presents the decay of the mean concentrations and the scalar variances, wherein the associated decay timescales

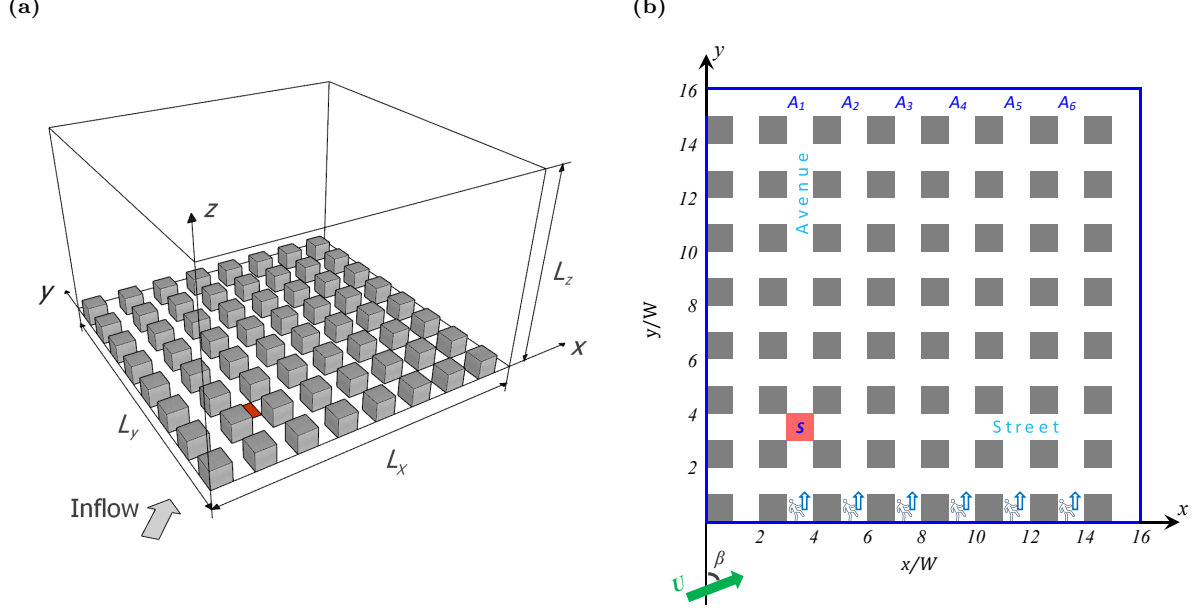


Figure 1: Schematic diagram of virtual agents walking along the avenues of an aligned building array. (a) 3D view of the computational domain; (b) plan view with the walking agents indicated. The blob highlighted in red in avenue A_1 denotes an instantaneous ground-level pollutant release (see Eq. 1). The virtual walkers move along the avenues in the spanwise direction, y , and β denotes the angle between the agent walking direction with respect to the dominant wind direction. $L_x = L_y = 16H$ and $L_z = 6.5H$ denote the domain dimensions, where H is the height of the building cuboid.

are quantified. The PDFs and CDFs of pollutant exposure are analysed in Sec. 3.2, wherein exposure risks are compared for moving and fixed receptors, and evacuation routes planning for four scenarios discussed in Sec. 3.3. Discussion and summary are given in Sec. 4 and Sec. 5, respectively.

2. Methodology

2.1. Urban geometry

As in many previous studies of urban pollutant dispersion (e.g. Davidson et al., 1995; Marucci and Carpentieri, 2020), we consider an idealised urban district represented by an array of regularly aligned building cuboids (see Fig. 1 for a schematic diagram). The building array consists of 8 building rows $\times$ 8 building columns. As in Duan and Ngan (2019), unblocked rows and columns are referred to as “streets” and “avenues”, respectively.

The domain dimensions are $L_x = 320 \times \Delta x = 320 \text{ m} (= 16H)$ in the east-west (or x) direction, $L_y = 320 \times \Delta y = 320 \text{ m} (= 16H)$ in the north-south (i.e spanwise or y

direction) and $L_z = 130 \times \Delta z = 130 \text{ m}$ ($= 6.5H$) in the vertical (z), comparable with Wang and Ngan (2021) and Ma and Cheng (2023). The spatial resolution is isotropic, i.e. $\Delta x = \Delta y = \Delta z = 1 \text{ m}$ ($= H/20$), which meets the suggested best practices for urban computational fluid dynamics that the canyon walls be separated by at least 10 grid points (Franke et al., 2011). The building widths (W), avenue widths and street widths are equal to the building height $H = 20 \text{ m}$, which implies a homogeneous urban topography, i.e. the canyon aspect ratios in x and y directions are unity ($AR_x = AR_y = H/W = 1$), and reduced ventilation in the turbulent flow of the skimming flow regime (Hunter et al., 1992).

2.2. Forcing and moving agents

An impulse area source is prescribed at the ground level of a street-avenue intersection from the leading corner of the array. After the flow has reached statistical stationarity, pollutant is released at time t_0 , implying a source flux,

$$S = S_0 \delta(x - \vec{x}_0, t - t_0), \quad (1)$$

where S_0 denotes a source emission strength, which is specified arbitrarily as a constant, and $\vec{x}_0$ denotes a source location. As opposed to a continuously released source (e.g. Marucci and Carpentieri, 2020; Wang and Ngan, 2021), the construction of the initial-value problem herein allows the quantification of pollutant decay rates and associated decay timescales (DePaul and Sheih, 1985).

The flow is forced by a prescribed pressure gradient, ΔP . Following Wang and Ngan (2021) and Blunn et al. (2022), an approaching wind of $\theta \in [0^\circ, 45^\circ]$ with regard to the x -axis is considered, which is equivalent to a $\beta \in [45^\circ, 90^\circ]$ wind with respect to the agent walking direction (along the y -axis). Because the current work is focused on the exposure of moving agents, the latter notation, β , is used (see Fig. 1). For $\beta = 90^\circ$, $\Delta P = 0.6 \times 10^{-3} \text{ Pa m}^{-1}$, which generates the familiar canyon circulations within the building rows and channel flows along the streets. For a 45° wind, the building obstacles form a staggered array (Coceal et al., 2014). For completeness, the flow patterns are presented in Fig. 2. It can be seen the counter-rotating wake vortices are altered as the dominant wind is rotated and the symmetry of the vortex pair is retained for the $\beta = 45^\circ$ diagonal wind. The streamline geometries agree well with previous studies of turbulent

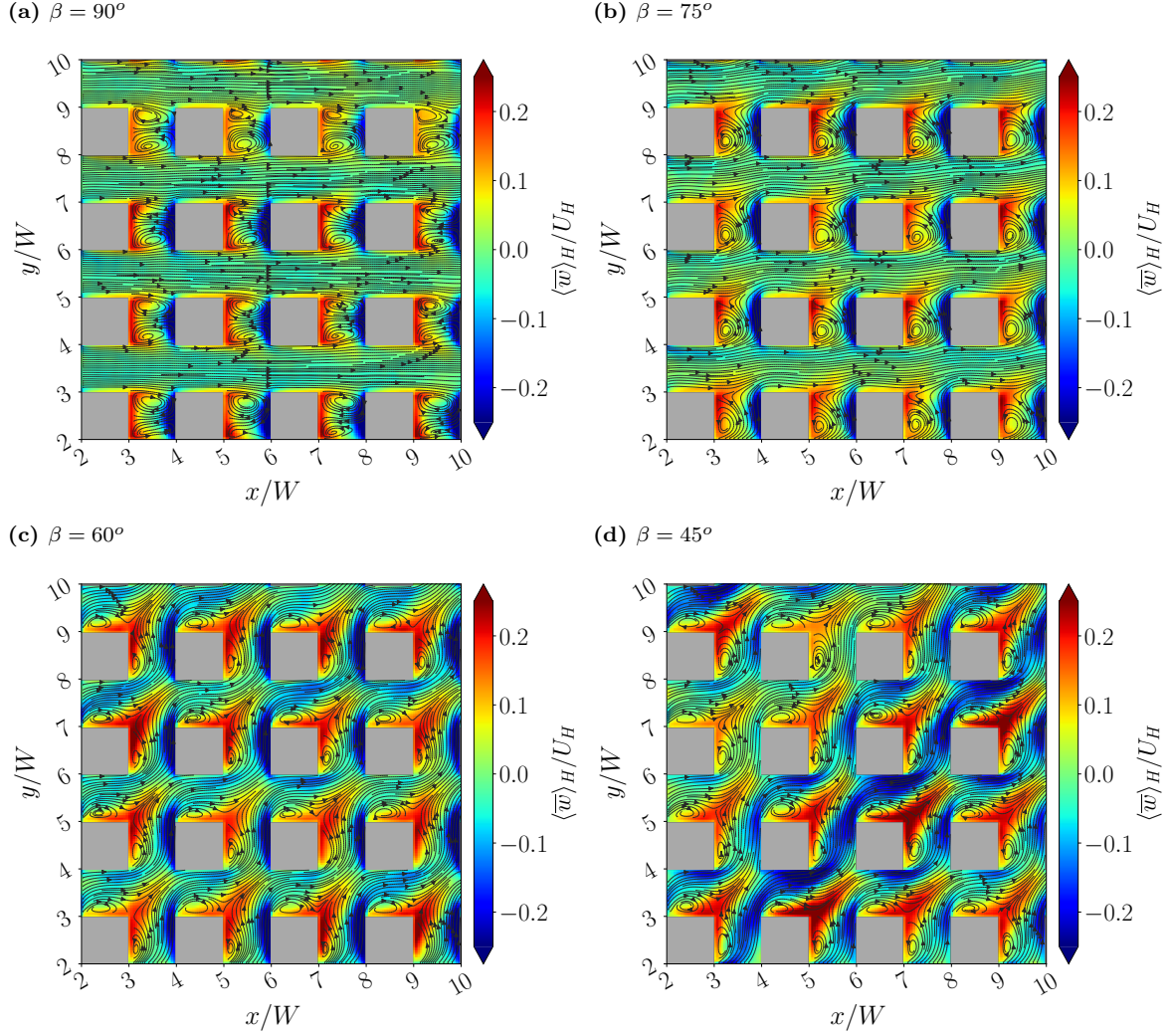


Figure 2: Streamline geometries for different β . The flows are shaded by the nondimensionalized mean vertical velocity component, wherein $\langle \bar{\cdot} \rangle_H$ denotes temporal and vertical averaging for $z/H = [0, 1]$. U_H corresponds to the absolute velocity slightly above the roof level.

flow around building cuboids of an aligned array (e.g. Claus et al., 2012; Coceal et al., 2014; Wang and Ngan, 2021).

The Reynolds number based on the building height (H) and the freestream wind speed (U_{ref}) is $Re \equiv U_{\text{ref}} H / \nu \sim \mathcal{O}(10^6)$, which is comparable with the LES study of Wang and Anderson (2019) and Blunn et al. (2022), but is a few orders of magnitude greater than Inagaki and Kanda (2008) and Cheng and Castro (2002) because they considered scaled urban topographies, and is smaller than Liu et al. (2022) by two orders of magnitude because the maximum building height (180 m) of a real urban district was used as the characteristic length scale. The Re implies that the turbulent flow is in the fully rough regime (Castro and Robins, 1977).

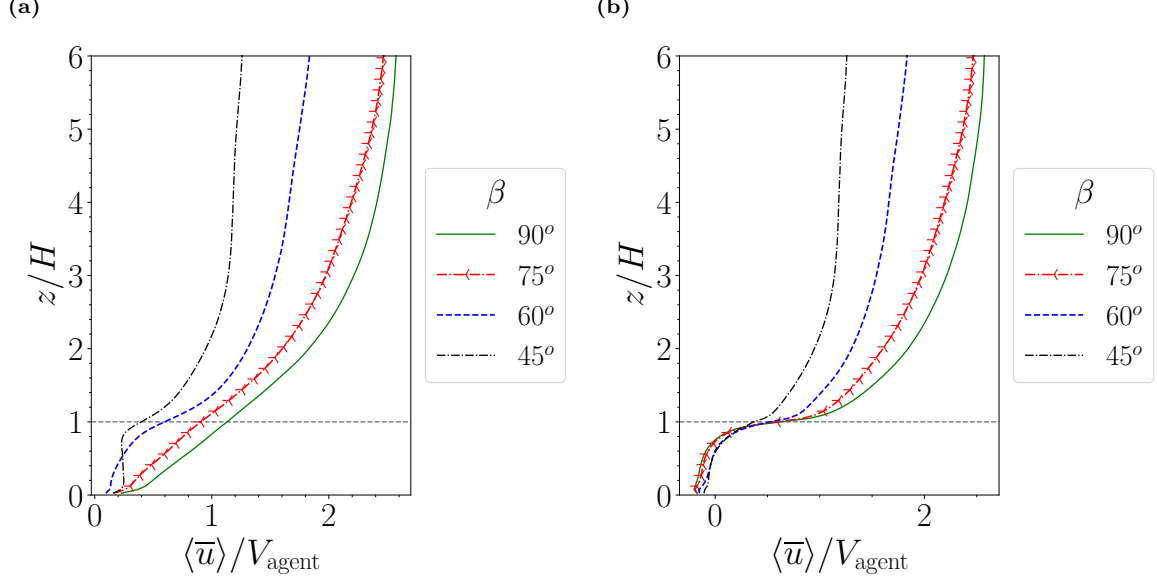


Figure 3: Vertical profiles of the streamwise velocity component, u , normalised by the agent walking speed, V_{agent} . (a) Ensemble average along the middle of the repeating streets, $y/W = 2N + 1.5$; (b) ensemble average along the middle of the repeating building rows, $y/W = 2N + 0.5$, where $N = 0, 1, \dots, 6$. Dashed horizontal line indicates $z/H = 1$. $\langle \bar{u} \rangle$ denotes temporal and horizontal averaging.

Virtual agents (i.e. moving receptors) initially set near the south boundary of the building array (see Fig. 1) start walking along the avenues at the instant of the tracer release (at t_0 , see Eq. 1). Once the north boundary is reached, the walkers reenter the domain from the south boundary and walk north once more. This prescription is maintained from the source release till the end of the simulation, whereby pollutant concentrations (C) experienced during the periodic walking along the avenues are recorded. It is noteworthy that the moving agents essentially emulate the pedestrian walking behaviour in real urban environments.

Implementation of the virtual walkers in LES essentially follows the virtual flight measurements of Schröter et al. (2000) and Sühling and Raasch (2013). The agent walking speed, $V_{\text{agent}} = 1.34 \text{ m s}^{-1}$, specified herein lies in the range of average walking speeds of $1.0 \text{ m s}^{-1} - 1.5 \text{ m s}^{-1}$ for adults (Mansfield et al., 2018; Mohamed and Appling, 2020). For a moderate wind considered in the current study, $V_{\text{agent}} / \langle \bar{u} \rangle > 1$ in the pedestrian region, where $\langle \bar{u} \rangle$ is the mean streamwise velocity component (see Fig. 3).

Data recorded by the moving receptors will be compared with that for fixed receptors (y_n), namely the grid points discretely distributed along the agent walking tracks in the y -direction. Therefore, the subscript n indicates the spanwise grid index.

2.3. Large-eddy simulation

The boundary-layer flow and scalar dispersion are simulated using PALM 6.0 (Maronga et al., 2020), which is a LES model developed specifically for atmospheric and oceanic boundary layer studies. The model is based on the implicitly filtered non-hydrostatic and incompressible Boussinesq equations. Subgrid-scale (SGS) fluxes are parameterised using a dynamic SGS model according to Germano et al. (1991) and Heinz (2008), which allows the occurrence of backscatter (namely negative values of SGS eddy viscosity) while ensuring stability. The SGS eddy viscosity and diffusivity are obtained from additional prognostic equations for the SGS turbulent kinetic energy based on the assumption that energy transport by SGS eddies is proportional to the local gradients of the mean quantities. Detailed descriptions of the governing equations of the LES model can be found in Lau and Ngan (2018) and Maronga et al. (2020). Therefore, they are not repeated here.

As in Liu et al. (2005), periodic boundary conditions are applied in the lateral directions, whereby an infinitely spread urban region is assumed. To prevent nonphysical accumulation of pollutants within the domain, concentrations at the lateral edges are set to zero after Wang et al. (2021). At solid surfaces, there is no-slip for the velocity components and Neumann (zero-gradient) for scalars. A Neumann boundary condition is also applied at the domain top. Unresolved Reynolds shear stresses near walls are parameterised by assuming a constant-flux layer between the roughness height, z_0 , and the first grid layer following the Monin-Obukhov similarity theory (MOST) (Monin and Obukhov, 1954). As in previous studies (Park et al., 2015; Yoshida et al., 2018; Duan and Ngan, 2020), the roughness lengths for momentum and passive scalar are identical, with $z_0 = 0.1$ m, which is representative of very rough walls (Letzel et al., 2012).

A third-order Runge-Kutta time-stepping scheme (Williamson, 1980) combined with an upwind-biased fifth-order finite differencing scheme is applied in solving the advection terms for momentum and scalar. This combination has proven effective for ensuring accuracy and algorithmic simplicity (Wicker and Skamarock, 2002). The Courant-Friedrichs-Lewy (CFL) criterion was set to 0.9 with variable integration timesteps (~ 0.2 s) to guarantee numerical stability. The Poisson equation for pressure is solved with the multigrid method, which is highly optimised for Intel processors used for running the current model.

The 3-D model was initialised with a stationary-state wind profile obtained from a 10-hour run of a 1-D model with a Reynolds-average based turbulence parametrisation

(Maronga et al., 2020). A 6-hour spin up, $\sim 200t^*$ (where $t^* \equiv H/u_*$ denotes the eddy turnover timescale and $u_* \sim 0.2 \text{ m s}^{-1}$ is the friction velocity), ensures that the turbulent boundary layer has become fully developed and the flow has reached statistical stationarity. Data are subsequently collected at time intervals of $\Delta t = 10 \text{ s}$ ($\sim 0.1t^*$, about four times higher than the temporal resolution of Blunn et al. (2022)) for a duration of 3600 s ($\sim 36t^*$), which are sufficient for the initial-value problem considered herein (Bernardini et al., 2014).

Validation of the LES model is presented in Appendix A.

3. Results and analyses

3.1. Scalar decay and mixing

3.1.1. Decay of volume-averaged concentrations

The removal of pollutants from the control domain (the region for $z/H \leq 1$, hereafter $\mathcal{D}$), i.e. ventilation, directly affects the scalar concentration inside the canyons and hence the exposure of walking agents to the polluted air at different locations. For a release of pollutants at an initial instant (Eq. 1), ventilation can be quantified by the decay rate of $\langle C \rangle(t)/C_0$, the normalised concentration spatially averaged over $\mathcal{D}$. Herein, C_0 denotes the bulk average of the concentration at initial time t_0 .

Physically, the change of β should not alter the exponentially decaying nature of $\langle C \rangle(t)/C_0$ (Davidson et al., 1996). The familiar exponential decay function (DePaul and Sheih, 1985), viz.

$$\langle C \rangle(t)/C_0 \sim \exp\left(-\frac{t}{\tau_r}\right), \quad (2)$$

where τ_r is known as the retention time (the time required for $\langle C \rangle(t)/C_0$ to reach e^{-1}), should always hold for a unit-aspect-ratio 2D street canyon (Duan et al., 2019) and a cubic 3D building array (Duan and Ngan, 2020). Fig. 4 plots the history of $\langle C \rangle(t)/C_0$. It can be seen that the exponentially decaying behaviour persists when β varies: the minimum R^2 is 0.98. The slight change of the slope reflects the sensitivity to the wind direction.

Longer retention of pollutants within the domain implies high risk of exposure. Fig. 5 shows that the removal of pollutants from $\mathcal{D}$ accelerates as the wind rotates towards the canyon axis (i.e. increased β). This is presumably because ventilation routes below

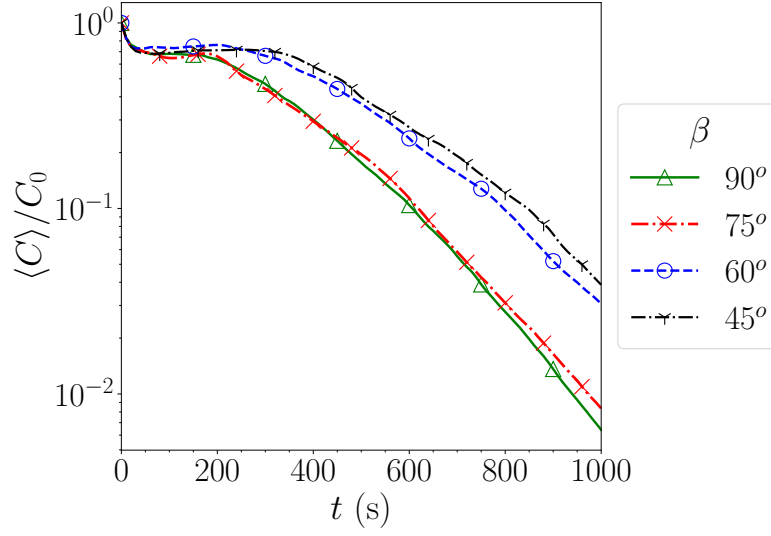


Figure 4: Decay of the normalised concentrations, $\langle C \rangle(t)/C_0$, for different β . As in Duan and Ngan (2020), the initial-stage spin up is excluded in the fitting. For clarity, the time axis is clipped at 1000 s.

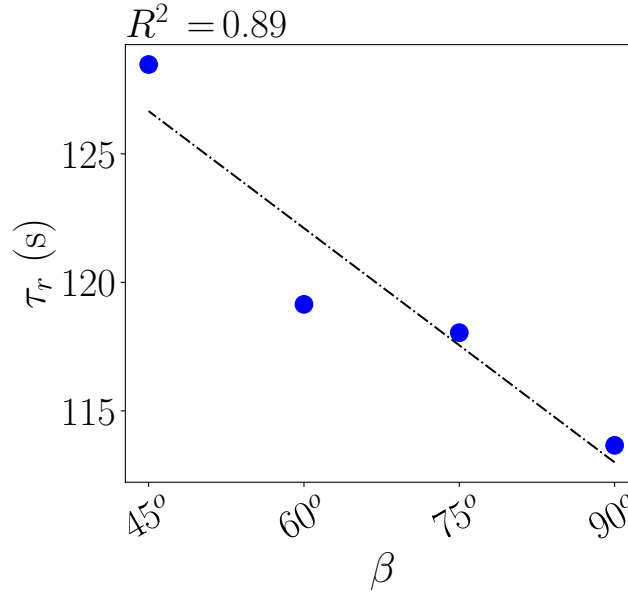


Figure 5: Retention time, τ_r (Eq. 2), associated with the decay of the mean concentrations for different β . The timescale is obtained from least squares regression of the decay of $\langle C \rangle(t)/C_0$ plotted in Fig. 4.

225 $z/H < 1$ are altered when β is changed. For $\beta = 90^\circ$, ventilation is enhanced by the
 226 channel flow along the streets (Blunn et al., 2022). By contrast, for $\beta = 45^\circ$, the wind
 227 blows diagonally and ventilation is similar to that in a staggered array (Claus et al.,
 228 2012), where the pollutant scalar undergoes a more winding trajectory (Coceal et al.,
 229 2014).

3.1.2. Variance decay

The decay of the mean concentration analysed in the above section measures how quickly pollutants are removed and the volume averaging tacitly assumes homogeneity of concentrations in the control domain. An obvious limitation is that it does not quantify inhomogeneity and little can be said about how rapidly air inside the canopy bulk gets polluted; however, this can be of particular importance for emergency response because it gives a sense of the effectiveness of evacuation to avoid exposure to the air that is highly mixed with the pollutants.

The scalar variance, $\sigma_C^2(t) \equiv (C - \langle C \rangle)^2$, has proven an effective probe to the inhomogeneity and was successfully applied to the quantification of scalar mixing (Duan et al., 2019). The variance-decay rate characterises the rapidity of mixing (Pierrehumbert, 1994), which provides a useful timescale for emergency response reference.

It can be seen in Fig. 6 that the decay stages of the nondimensionalized scalar variance, $\langle \sigma_C^2 \rangle(t)/C_0^2$, differ slightly between early and late times, similarly to the decay of the mean concentrations (Fig. 4 in Sec. 3.1.1). However, unlike that for a 2D canyon (Duan et al., 2019), the initial-stage decay is established almost immediately after the source release and the transition to the late stage occurs much smoother. This is likely due to the fact that for a 2D canyon the variance decay (at long times) is dominantly driven by ventilation across the roof-level open boundary, whilst for a 3D array, pollutants also escape through the sides (Kastner-Klein and Plate, 1999; Jiang and Yoshie, 2018).

Given that the late-time change of scalar variances is primarily driven by the removal of pollutants from the control domain (Duan and Ngan, 2020), the timescale associated with the variance decay, τ_σ , can be defined in a similar manner as that for the decay of the mean (Eq. 2), viz.

$$\langle \sigma_C^2 \rangle(t)/C_0^2 \sim \exp\left(-\frac{t}{\tau_\sigma}\right). \quad (3)$$

Fig. 7 plots τ_σ for different β . Although the amplitudes do not differ much, τ_σ exhibits a clear linear scaling with β ($R^2 = 0.89$, as τ_r does, cf. Fig. 5), implying that a well planned β , namely evacuation direction with respect to the dominant wind, could reduce the risk of exposure to the air before it is highly mixed with the pollutants.

It is noteworthy that even a small difference in the variance decay timescale can be non-negligible during emergency response when this time difference is translated into a spatial difference. For example, a 10 s difference in time can lead to around 15 m difference

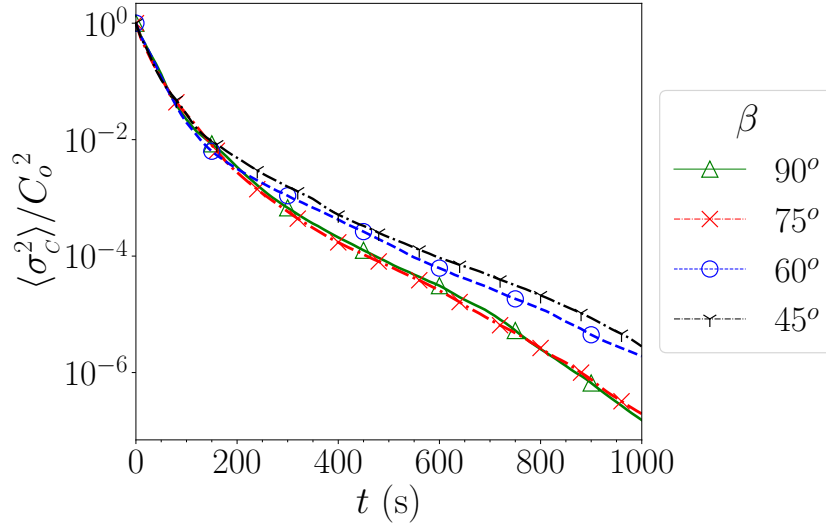


Figure 6: Decay of the normalised scalar variances, $\langle \sigma_c^2 \rangle(t)/C_0^2$. For clarity, the time axis is clipped at 1000 s.

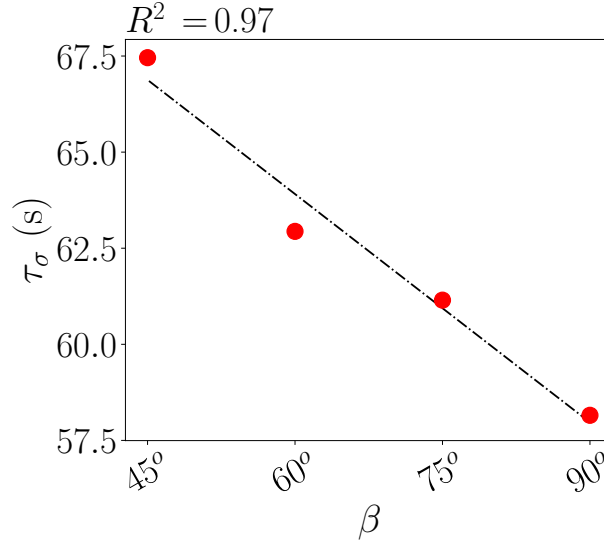


Figure 7: Scalar variance-decay timescales, τ_σ , for different β . Similarly to Fig. 4, the initial transition is excluded in the least squares regression of the exponentially decaying function, Eq. (3).

in space (even under the current normal walking speed, $1.34 \text{ m s}^{-1} \times 10 \text{ s} \approx 13.4 \text{ m}$), which measures the distance from one avenue to another for densely-packed urban regions.

3.1.3. Avoidance of air mixed with pollutants

A practical concern is if a normal agent walking speed specified in the current study ensures a safe avoidance of the contaminated air. While an accurate calculation needs to account for time-varying meteorological forcing, the geometrical complexity of the urban

topography and the uncertainty of the pedestrian walking behaviour in realistic scenarios, a rough estimate follows.

The calculation of the timescale associated with the virtual walker, $\tau_{\text{agent}} \equiv L/V_{\text{agent}}$, is straightforward; however, the characteristic length scale, L , is not unique. Taking the domain dimension as the characteristic length scale ($L_y = 320$ m, see Sec. 2.2) and given $V_{\text{agent}} = 1.34 \text{ m s}^{-1}$, $\tau_{\text{agent}} = 238$ s; taking the avenue width as the characteristic length scale ($W = 20$ m), $\tau_{\text{agent}} = 15$ s. The former τ_{agent} is larger than the timescale associated with the scalar mixing (evaluated for the entire domain, cf. Fig. 7), implying an insufficient time at the current walking speed to escape out of the control domain to completely avoid exposure to the polluted air, whilst the latter is smaller than τ_{agent} , indicating that if a walker is near the source (on a spatial scale of one avenue width), there is still adequate time for an effective evacuation to be made.

3.2. Exposure risks

3.2.1. Exposure to $\max C/C_0$

The spatial variability of exposure, which cannot be captured by the mean and variance, is now examined. While the decay of the mean (Sec. 3.1.1) and variance (Sec. 3.1.2) cannot be applied directly to walking agents, because they correspond to an Eulerian calculation, one can quantify the maximum pollutant concentration, $\max C/C_0$, to which a virtual walker is exposed. Letting C_{walker} denote the concentrations recorded by a walker (i.e. C_{walker} are a subset of the Eulerian concentrations, C), $\max C/C_0$ reads

$$\max C/C_0(A_i, \beta) \equiv \max(C_{\text{walker}})(A_i, \beta). \quad (4)$$

Obviously, $\max C/C_0$ depends on which avenue (A_i) the agent walks along and the wind direction, β .

Figs. 8a,b summarise the $\max C/C_0$ recorded by the agents walking along different avenues (A_i , panel a) and for different β (panel b). Fig. 8a shows that $\max C/C_0$ decreases rapidly away from the source, particularly for large β in the first few avenues (note the logarithmic scale of the ordinates and the least-squares regression plotted in the inset for reference). The $\max C/C_0$ for $\beta = 45^\circ$ remains smaller than that for other β across all A_i . This is because the building blockage, which protects pedestrians from immediate exposure to peak concentrations (Wang and Ngan, 2021; Melo et al., 2023), is more prominent for the $\beta = 45^\circ$ diagonal wind (for which the building arrangement is effectively

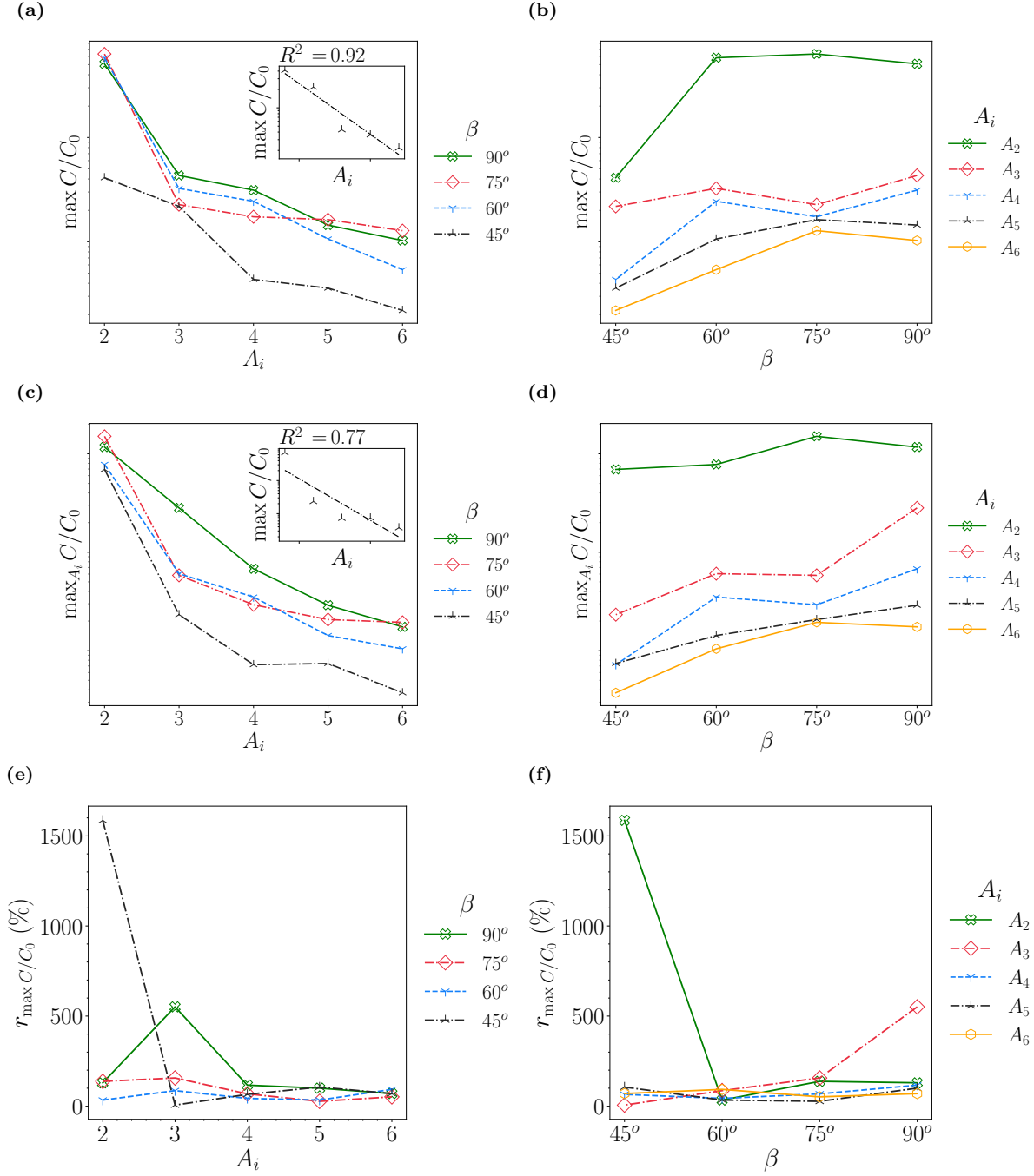


Figure 8: Sensitivity of (a,b) $\max C/C_0$ (Eq. 4) recorded by the walking agents and (c,d) $\max_{A_i} C/C_0$ (Eq. 5) recorded by the fixed receptors discretely distributed along the agent walking tracks to A_i and β ; (e,f) relative differences between $\max C/C_0$ and $\max_{A_i} C/C_0$ (Eq. 6). For reference, the dash-dotted lines in the insets of panels a and c plots the least-squares regression of $\max C/C_0$ versus A_i for $\beta = 45^\circ$. Note the logarithmic scale of the ordinates for panels a-d.

staggered, see Fig. 2). It will be seen in the latter section (Sec. 3.2.2) that this result is also supported by the PDFs. Fig. 8b shows that the $\max C/C_0$ exhibits an increasing trend with β (when the dominant wind direction deviates more from the agent walking

direction), and the amplitude of $\max C/C_0$ is particularly high for A_2 , the avenue close to the source. If an agent is walking in the avenue near the pollutant source (e.g. in A_2), the results suggest evacuation routes towards farther avenues so as to quickly reduce the exposure to $\max C/C_0$, and to decrease β so as to keep $\max C/C_0$ at a relatively lower level.

The $\max C/C_0$ recorded by the walking agents, Eq.(4), may be compared with the maximum concentration recorded by the fixed receptors (y_n) discretely distributed along the same walking track (A_i) of concern (see Sec. 2.2), $\max_{A_i} C/C_0$,

$$\max_{A_i} C/C_0(A_i, \beta) \equiv \max(C)(y_n \in A_i, \beta), \quad (5)$$

Although the patterns of $\max C/C_0$ versus A_i and β (Figs. 8a,b, respectively) and $\max_{A_i} C/C_0$ versus A_i and β (Figs. 8c,d, respectively) appear quite similar, it can be seen that the relative differences (Figs. 8e,f, respectively), viz.

$$r_{\max C/C_0} = \frac{\max_{A_i} C/C_0 - \max C/C_0}{\max C/C_0}(\%), \quad (6)$$

are markedly high. While it may seem unsurprising that the concentrations collected for fixed locations can differ from that recorded in a moving frame, the difference is surprisingly large for the initial-value problem considered herein, especially for the avenue adjacent to the pollutant source (i.e. A_2) and under the forcing of $\beta = 45^\circ$. The results indicate that the exposure of a walker to the maximum concentration interpreted from data recorded by the fixed receptors can be significantly overestimated and the actual maximum concentration experienced by the walker can be much smaller.

3.2.2. PDFs and CDFs for moving receptors

The maximum concentrations, $\max C/C_0$, analysed in the above section do not provide a complete picture of exposure. Furthermore, decreasing the exposure to $\max C/C_0$ does not necessarily ensure safety and there could be non-negligible risk (or probability) of exposure to high concentrations (though smaller compared to $\max C/C_0$). This section examines the probability density functions (PDFs) and the cumulative density functions (CDFs) associated with the exposure to pollutants.

The PDFs of concentrations recorded by the virtual walkers (Fig. 9a, c, e, g) show a much fatter tail for A_2 , indicating high probability of exposure to peak concentrations for agents walking in this avenue due to its immediate vicinity to the source. As dispersion occurs on larger spatiotemporal scales, the tail becomes progressively thinner for

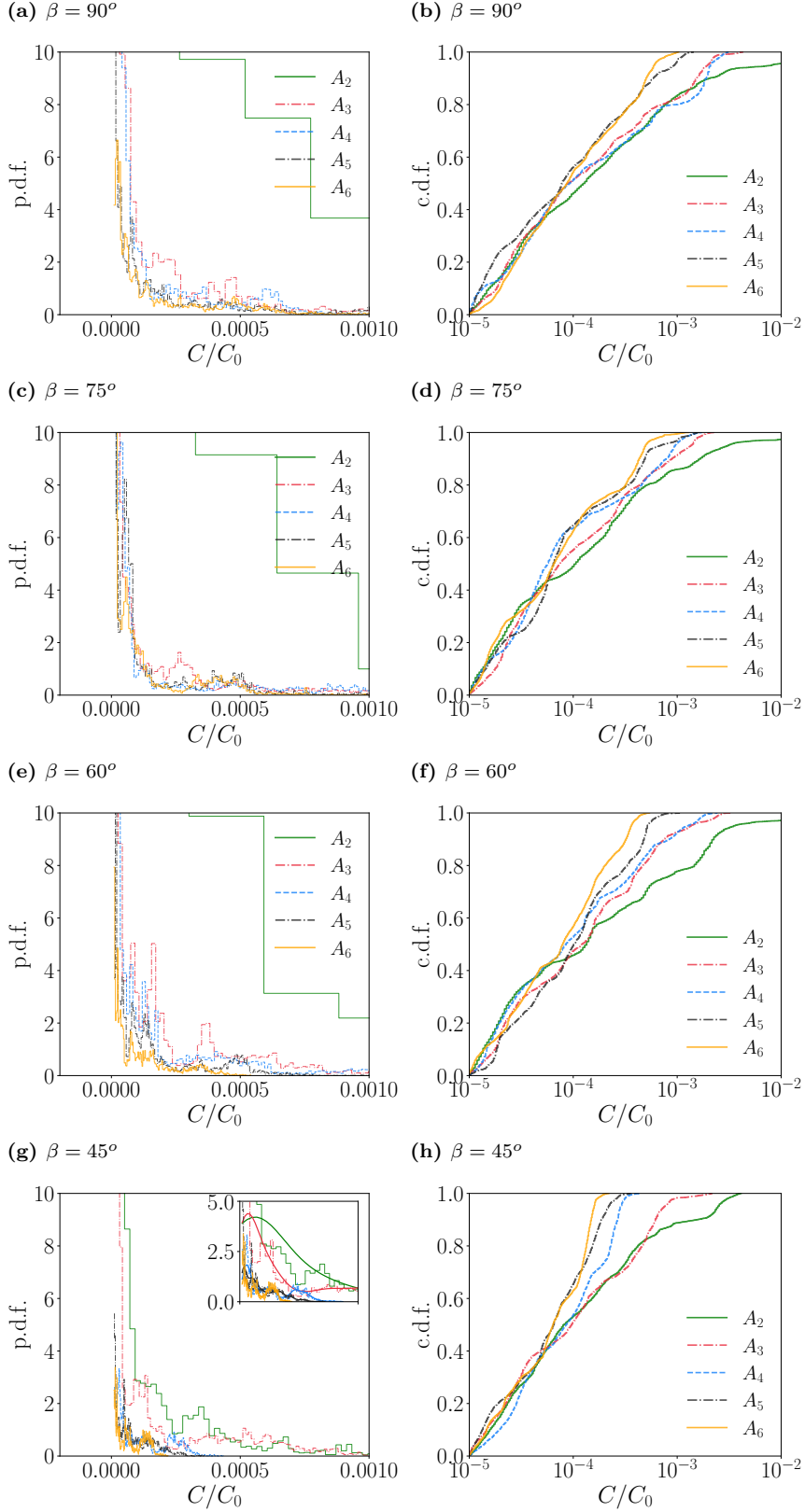


Figure 9: Probability statistics of the normalised scalar concentrations (C/C_0) recorded by the walking agents. (left panels) PDFs (shown as step functions). For clarity, statistics in each bin are normalised such that the bar heights sum to 100, x -axis is clipped at $C/C_0 = 0.001$, and y -axis capped at 10. The smoother curves in the inset of panel g plot the kernel density estimates of the step functions. (right panels) CDFs.

increasing A_i and a few local peaks are seen, e.g. around $C/C_0 = 0.5 \times 10^{-3}$ for A_3 and A_4 in panel a ($\beta = 90^\circ$), which reflect the spatial variability of the exposure risk during pedestrian walking. Emergence of the local peak concentrations is presumably attributed to the atmospheric turbulence, which occurs in very short-time intervals and is more sensitive to the spatial location than to the wind direction (Roth et al., 2015). As an agent moves along the avenue, perturbations of the atmospheric turbulence from the canyon circulations and the channel flows set in alternately.

As β is decreased, influence of the channel flow is gradually diminished and pollutants disperse more evenly in the crosswind direction, which agrees with the numerical results of Branford et al. (2011) and Coceal et al. (2014). For $\beta = 45^\circ$ (panel g), the PDF looks relatively smoother (evidently for A_2) and the flow is statistically symmetric about the dominant wind direction. The results imply that staggered arrangement of the building array may help avoid early exposure to high concentrations for agents walking in the avenue near the pollutant source due to the immediate blockage of the building obstacles.

The CDFs help quantify the cumulative risks of exposure to different ranges of concentrations. It can be seen the CDF curves (Fig. 9b, d, f, h) start to diverge for increased C/C_0 . The curve associated with downwind A_i (more notably for small β , e.g. panel h) spans relatively narrower range of C/C_0 , indicating that agents walking in avenues far from the pollutant source are less likely exposed to extremely high concentrations (hereafter C_{extreme} , herein $C/C_0 \gtrsim 1 \times 10^{-3}$ for example), in contrast to agents in the avenues near the pollutant source. However, the CDF curves become increasingly steeper at the high-concentration end when A_i is increased, implying the growing cumulative risk, F_{C/C_0} , of exposure to highly polluted air (hereafter C_{high} , though smaller than the extremes, C_{extreme}).

3.2.3. PDFs and CDFs for fixed receptors

Fig. 10 plots the PDFs and CDFs for fixed receptors distributed along the agent walking tracks (cf. Eq. 5). Although they exhibit quite similar patterns compared to the results recorded by the moving agents (see Fig. 9 analysed in Sec. 3.2.2), the curves herein are obviously more smoother. The difference implies that the spatial variability of the exposure risk during pedestrian walking cannot be sufficiently captured using data recorded by fixed receptors, which corresponds to an Eulerian type of analysis.

Another notable difference is the behaviour of the PDF tail for the near-source avenue,

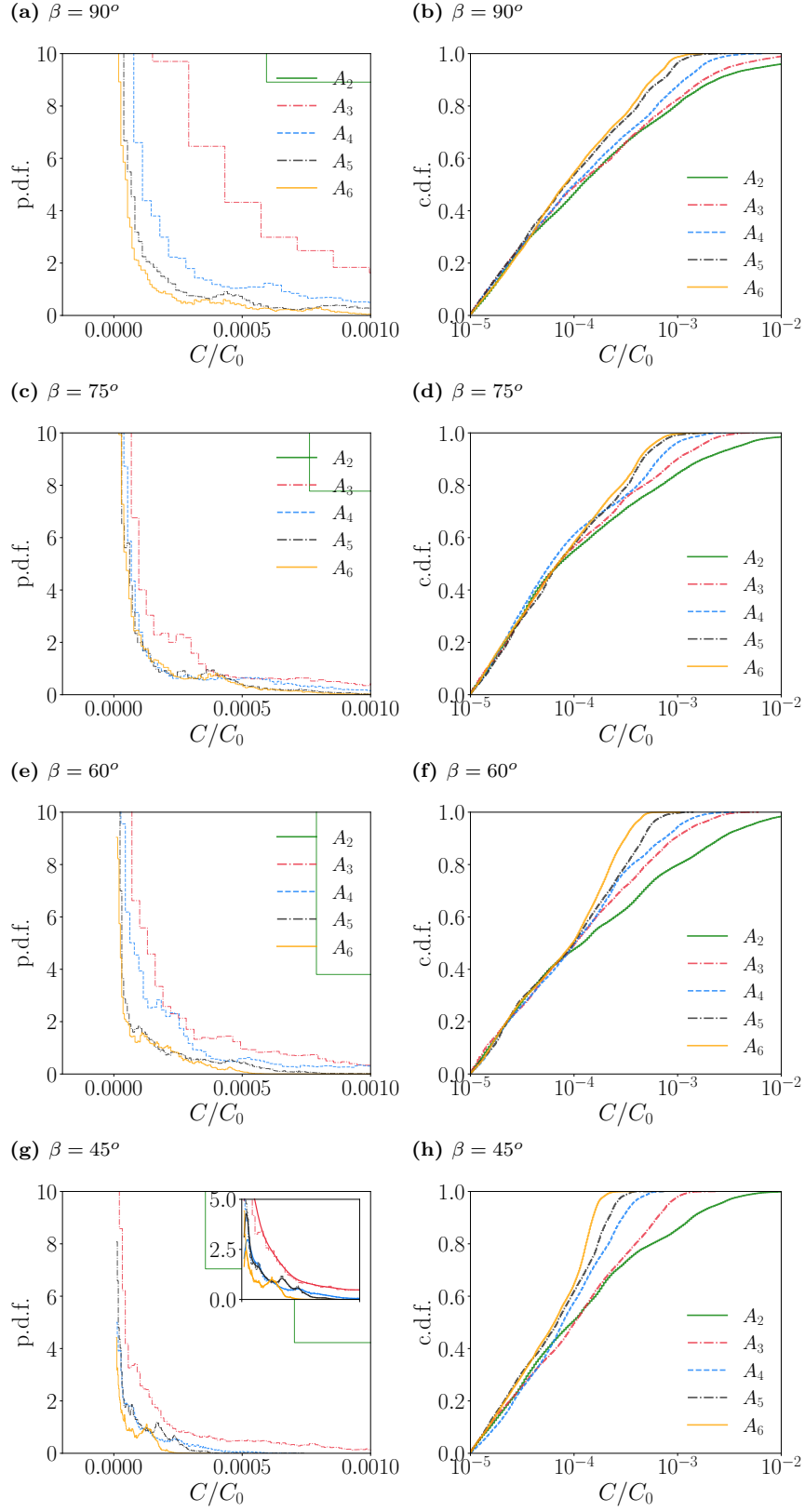


Figure 10: As in Fig. 9, but for fixed receptors, namely the spatial data collected at fixed grid points discretely distributed along the agent walking tracks.

i.e. A_2 (the step functions plotted in green in left panels). For the fixed receptors herein, the fat PDF tail persists across all β . By contrast, the sensitivity to β is well reflected in the data recorded by the walking agents (cf. Fig. 9 left panels). This is because the concentrations collected by the moving receptors along walking track A_2 may not contain a wide range of concentrations before dispersion occurs on larger spatiotemporal scales, irrespective of the wind direction. In other words, data collected by fixed receptors throughout the entire simulation period naturally contain a wider range of concentrations than that recorded by the walking agents during dispersion.

A direct implication of the thicker PDF tail for A_2 under $\beta = 45^\circ$ (see the step function in Fig. 10g) compared to that recorded by the walkers (see Fig. 9g) is that pollutant exposure to the extremes in A_2 interpreted from the data for fixed receptors tends to be overestimated. A similar trend tends to be so for A_3 under $\beta = 90^\circ$ (see Fig. 10a versus Fig. 9a); however, the sensitivity to β is gradually diminished for avenues further downstream, wherein the pollutant cloud has grown substantially in size and dispersion occurs on much larger spatiotemporal scales.

3.3. Route evaluation

3.3.1. Moving receptors

PDFs and CDFs assess the probability aspects of exposure to the entire spectrum of recorded concentrations; however, it is more important to quantify the exposure risk to the air that is more severely polluted. For a high-concentration range of concern, $C/C_0 \in [a, b]$, the integrated probability of exposure, P (or exposure risk), can be quantified as

$$P_{C_{\text{high}}} \equiv F_{C/C_0}(b) - F_{C/C_0}(a), \quad (7)$$

where F denotes the cumulative probability, and see Fig. 9 for reference of the high-concentration range, $[a, b] \equiv [0.9 \times 10^{-4}, 2.0 \times 10^{-4}]$, which is chosen herein purely for demonstration purpose with no loss of generality. Similarly, the integrated exposure risk to the extremes reads

$$P_{C_{\text{extreme}}} \equiv 1 - F_{C/C_0}(b). \quad (8)$$

Fig. 11 plots the exposure risks for different A_i and β . It can be seen that the integrated probability of exposure to the high concentrations, $P_{C_{\text{high}}}$, roughly ranks as $P(A_6) > P(A_5) > P(A_4) > P(A_3) > P(A_2)$ (Fig. 11a). $P_{C_{\text{high}}}$ shows a similar monotonic

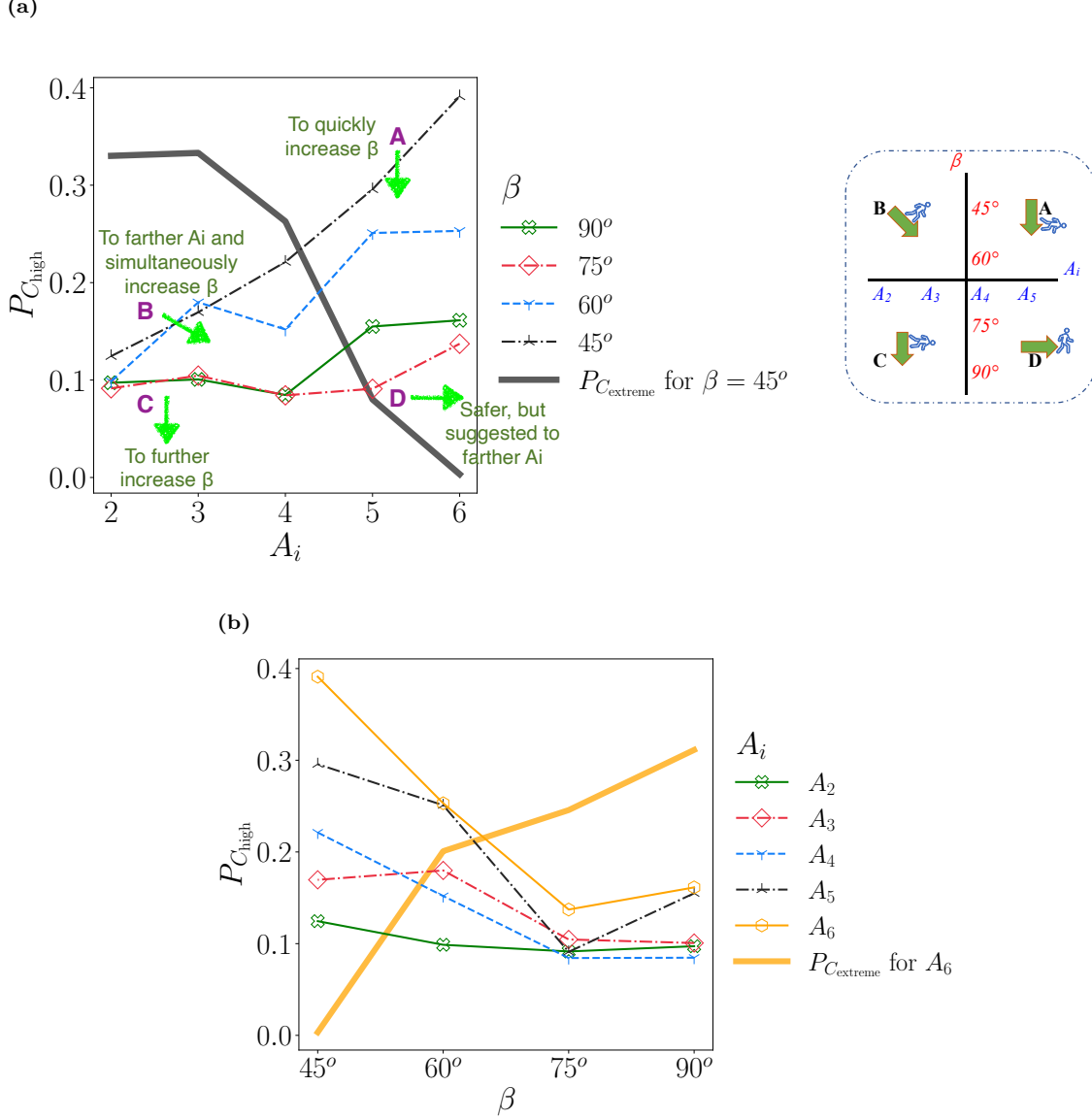


Figure 11: Integrated probability of exposure to high concentrations, $[a, b]$, $P(a < C/C_0 \leq b)$ (i.e. $P_{C_{\text{high}}}$, see Eq. 7) for different (a) A_i ; and (b) β . Note that the thicker line (colored in black in panel a and in orange in panel b) plots $P(C/C_0 > b)$ (i.e. $P_{C_{\text{extreme}}}$, see Eq. 8) and for clarity, results are only shown for one case: $\beta = 45^\circ$ in panel a and A_6 in panel b. To the right of panel a is a schematic representation of four evacuation scenarios, A, B, C and D. Each scenario corresponds to different values of A_i and β .

sensitivity to β (Fig. 11b), and there is $P(\beta_{45^\circ}) > P(\beta_{60^\circ}) > P(\beta_{75^\circ}) > P(\beta_{90^\circ})$. For the integrated probability of exposure to the extremes, $P_{C_{\text{extreme}}}$, an opposite dependence (by definition) is seen on A_i and β , respectively.

The results in Fig. 11 indicate that evacuation routes during pollutant dispersion strongly depend on the meteorological condition (herein β) and the position of the receptor (namely the dynamically changing location of the agents walking along A_i). During

emergency response, the risk of pollutant exposure may be greatly reduced if one could scientifically decide the priority of moving to further avenues first or adjusting the walking direction immediately for given A_i and β . With no loss of generality, we analyse four scenarios: A, B, C and D (annotated in Fig. 11a left panel and schematically sketched in Fig. 11a right panel), with each scenario corresponding to different values of β and A_i .

It can be seen if agents are located in avenues very close to the pollutant source (as scenarios B and C) and are walking at small β (e.g. 45° , as scenario B) with respect to the dominant wind, it is always safe for agents to move towards farther avenues and simultaneously increase β to reduce $P_{C_{\text{extreme}}}$ meanwhile keeping $P_{C_{\text{high}}}$ low. If agents are in the same avenue, but walking at large β (e.g. 90° , as location C), they are suggested to further increase β (i.e. to deviate more from the dominant wind direction). Although spending time moving to farther avenues also reduces $P_{C_{\text{extreme}}}$, it is perhaps not the primary concern during emergency response as $P_{C_{\text{extreme}}}$ is already at a very low level.

If agents are located in remote avenues of a few blocks to the accidental venue (as scenarios A and D) and are walking at small β (e.g. 45° , as scenario A) with respect to the dominant wind, they are suggested to increase β first to quickly decrease $P_{C_{\text{high}}}$ and then direct towards even farther avenues. The evacuation pathway is the same as that for scenario C. If agents are in the same avenue, but walking at large β (e.g. 90° , as scenario D), they are in a relatively much safer condition, but are suggested to stay as far as possible to further decrease $P_{C_{\text{extreme}}}$. The evacuation route planning is similar to that for scenario B.

It is obvious that if agents' locations are in the same avenue with the pollutant source (i.e. in A_1), evacuation routes should be immediately opposite to the dominant wind.

3.3.2. Fixed receptors

Similarly to Fig. 11, Fig. 12 plots the integrated probability of exposure to the high concentration range, C_{high} , but for fixed receptors. Although the general patterns seem quite similar to Fig. 11, a few nontrivial differences in the details of $P_{C_{\text{high}}}$ versus A_i (panel a) and β (panel b) are noteworthy.

For avenues near the source, $P_{C_{\text{high}}}$ appears lower than that experienced by the walkers (cf. Fig. 11a), indicating an underestimation of the exposure risk to the high concentrations actually experienced by a walker. This is particularly so for large β (cf. Fig. 11b). The results imply that although similar evacuation routes as described in the above sec-

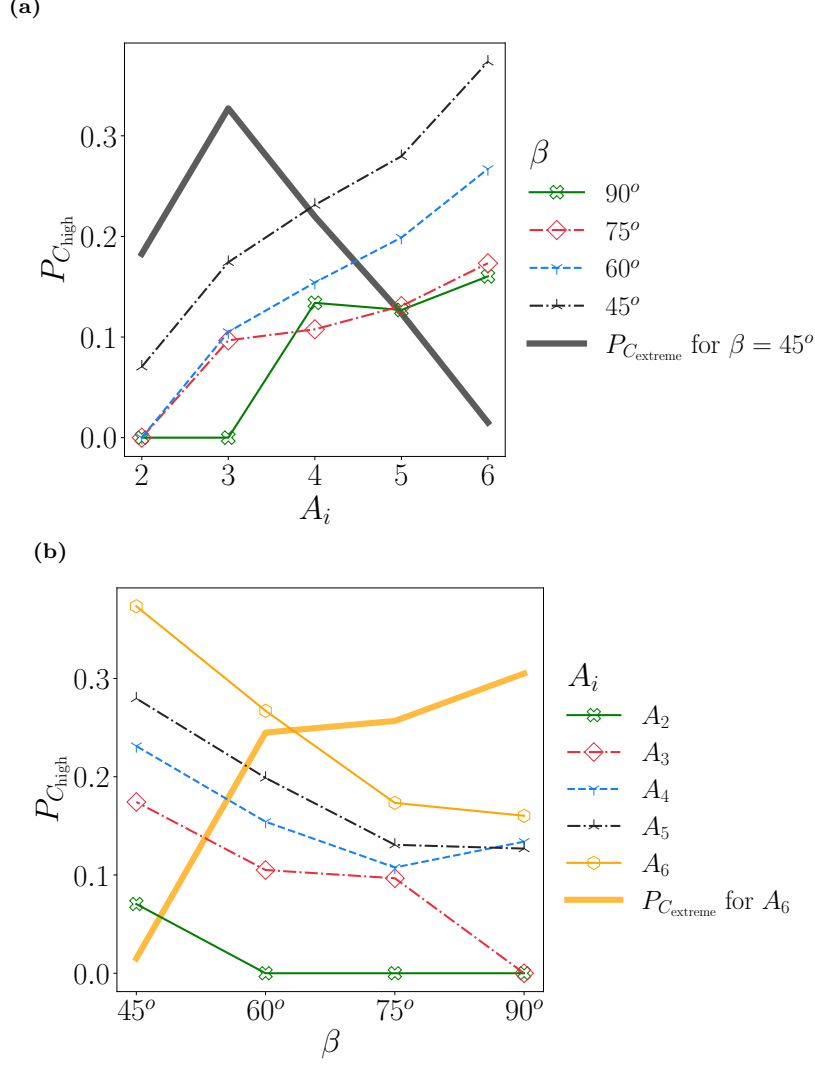


Figure 12: As in Fig. 11, but for fixed receptors, namely the spatial data collected at fixed grid points discretely distributed along the agent walking tracks.

tion (Sec. 3.3.1) may be suggested, the integrated probability of exposure along the same route cannot be accurately predicted based on the Eulerian estimates.

4. Discussion

A modified arrangement of the roughness grid may be thought as equivalent to rotating the wind (Branford et al., 2011; Marucci and Carpentieri, 2020; Blunn et al., 2022). The layout of the building obstacles directly affects pollutant exposure. For agents moving along an avenue near the pollutant source, a staggered array (for which the wind perpendicular to the avenue is rotated) is shown to help in the avoidance of early exposure to high concentrations due to the immediate blockage of the near-field building blocks. The simplified urban topography represents a convenient starting point in the

literature (e.g. Wang and Ngan, 2021; Li and Katul, 2022); however, spatial characteristics of the mean flow and turbulence in realistic urban districts of high inhomogeneity may vary greatly (Giometto et al., 2016; Hadavi and Pasdarshahri, 2021), wherein the obstruction of solid obstacles could change ventilation and hence exposure qualitatively (Blunn et al., 2022; Liu et al., 2022).

As a typical simplification, neutral stratification, which represents an idealised micro-meteorological condition (cf. Nazarian et al., 2018; Hadavi and Pasdarshahri, 2021; Lee et al., 2023; Li et al., 2023), was assumed in the current work. Under thermal stratification, the center of mass of the pollutant cloud can either descend or be elevated by the buoyancy forcing (Park and Baik, 2013; Ma and Cheng, 2023). It was shown in Duan and Ngan (2020) that the thermal internal boundary layer for an aligned building array can be four times thicker for a $\Delta T = 12$ K ground heating compared to that for a $\Delta T = -2$ K ground cooling, where ΔT denotes the temperature increase at the ground level. Ventilation improves for the former and deteriorates for the latter, leading to varying ventilation timescales (the mean tracer age was found to increase by up to 25% for $\Delta T = -4$ K and to decrease by up to 80% for $\Delta T = 8$ K) and hence that the PDFs and CDFs of pollutant concentrations experienced by the virtual walkers would differ significantly compared to that under neutral stratification. However, the exact sensitivity of pollutant exposure for moving agents to the the boundary-layer stability remains unclear.

During accidental releases of hazardous pollutants, both the toxicity and the duration of exposure are important concerns (Greene and Morris, 2006; Scungio et al., 2018). The latter is being investigated in ongoing work using tracer age statistics; however, the former has remained not fully addressed because as in many studies in the literature a tracer gas is oftentimes assumed to be passive and inert for simplicity (e.g. Gao et al., 2022). The toxicity aspect could be worth exploring in future work. Although a continuously-released source (opposed to the impulse source specified in the current study) may preclude the quantification of pollutant decay (this is why it is not used herein), it allows the calculation of exposure for a statistically-steady pollutant field, which is also of great concern in the literature (e.g. Marucci and Carpentieri, 2020; Wang and Ngan, 2021).

A few other simplifications are also enforced to simplify the problem, such as the fixed agent departure location, departure time and the constant walking speed. Although a direct extrapolation of the results to real urban environmental scenarios is not straight-

forward, they should serve as a useful baseline reference for exposure risk assessment and evacuation route planning for urban regions with well-aligned avenues. Despite the idealised agent walking routes, no assumptions are imposed on the implementation of the methodology presented in the current work, therefore it can be applied to more interesting cases, e.g. for more real origin-destination-based walking trajectories (Tilahun and Levinson, 2010; Kim and Chung, 2018), which requires further efforts.

5. Conclusions

Pollutant dispersion and exposure have been conventionally quantified based on statistics for fixed receptors, namely fixed grid points discretely distributed in a computational domain. Subsequent spatial or temporal averages may not accurately quantify the exposure of walkers (or moving receptors). The current study investigates pollutant exposure of virtually walking agents (which essentially emulate the pedestrians that walk along the avenues of a real urban district) to an impulse release of gaseous pollutants. The implementation of virtual walkers in LES for pollutant exposure represents the main novelty of this study.

The dispersion of pollutants is driven by a turbulent flow developed over an idealised urban district, an aligned array of unit-aspect-ratio canyons, which implies a skimming flow regime. Impacts of the angle (β) between the agent walking direction (which is fixed to simplify the problem) and the dominant wind direction is examined. Timescales associated with the decay of the scalar mean and variance both exhibit a monotonic dependence on β (Sec. 3.1), indicating temporally variable exposure risks. It is shown that timely evacuation is still possible even if agents are in an avenue adjacent to the release point; however, the results suggest that higher walking speeds must be considered as a walker moves towards avenues further downwind of the domain to ensure an adequate time for evacuation.

For the initial-value problem considered herein, we demonstrate that the actual exposure can differ from simple Eulerian estimates: the maximum concentration exposed by a walker interpreted from data recorded by the fixed receptors along the same walking track is found to be overestimated by a few orders of magnitude. The exposure risks for moving receptors along different avenues, A_i , are quantified using the PDFs and CDFs of the recorded concentrations for different β (Sec. 3.2), and evacuation route planning

for minimised exposure risks to the polluted air analysed.

Intuitively, one would expect the exposure risk to be lower along an evacuation route that deviates more from the dominant wind direction and be farther from the release point. The former is based on the fact that lateral spread of pollutants is much slower than dispersion downwind; for the latter, far-field pollutant concentrations generally have decayed to a substantially low level. In most of the scenarios that differ in β and A_i , the results suggest evacuation routes towards a direction that deviates as much as possible from the dominant wind direction (Sec. 3.3) and, under certain circumstances, walkers are recommended to be contemporarily evacuated towards avenues further downstream; however, this does not always ensure reduced exposure (further demonstrated in Appendix B). The results imply that decision of the priority of moving to further avenues downstream first or deviating immediately from the dominant wind direction for given A_i and β can be important during emergency response.

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Appendix A. Model validation

The current LES model has been extensively validated for urban-scale turbulent boundary-layer flows (Gronemeier et al., 2020) and pollutant dispersion (Resler et al., 2020). We have previously validated this model for a single street canyon (Duan et al., 2019) and an idealised building array (Duan and Ngan, 2020). Following Belcher et al. (2015), the model herein is validated against the experimental data obtained from the EnFlo wind tunnel at the University of Surrey and the DNS data of Branford et al.

(2011). We consider a grid of aligned cubic building blocks and a 45° wind with respect to the frontal building facades, identical in setup to that in the DNS (see Fig. A.13).

In both the DNS and the wind-tunnel experiments, a continuous pollutant source was applied, whereby a statistically-steady state scalar field was obtained. By contrast, the current work is focused on an instantaneous source (Eq. 1). To better align with the initial-value problem investigated in the current study, we attempt to expand the validation in a harder way that differs from the conventional ones (e.g. Cheng et al., 2008; Duan et al., 2019), namely a steady scalar field is reconstructed via integration of the results for an instantaneous release. A formal description of the integration can be found in Lo and Ngan (2015) and is therefore not elaborated here.

Fig. A.14 compares the normalised centreline concentrations. While the decay downwind of the source is well captured, the overprediction of the concentration in the first sampling cell is notable. The discrepancy may be attributed to the differences between the source setups: the source was discretised as a Gaussian bell over a few grid points and was prescribed at $z = 0.0625H$ in the DNS, while the LES applied a purely areal source. Far from the source ($x/H > 6$), the LES shows excellent agreement with the measurements and the DNS.

Fig. A.15 plots the lateral concentration profiles at different distances ($2\sqrt{2}H$, $3\sqrt{2}H$, $6\sqrt{2}H$ and $8\sqrt{2}H$) from the source cell measured along the diagonal. There are a few large discrepancies near the plume centre, e.g. in panels a and b. Similar discrepancies are also seen in the DNS of Branford et al. (2011). Despite that, the lateral distributions are reasonably well estimated for various downwind distances and the current LES actually shows improved agreement with the experiments compared to the DNS at some locations (e.g. $x/H = 4$ and 10 in panel b). It is noteworthy that excellent agreement with the wind-tunnel measurements and the DNS data is obtained for the profile tails, suggesting that the plume width is well predicted.

Appendix B. Exposure risks along a diagonal route

In real urban districts, pedestrians may either walk along an avenue or cross a street. While it is difficult to specify a walking trajectory that satisfies personal preferences, we estimate the integrated probabilities of exposure to highly and extremely polluted air (i.e. $P_{C_{\text{high}}}$ (Eq. 7) and $P_{C_{\text{extreme}}}$ (Eq. 8), see Sec. 3.3) along the diagonal of the domain. This

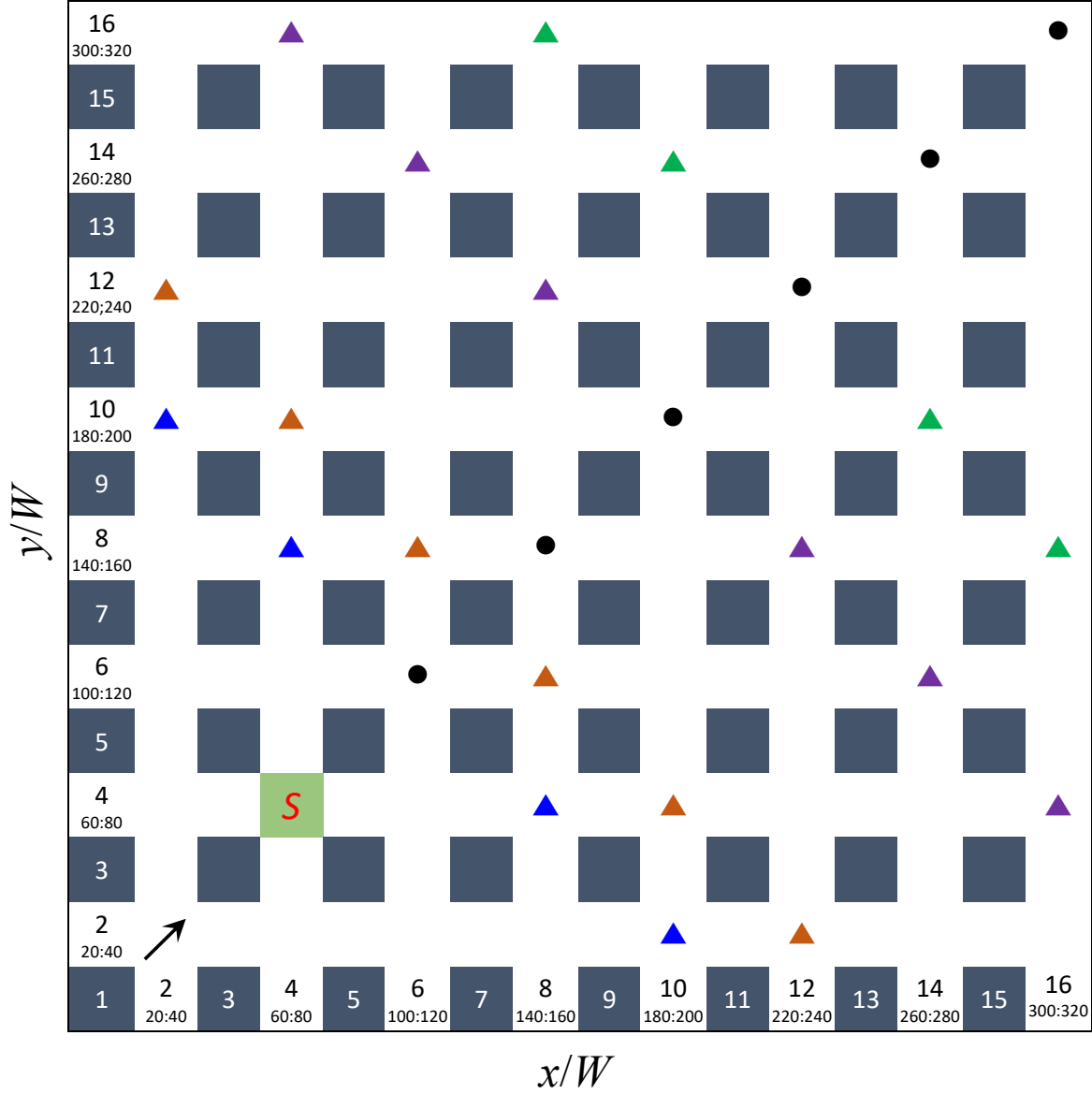


Figure A.13: Schematic diagram of an aligned building array considered in the DNS of [Branford et al. \(2011\)](#) and used for the validation of the current LES model. The arrow denotes the 45° wind. The numbers annotate the rows (y/W) and columns (x/W), as well as the associated grid points. Filled triangles and circles indicate sampling positions for the lateral (crosswind) and centreline (diagonal) profiles, respectively. A delta-function ground-level source (Eq. 1) covers the grid points of 60 – 80 (highlighted in green).

specification represents a scenario that includes both pedestrian walking and crossing behaviour in a real pedestrian network.

While one would intuitively expect the exposure risk to be lower along an evacuation route that deviates more from the dominant wind direction and be farther from the release point (the diagonal route accounts for the impact of both), a monotonic dependence is

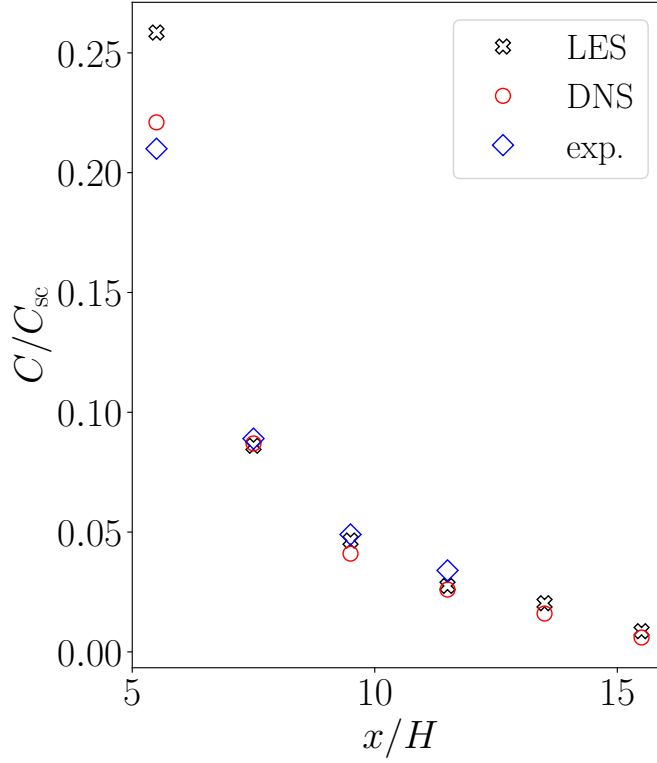


Figure A.14: Comparison of the centreline concentrations normalised by the concentration in the source cell, C_{sc} . Crosses: the current LES model; Circles: DNS of [Branford et al. \(2011\)](#); Squares: wind-tunnel data from the EnFlo wind tunnel at the University of Surrey ([Belcher et al., 2015](#)).

not guaranteed. Fig. [B.16](#) shows that $P_{C_{high}}$ and $P_{C_{extreme}}$ do not change monotonically with β .

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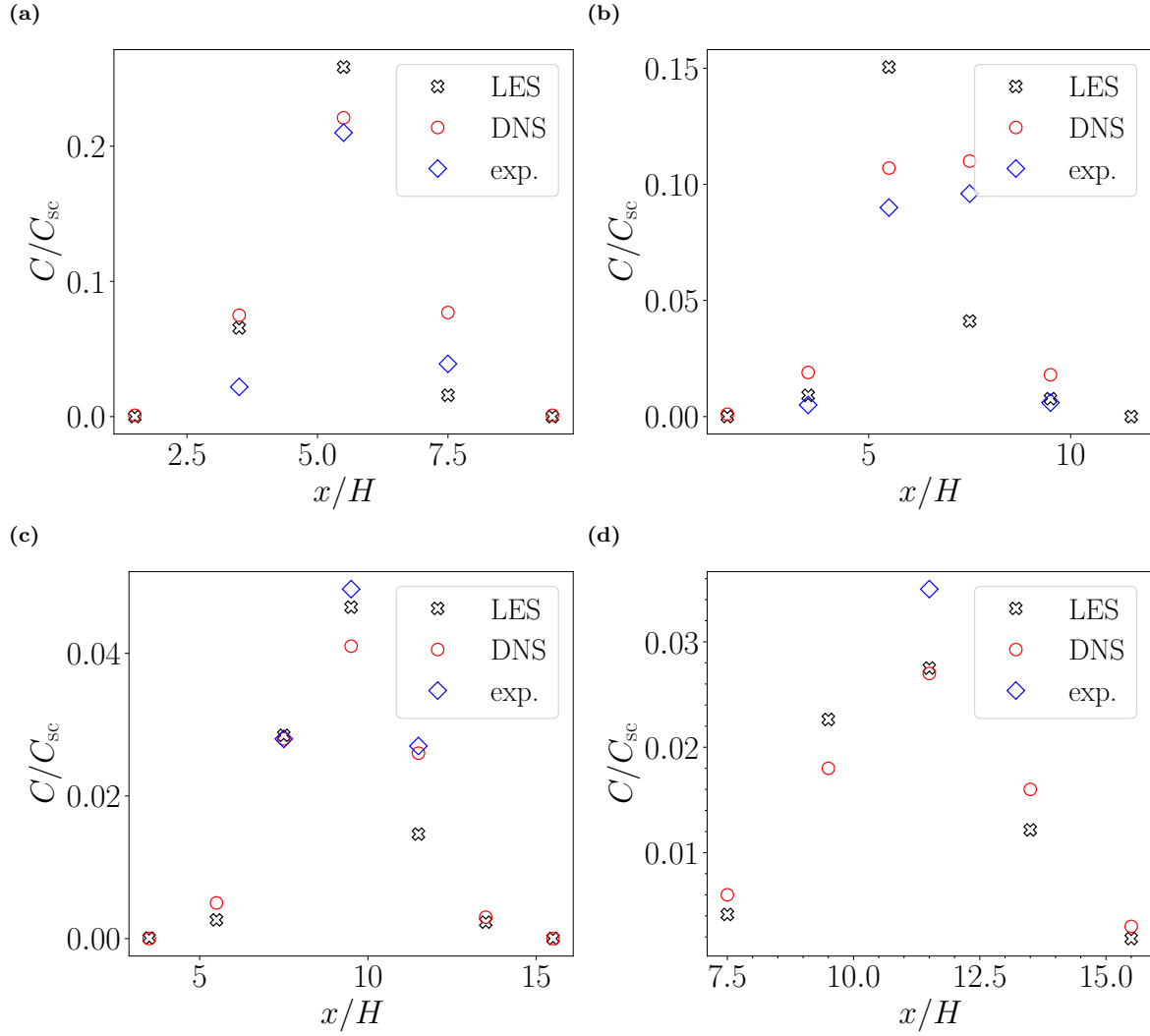


Figure A.15: Lateral profiles of the normalised concentrations at different perpendicular distances from the source: (a) $2\sqrt{2}h$; (b) $3\sqrt{2}h$; (c) $6\sqrt{2}h$; (d) $8\sqrt{2}h$. Crosses: the current LES model; Circles: DNS of Branford et al. (2011); Squares: wind-tunnel data from the EnFlo wind tunnel at the University of Surrey (Belcher et al., 2015).

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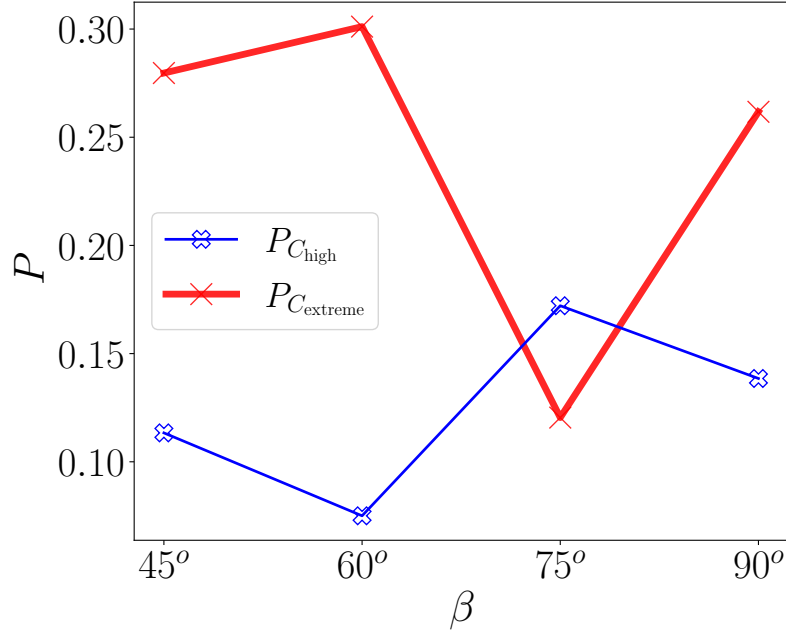


Figure B.16: $P_{C_{\text{high}}}$ and $P_{C_{\text{extreme}}}$ for a diagonal walking route for different β .

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