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## Evaluation of fast atmospheric dispersion models in a regular street network

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► **To cite this version:**

Denise Hertwig, Lionel Soulhac, Vladimír Fuka, Torsten Auerswald, Matteo Carpentieri, et al.. Evaluation of fast atmospheric dispersion models in a regular street network. *Environmental Fluid Mechanics*, 2018, 10.1007/s10652-018-9587-7 . hal-01761232

**HAL Id: hal-01761232**

**<https://hal.science/hal-01761232>**

Submitted on 8 Apr 2018

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1 **Evaluation of fast atmospheric dispersion models in a regular**  
2 **street network**

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8 Received: date / Accepted: date

9 **Abstract** The need to balance computational speed and simulation accuracy is a key chal-  
10 lenge in designing atmospheric dispersion models that can be used in scenarios where near  
11 real-time hazard predictions are needed. This challenge is aggravated in cities, where mod-  
12 els need to have some degree of building-awareness, alongside the ability to capture effects  
13 of dominant urban flow processes. We use a combination of high-resolution large-eddy sim-  
14 ulation (LES) and wind-tunnel data of flow and dispersion in an idealised, equal-height  
15 urban canopy to highlight important dispersion processes and evaluate how these are repro-  
16 duced by representatives of the most prevalent modelling approaches: (i) a Gaussian plume  
17 model, (ii) a Lagrangian stochastic model and (iii) street-network dispersion models. Con-  
18 centration data from the LES, validated against the wind-tunnel data, were averaged over  
19 the volumes of streets in order to provide a high-fidelity reference suitable for evaluating  
20 the different models on the same footing. For the particular combination of forcing wind

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direction and source location studied here, the strongest deviations from the LES reference were associated with mean over-predictions of concentrations by approximately a factor of 2 and with a relative scatter larger than a factor of 4 of the mean, corresponding to cases where the mean plume centreline also deviated significantly from the LES. This was linked to low accuracy of the underlying flow models/parameters that resulted in a misrepresentation of pollutant channelling along streets and of the uneven plume branching observed in intersections. The agreement of model predictions with the LES (which explicitly resolves the turbulent flow and dispersion processes) greatly improved by increasing the accuracy of building-induced modifications of the driving flow field. When provided with a limited set of representative velocity parameters, the comparatively simple street-network models performed equally well or better compared to the Lagrangian model run on full 3D wind fields. The study showed that street-network models capture the dominant building-induced dispersion processes in the canopy layer through parametrisations of horizontal advection and vertical exchange processes at scales of practical interest. At the same time, computational costs and computing times associated with the network approach are ideally suited for emergency-response applications.

**Keywords** Pollutant dispersion · Urban environment · Street-network model · Gaussian plume model · Lagrangian stochastic model · Model inter-comparison

## 1 Introduction

In the event of hazardous materials being released into the atmosphere, either by accident or intentionally, dispersion models are key to coordinate actions to avoid or mitigate impacts on human health [11, 31, 63]. Emergency response dispersion models are applied both *proactively*, e.g. to assess exposure risks and vulnerability of sensitive public structures, and *reactively* as part of emergency management protocols and decision making frameworks [34]. Principal areas of application can be grouped into (i) planning (pre-incident), (ii) response (mid-incident) and (iii) analysis/evaluation (post-incident).

In general, an emergency response dispersion model needs to have short latency times to enable timely actions (fast), it should make low demands on computational resources required, be easy to use and fast to set up (cheap) and the results produced should be accurate and interpretable in an unambiguous way. Figure 1 illustrates these requirements in terms of a ‘*feasibility triangle*’. The dilemma faced in emergency response modelling is that once two of these requirements are met, fulfilling the remaining third becomes a challenge. For example, in order to make accurate calculations quickly, computational requirements and costs are high; fast and cheap models have accuracy limitations; accurate and computationally expensive models require long run times. Hence, as long as computational resources remain limited, model developers are tasked with finding an optimal balance between these requirements.

### 1.1 Challenges in urban areas

High population density and limited evacuation options increase human exposure risks in cities, making them particularly vulnerable to hazards from air-borne contaminants. Quality requirements on urban dispersion models hence are high. The challenge to balance speed and accuracy is exacerbated since urban dispersion models need to have some degree of building-awareness, alongside the ability to capture complex effects of urban flow patterns

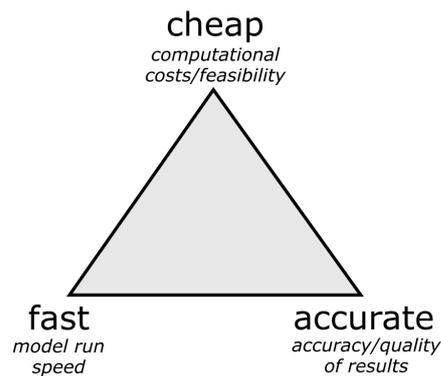


Fig. 1: ‘Feasibility triangle’ for emergency response dispersion modelling.

64 on the dispersion process [18,5]. Numerous field, laboratory and numerical experiments  
 65 of the past have shown that the impact of buildings on pollutant dispersion is significant,  
 66 particularly in the near-field close to the source [27, 14, 50, 82, 79]. Due to building-induced  
 67 flow effects like channelling, branching in intersections, wake recirculation or vortex shed-  
 68 ding at roof and building corners, plume dispersion within the urban canopy layer (UCL)  
 69 is distinctively different from dispersion well above the roughness sublayer. Building ar-  
 70 rangements and street layouts uniquely determine this so-called *topological* component of  
 71 urban dispersion. Material can travel significant distances upstream of the source if trapped  
 72 in recirculating wind regimes [82]. Localised trapping of pollutants in building wakes can  
 73 create secondary sources whose emission characteristics are governed by local flow proper-  
 74 ties and can vastly differ from those of the primary source [5]. In addition, strong variations  
 75 in building heights can result in significant asymmetries of the vertical plume structure with  
 76 material being lifted out of the canopy layer, resulting in a shift of the effective source height  
 77 [44, 45, 15].

78 Computational fluid dynamics (CFD) approaches like Reynolds-Averaged Navier-Stokes  
 79 (RANS) modelling or large-eddy simulation (LES), and to a lesser extent wind-tunnel ex-  
 80 periments, can deliver detailed information about flow and dispersion processes in built  
 81 environments [79]. While CFD models can be specifically designed for emergency response  
 82 planning and preparation [44,30], associated computing times currently are too long for  
 83 operational use during emergency events [80].

84 Instead, simpler model formulations are needed that represent processes relevant for the  
 85 scenario through suitable parametrisations and ideally can also be operated in inverse mode  
 86 for source detection. Approaches for fast urban dispersion modelling are discussed below.  
 87 For an overview of urban dispersion models see e.g. Andronopoulos et al. [2].

## 88 1.2 Options for fast urban dispersion modelling

89 Urban emergency response models are primarily applied to the dispersion of air-borne sub-  
 90 stances from localised releases from a limited number of sources. Typical time scales of  
 91 interest range from seconds to a few hours and length scales from streets to city extents.  
 92 Models currently used for fast dispersion simulations differ significantly in the way they

Table 1: Characteristics of different modelling approaches for dispersion from localised releases in cities.

Type	Dispersion	Flow	Buildings
CFD	Eulerian or particle tracking	internally computed mean or turbulent velocities	explicit
Gaussian	analytical, empirical	mean plume advection velocity (prescribed or modelled)	implicit
Lagrangian	particle tracking	externally computed mean flow, turbulent variances, Lagrangian time scales	explicit / implicit
Street-network	flux balance	mean horizontal advection velocities, vertical exchange velocities (prescribed or modelled)	street topology
Hybrid	nomographs	externally computed flow statistics	explicit / implicit

93 represent the built environment and account for urban flow and dispersion processes, as  
 94 summarised in Tab. 1.

95 Here, the comparatively expensive flow-resolving and building-representing CFD solu-  
 96 tions are included as a reference. At the other end of the complexity spectrum we find the  
 97 widespread class of Gaussian dispersion models. *Gaussian plume models* are based on an  
 98 empirical-analytical representation of the downwind concentration spread, with the plume  
 99 shape being determined through empirically defined concentration standard deviations in  
 100 lateral and vertical direction. In its simplest configuration, this model needs as input only an  
 101 estimate of the mean velocity along the plume trajectory  $U_p$ . Gaussian plume models have  
 102 been extensively tested and advanced model versions include parametrisations of effects  
 103 of atmospheric stratification, complex terrain or built environments. The US EPA’s model  
 104 AERMOD [25] takes into account urban effects through enhanced turbulence levels relative  
 105 to rural areas and includes a module (PRIME) that accounts for plume downwash in the  
 106 wake of single buildings. The UK’s ADMS model [22] in its urban version ADMS–urban  
 107 [51] uses the Operational Street Pollution Model (OSPM) [46, 8] to model street canyon  
 108 effects. Flow and dispersion effects around isolated buildings are modelled in the ADMS–  
 109 BUILD module [58].

110 With *Gaussian puff models* short-duration, non-steady-state releases are modelled by  
 111 tracking the path of individual pollutant clouds in the flow (in a Lagrangian sense). Within  
 112 the Urban Dispersion Model (UDM) [16] bulk effects of single buildings, building clusters,  
 113 or entire cities on puff trajectories are parametrised. This distinguishes UDM from  
 114 Lagrangian Gaussian puff models like RIMPUFF [77], SCIPUFF [75, 1] or CALPUFF [62],  
 115 which are used on the regional/meso-scale and treat cities in a bulk way as an urban rough-  
 116 ness. All of these models are integral components of several national and multi-national  
 117 emergency response support systems.

118 *Lagrangian stochastic dispersion models* compute trajectories of computational parti-  
 119 cles in 3D wind fields using random-walk methods to represent the stochastic component  
 120 of the dispersion process. Compared to typical Gaussian or building-resolving CFD models,  
 121 Lagrangian models can be applied to problems ranging from local to global scales. Usually,  
 122 Lagrangian models are run off-line on wind fields supplied by diagnostic or prognostic mod-  
 123 els, e.g. numerical weather prediction models for applications from regional to global scales

124 and CFD or diagnostic wind models for urban-scale problems. Well-known representatives  
125 of off-line Lagrangian models used operationally across scales are the UK Met Office's  
126 NAME model [49] or NOAA's HYSPLIT model [74]. Examples of Lagrangian random-  
127 walk dispersion models applied in built environments are LANL's QUIC-PLUME model  
128 [81] and Micro-Swift-Spray (MSS) [78]. In both QUIC-PLUME and MSS flow informa-  
129 tion is provided by built-in wind models based on empirical-diagnostic representations of  
130 building-induced flow effects.

131 *Street-network models* are a comparatively recent addition to the family of urban dis-  
132 persion models, first brought forward by Soulhac [67]. Here, urban areas are represented  
133 through a network of connected boxes, covering street canyons and intersections, and canopy-  
134 layer dispersion is simulated by parametrising concentration fluxes between these boxes  
135 [38,6]. While not representing buildings explicitly, the model is directly aware of the street  
136 topology of the city. Like Gaussian dispersion models, street-network models require only  
137 few flow specifications, which can be either imported from an external flow simulation or  
138 obtained through suitable parametrisations. The only street-network models currently used  
139 operationally are the SIRANE [71,72] model and its unsteady version SIRANERISK [69],  
140 which both contain built-in flow parametrisations.

141 A further approach was introduced by the US Naval Research Laboratory with the *hy-*  
142 *brid plume dispersion model* CT-Analyst [11]. This model produces real-time urban con-  
143 centration predictions by interrogating databases containing possible contaminant pathways  
144 for the release scenario [10]. These pathways have to be calculated in advance from detailed  
145 3D flow simulations with building-resolving LES for different ambient wind directions and  
146 atmospheric conditions.

### 147 1.3 Aims of this study

148 In this study we aim to document strengths and limitations of prevalent dispersion mod-  
149 elling approaches with regard to the physical processes they capture. We choose the canon-  
150 ical test case of a localised release in an array of cuboidal buildings with oblique wind  
151 forcing. The models considered here are: (1) a baseline Gaussian plume dispersion model,  
152 (2) a Lagrangian stochastic plume model driven by 3D wind fields from models of varying  
153 complexity, and (3) two street-network dispersion models. While in some cases well-known  
154 representatives of these categories are used, the chief aim of this study is to highlight dif-  
155 ferences in modelling frameworks rather than ranking particular models. The fact that these  
156 approaches represent urban dispersion processes through vastly different modelling helps to  
157 identify which of these processes are of importance. By including the comparatively new  
158 street-network modelling approach as an alternative to traditional approaches and putting  
159 the focus on near-field dispersion patterns, this study adds further insight to previous model  
160 inter-comparison studies [57,56,60,41,3,4].

161 Furthermore we aim (i) to assess where in the hierarchy of fast dispersion modelling  
162 approaches the street-network model is situated by assessing its performance against more  
163 established methods, (ii) to investigate the effect of the accuracy and level of detail of the  
164 flow representation in the different types of models, and hence (iii) to gain insight into  
165 how existing parametrisations in such models could be improved. The dispersion character-  
166 istics are analysed based on datasets from boundary-layer wind-tunnel measurements and  
167 high-resolution large-eddy simulation of plume dispersion in an idealised urban environ-  
168 ment comprised of a regular uniform array of cuboidal buildings. The performance of the  
169 LES has previously been validated successfully regarding its representation of flow and

170 dispersion processes for this geometry based on the wind-tunnel experiments [23,32]. We  
 171 extend this evaluation with a focus on particular aspects of the dispersion characteristics and  
 172 then use the LES as a reference to establish differences between the output from the sim-  
 173 pler models, averaged over the volumes of streets to reflect a common representation that  
 174 matches the output from street-network models.

175 This work is part of the DIPLOS project (DIspersion of LOcalised releases in Street net-  
 176 works; [www.diplos.org](http://www.diplos.org)) that aimed to improve parametrisations of dispersion processes  
 177 in cities through a better understanding of time-dependent canopy-layer flow processes. De-  
 178 tails about the test case and the reference data are presented in Sect. 2, followed by a brief  
 179 introduction of the dispersion models used (Sect. 3). Flow and dispersion characteristics  
 180 are discussed in Sect. 4, followed by an overview of the model inter-comparison study in  
 181 Sect. 5. Conclusions are presented in Sect. 6.

## 182 2 Reference experiment and simulation

### 183 2.1 Urban test geometry

184 Given the interest in hazard modelling in populous areas, we are particularly interested in a  
 185 geometric regime characteristic of city centres, and more specifically of European cities. To  
 186 a fair degree of realism, such urban environments may be approximated by large rectangular  
 187 blocks sufficiently close together as to produce a measure of decoupling between canopy-  
 188 layer flow and the external boundary layer. This means that street-canyon flow is fully de-  
 189 veloped and the city centre may be viewed as a network of streets joined at intersections [6].  
 190 With this in mind, the DIPLOS test geometry was designed as an array of aligned rectangu-  
 191 lar buildings of uniform height  $H$  and street width  $W = H$  (Fig. 2a), corresponding to the  
 192 so-called skimming-flow regime. Each building has a dimension of  $1H \times 2H \times 1H$  in  $x$ ,  $y$   
 193 and  $z$ . In contrast to canonical cube-array settings, the rectangular buildings of the DIPLOS  
 194 array introduce a geometrical asymmetry that is more typical of actual street topologies.  
 195 A similar set-up is that of the well-studied MUST field-experiment configuration consist-  
 196 ing of an aligned array of shipping containers [9]. However, with a canyon aspect ratio  
 197 of  $H/W = 1$  the DIPLOS array produces more pronounced street-canyon flow behaviour  
 198 typical for skimming-flow regimes compared to the rather ‘open’ MUST geometry with  
 199  $H/W \simeq 0.2$  [61]. The plan area density, defined as the ratio of the area covered by buildings  
 200 to the total area, has a value of  $\lambda_p = 0.33$  irrespective of model orientation. The frontal area  
 201 density (ratio between the silhouette area of the buildings to the total plan area) is  $\lambda_f = 0.35$   
 202 for a model orientation of  $-45^\circ$  that is investigated in this study.

### 203 2.2 Reference data

#### 204 2.2.1 Wind-tunnel experiment

205 Flow and dispersion experiments under neutral stratification conditions were conducted in  
 206 the Enflo laboratory at the University of Surrey. The open-return boundary-layer wind-  
 207 tunnel used in this study has a 20 m test section and a cross section of  $3.5 \text{ m} \times 1.5 \text{ m}$ .  
 208 The urban scale-model consisted of a regular array of  $14 \times 21$  rows of wooden blocks of  
 209 height  $H = 70 \text{ mm}$ . The model was mounted on a turntable whose centre was located about  
 210 14 m downstream of the test-section entrance. In this study we focus on a model orientation

211 of  $-45^\circ$  to the approaching boundary-layer flow; i.e. none of the streets are aligned with  
212 the inflow direction. As can be seen in Fig. 2a, in this set-up the corners of the model array  
213 were slightly curtailed in order to fit the array into the tunnel. In the flow development sec-  
214 tion upstream of the model, a fully-rough boundary-layer flow was modelled by the use of  
215 1.26 m tall vorticity generators (Irwin spires) placed at the tunnel entrance and a staggered  
216 array of roughness elements covering the tunnel floor, resulting in a boundary-layer depth  
217 of about  $14H$ . Measurements within the model took place sufficiently far away from the  
218 leading edge of the model where the mean flow in any repeating unit as shown in Fig. 2b  
219 was verified to be independent of the location within the centre of the array. The tunnel free-  
220 stream velocity of  $U_e = 2 \text{ m s}^{-1}$  was constantly monitored downwind of the model by two  
221 reference ultrasonic anemometers positioned at a height of approximately  $14.5H$ . Castro et  
222 al. [23] estimate the friction velocity above the array to be  $u_* / U_e = 0.0891$ , i.e.  $0.178 \text{ m s}^{-1}$ .  
223 The roughness length,  $z_0$ , was determined by a fit of the data to the logarithmic wind profile  
224 using a von Kármán constant of  $\kappa = 0.39$  and a zero-plane displacement height derived from  
225 the LES (detail provided in Sect. 2.2.2). This resulted in a value of  $z_0 / H = 0.039$ .

226 Plume dispersion from a ground source was realised through the continuous release of  
227 a passive trace gas, for which a sufficiently diluted propane-air mixture was used to elimi-  
228 nate buoyancy effects. The source had an internal diameter of 20 mm (i.e. approx.  $0.29H$ )  
229 and was located in the middle of one of the long streets close to the centre of the model  
230 (Fig. 2c). The relatively large source diameter in combination with a very low flow rate  
231 of  $Q = 1.4 \text{ l min}^{-1}$  minimised momentum effects associated with the release through the  
232 source area and tests showed that residual effects are only non-negligible very close to the  
233 release location.

234 Point-wise concentration time-series were recorded using a Cambustion fast flame ion-  
235 isation detector (FFID), capable of measuring hydrocarbon concentration fluctuations at a  
236 frequency of 200 Hz. Velocity measurements were conducted with a two-component Dantec  
237 LDA system with a focal length of 160 mm providing a measuring volume with a diameter of  
238 0.074 mm and a length of 1.57 mm. The flow was seeded with micron-sized sugar particles  
239 at a sufficient level to attain flow sampling rates around 100 Hz. All data were acquired over  
240 a measurement duration of 2.5 min. The measurement sites analysed in this study are shown  
241 in Fig. 2c. Horizontal transects for the mapping of the plume footprint were conducted at  
242 nominal heights of  $z/H = 0.5$  and  $1.5$ , measuring concentrations and horizontal flow com-  
243 ponents. As discussed by Castro et al. [23], positional errors of the probes in the horizontal  
244 plane relative to the height of the buildings were corrected for in a post-processing step.  
245 In the data analysed here, the height range for individual measurement points was  $0.44H$   
246 to  $0.54H$  and  $1.44H$  to  $1.54H$ , respectively. Further uncertainties have to be expected with  
247 regard to the accuracy of the turntable orientation. Particularly for cases where the array is  
248 aligned with the approach flow, slight offsets can lead to strong differences in dispersion  
249 features as discussed by Fuka et al. [32]. Vertical profiles of paired velocity (all compo-  
250 nents) and concentration signals are available over a height range of  $z/H = 0.29$  to  $5$ . Scalar  
251 fluxes were measured using a laser Doppler anemometer (LDA), acquiring velocity signals,  
252 together with the concentrations signals measured by the FFID. For the vertical turbulent  
253 concentration fluxes,  $\overline{c'w'}$ , analysed here the FFID probe had a constant positional offset to  
254 the LDA measuring volume of  $+2 \text{ mm}$  in  $x$  direction ( $3\%$  of  $H$ ) and  $-5 \text{ mm}$  in  $y$  direction  
255 ( $7\%$  of  $H$ ). The implications of these spatial offsets obviously depend on local velocity and  
256 concentration gradients and will be discussed in the analysis of the data. Details of the flux-  
257 measurement set-up and associated uncertainties are described by Carpentieri et al. [19,20]  
258 for similar experiments conducted in another city geometry.

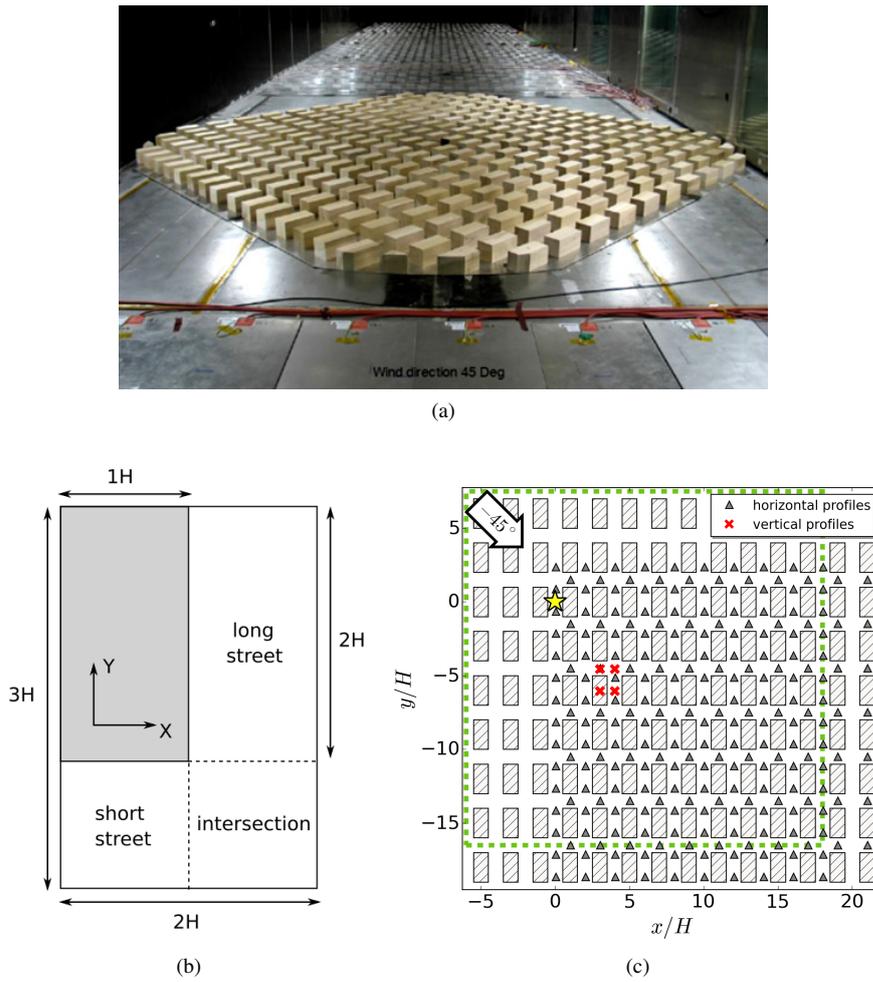


Fig. 2: (a) Upstream view of the DIPLOS array mounted in the Enflo wind tunnel for a model orientation of  $-45^\circ$ . Floor roughness elements and vorticity generators used to produce a thick approach-flow boundary-layer can be seen upstream of the array. (b) Plan-view of the repeating unit of the array, including the  $1H \times 2H$  building (grey shading), long and short streets and an intersection. (c) Plan-view of a cut-out of the DIPLOS wind-tunnel array. The ground source is located at  $x/H = y/H = 0$  (star symbol). Wind-tunnel measurement locations (triangles: horizontal profiles; crosses: vertical profiles) and the horizontal extent of the  $24H \times 24H$  LES computational domain (dashed square) are indicated. In (b) and (c) a coordinate system aligned with the streets is used (short streets along  $x$  direction; long streets along  $y$  direction).

### 2.2.2 Large-eddy simulation

LES of flow and scalar dispersion was carried out at the University of Southampton using the open-source CFD package OpenFOAM (v2.1) and a mixed time-scale eddy-viscosity subgrid model [47]. The DIPLOS test case was simulated in a computational domain of size  $24H \times 24H \times 12H$  using a uniform Cartesian grid with a resolution of  $\Delta = H/16$ .

As in the wind-tunnel experiment, passive, non-buoyant scalars were released continuously from a localised ground-source. The quasi-circular area source comprised 12 grid cells resulting in an effective source diameter of  $0.244H$ , which is comparable to the experimental set-up. No-slip conditions were imposed on all solid surfaces. With a stress-free boundary condition at the top of the domain and periodic boundary conditions in horizontal directions, the case was effectively realised as a planar channel flow. For the concentration fields, sponge layers were implemented at the outlet boundaries to prevent material from re-entering the domain through the inlet boundaries as part of the flow recycling process. Flow and concentration statistics were obtained over averaging periods of  $1000 T$ , where  $T = H/u_*$  is the eddy-turnover time and  $u_*$  is the friction velocity. The flow simulation was started from an initial field of resolution  $\Delta = H/16$ , which was interpolated from a fully-developed precursor simulation of reduced resolution ( $\Delta = H/8$ ). A spin-up time of  $100 T$  was allowed before starting the pollutant release. Concentration statistics were computed by ensemble-averaging the time-averaged statistics derived from four independent realisations of the dispersion scenario.

As documented by Castro et al. [23] and Fuka et al. [32], for the same computational set-up the flow and dispersion simulations in a smaller domain ( $12H \times 12H \times 12H$ ) were successfully validated against wind-tunnel measurements and data from direct numerical simulations (DNS) based on mean flow and turbulence statistics. Detailed descriptions of the flow simulations and the numerical techniques involved can be found in these publications. The friction velocity derived from the LES for the test case presented here (larger domain of  $24H \times 24H \times 12H$ ) had a value of  $u_* = 0.305 \text{ m s}^{-1}$ . This results in relations of  $u_*/U_{2H} = 0.131$  and  $u_*/U_e = 0.0828$ , where  $U_{2H} = 2.34 \text{ m s}^{-1}$  is the horizontal velocity magnitude at twice the building height and  $U_e = 3.69 \text{ m s}^{-1}$  the free-stream velocity at  $z/H = 12$ . The roughness length  $z_0/H = 0.076$  was determined from a fit of the logarithmic wind profile with a von Kármán constant of  $\kappa = 0.39$  and using a zero-plane displacement height  $d/H = 0.58$  that was computed before from the pressure and shear stress distributions on the walls using Jackson's [48] approach (see Castro et al. [23] for details). For the purpose of non-dimensionalising the results from the LES, we use  $H = 1 \text{ m}$ .

## 3 Dispersion models

The dispersion modelling approaches and set-ups of the specific models used in this study are described below. A summary is presented in Tab. 2. In all formulations below and in Sect. 4 and 5, a Cartesian coordinate system is used that is aligned with the streets of the DIPLOS array (see Fig. 2c), where  $x$ ,  $y$ ,  $z$  denote lateral and vertical directions. Time-averaged variables are written in upper case letters, i.e.  $c = C + c'$ , where  $C = \bar{c}$  is the time mean,  $c'$  the fluctuation about the mean and  $c$  the instantaneous value. Volume-averaged quantities are indicated by square brackets,  $[C]$ ; spatial averages over 2D facets/areas by angled brackets,  $\langle C \rangle$ .

### 3.1 Gaussian plume model

We use the Gaussian plume model formulation introduced by Hanna et al. [42] as a baseline urban dispersion model. Previous evaluations of this model against two field experiments showed a satisfactory performance in high-density, high-rise urban environments, for which *a priori* information on the initial lateral and vertical plume spread were provided to the model [39]. While there are certainly more sophisticated (operational) Gaussian dispersion models available (see Sect. 1.2), they share the same underlying modelling framework with Hanna et al.'s baseline model, which will therefore be the subject of interest in our model inter-comparison.

In the model formulation used on this study, the spatial distribution of the mean scalar concentration  $C$  originating from a continuous point-source release is given by the classic Gaussian plume equation with ground reflection at  $z = 0$  m

$$C(x, y, z) = \frac{Q}{2\pi U_p \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \times \left[ \exp\left(-\frac{(z-h_Q)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z+h_Q)^2}{2\sigma_z^2}\right) \right], \quad (1)$$

where  $U_p$  is a representative UCL wind speed,  $Q$  is the constant mass emission rate and  $h_Q$  the release height ( $h_Q = 0$  m in this study). The dispersion coefficients,  $\sigma_y$  and  $\sigma_z$ , are given by the classic Briggs [12] parametrisations for urban areas, including a modification of the lateral plume spread parameter,  $\sigma_y$ , for light-wind situations proposed by Hanna et al. [42]:

$$\sigma_y = \sigma_{y0} + \max(0.16, (A/U_p))x / (1.0 + 0.0004x)^{-\frac{1}{2}}, \quad (2)$$

$$\sigma_z = \sigma_{z0} + 0.14x / (1.0 + 0.0003x)^{-\frac{1}{2}}, \quad (3)$$

where  $A = 0.25$  m s<sup>-1</sup>. Hence, the modification in Eq. (2) comes into play when  $U_p$  is less than about 1.6 m s<sup>-1</sup>. The initial plume spread is set to  $\sigma_{y0} = \sigma_{z0} = H/3$ , which is lower than the value of  $H/2$  proposed by Hanna et al., but leads to more realistic results in terms of the initial upwind spread for the scenario investigated here, where the source is located in a street with strong flow channelling. It has to be noted that such *a priori* knowledge about the flow in the source street is usually not available when running dispersion models for emergency-response scenarios. As in the LES the spatial resolution was uniform in all direction with a grid spacing of  $\Delta = H/16$ .

The bulk travel speed of the plume within the canopy layer,  $U_p$ , was approximated by spatially averaging the horizontal flow from the LES over a depth of  $z = 0$  m to  $H$ , resulting in a canopy-layer advection velocity of  $U_c = 0.67$  m s<sup>-1</sup>. In actual operational dispersion modelling the cloud speed cannot usually be derived from such detailed, space-resolved information as was the case here. Instead, this quantity has to be approximated through parametrisations based on more accessible quantities. We note here that the value of  $U_c$  stated above is quite close to the value of 0.73 m s<sup>-1</sup> determined from the relationship  $U_c = u_* (2/\lambda_f)^{1/2}$  proposed by Bentham and Britter [7] where  $u_*$  is the LES friction velocity. Hanna and Britter [43] suggest the relation  $U_c = 0.45U_{2H}$  for typical built-up inner-city areas with  $\lambda_f > 0.3$  (as in our study), which results in a value of 1.05 m s<sup>-1</sup> based on  $U_{2H} = 2.34$  m s<sup>-1</sup> in the LES (Sect. 2.2.2).

Table 2: Overview of dispersion model set-ups used in this study.

Name	Type	Flow
GAUSS-1	Gaussian plume	LES mean UCL velocity; RSL plume deflection
GAUSS-2	Gaussian plume	LES mean UCL velocity; UCL plume deflection
QUIC (URB)	Lagrangian stochastic	QUIC-URB (diagnostic model)
QUIC (CFD)	Lagrangian stochastic	QUIC-CFD (prognostic model)
QUIC (LES)	Lagrangian stochastic	3D LES field (prognostic model)
UoR-SNM	street network	LES velocities
SIRANE-1	street network	parametrisations
SIRANE-2	street network	LES velocities

337 To add some degree of building-awareness, the average horizontal plume deflection was  
338 taken into account. Two deflections from the  $-45^\circ$  forcing direction were considered: (1)  
339 based on the average horizontal wind direction of  $-54^\circ$  determined from the LES over a  
340 depth of  $1 \leq z/H \leq 2$ , covering the roughness sublayer (RSL) and (2) based on the LES  
341 UCL-averaged horizontal wind direction of  $-78^\circ$ . While the former is a quantity that could  
342 be approximated through measurements in an emergency, e.g. from tower or roof-level mea-  
343 surements, the latter is usually not easily obtainable from sparse *in-situ* measurements within  
344 the canopy layer. Initial tests of the model have shown a high sensitivity of the results to the  
345 plume-turning parameter in comparison to the plume orientation observed on the LES and  
346 the wind tunnel.

### 347 3.2 Lagrangian dispersion model

348 We use the Quick Urban & Industrial Complex (QUIC) dispersion modelling system (v6.2  
349 and v6.29) developed by LANL and the University of Utah [53]. The core of the system  
350 is the Lagrangian model QUIC-PLUME that introduces additional terms to the classic  
351 Langevin random-walk equations in order to account for urban dispersive effects arising  
352 from spatial inhomogeneities of UCL turbulence and particle reflections on surfaces. A de-  
353 tailed description of the model components is presented by Williams et al. [81].

354 In this study, QUIC-PLUME is run on 3D wind fields from two system-integrated flow  
355 models. (i) the building-aware mass-consistent wind solver QUIC-URB that is based on  
356 the empirical-diagnostic modelling strategy developed by Roeckle [59] and expanded upon  
357 by Brown et al. [17]. QUIC-URB computes mean wind fields around buildings by using  
358 empirical relationships to produce backflow in low pressure zones (e.g. street canyons) in  
359 combination with a mass consistency constraint which results in flow recirculation in the  
360 regions of interest [55]. (ii) QUIC-CFD that is based on the RANS equations in combina-  
361 tion with a zeroth-order turbulence model using a mixing-length approach [37]. In order to  
362 disentangle the performance of the dispersion model from the accuracy of the wind models,  
363 in the final variant (3), QUIC-PLUME is driven directly by the mean 3D LES reference  
364 wind field.

365 In both QUIC-URB and QUIC-CFD a logarithmic wind profile for neutral stratification  
366 is prescribed at the inflow edges based on the LES roughness parameters and  $H$  was set to

367 16 m. The reference wind speed  $U_{ref}$  was  $4 \text{ m s}^{-1}$  in a height of  $z_{ref} = 4.5H$ . In agreement  
 368 with the LES, a uniform grid resolution of  $\Delta = H/16$  was used. In order to ensure a fully  
 369 converged wind environment upstream of the source, the DIPLOS array set-up was realised  
 370 in a slightly larger domain of  $28H \times 27H \times 12H$ . QUIC-URB was run with the recom-  
 371 mended settings [53], including a modified wake-zone model [52]. For QUIC-CFD, model  
 372 parameters like the time step or the maximum allowable mixing length were automatically  
 373 generated by the system based on the specified geometry, cell size and wind speed.

374 With  $\Delta_x = \Delta_y = H/8$  and  $\Delta_z = H/16$  the collecting boxes for the particles were slightly  
 375 larger than the flow grid cells in order to reduce the statistical noise of the output. As in the  
 376 LES, computational particles with passive-tracer characteristics were released continuously  
 377 through a circular area ground source with a diameter of  $0.244H$ . In each run, 612,000  
 378 particles were released over a duration of 30 min. The model time step was set to 0.1 s.

### 379 3.3 Street-network dispersion models

380 The street-network dispersion modelling approach is based on the balance equation for the  
 381 volume-averaged scalar concentration  $[C]_V$  within a street or intersection box of volume  $V$   
 382 in the UCL

$$\frac{d[C]_V}{dt} + \frac{1}{V} \sum_{k=1}^K \Phi^k = [Q]_V, \quad (4)$$

383 where  $[Q]_V$  is the volume-source term and  $\Phi^k$  is the total scalar flux through the  $k$ th facet  
 384 of the box [67,38,6]. The total scalar flux  $\Phi^k$  can be partitioned into an advective and  
 385 a turbulent component. The horizontal exchange between street and intersection boxes is  
 386 assumed to be mainly *advective* and the associated scalar flux is

$$\Phi_{adv}^k = CU_i A^k \equiv [C]_V U_i^k A^k, \quad (5)$$

387 where  $U_i^k$  ( $i = 1, 2$ ) is the horizontal advection velocity aligned with the street, with which  
 388 material is transported through facet  $k$  of area  $A^k$ . The inherent assumption of this approach  
 389 is that the material is well-mixed within each street or intersection box, i.e. spatial concen-  
 390 tration fluctuations are small compared to the spatial mean.

391 On the other hand, the vertical exchange between the UCL and the external flow above  
 392 the buildings is assumed to be mainly *turbulent* and can be approximated by an exchange  
 393 velocity approach

$$\Phi_{turb}^{top} = \overline{c'w'} A^{top} \equiv ([C]_V - [C]_{ext}) E A^{top}, \quad (6)$$

394 where  $E$  is the vertical turbulent exchange velocity through the top facet of the box that  
 395 has an area of  $A^{top}$  [71]. The direction of exchange is determined by the difference between  
 396 the UCL and external concentrations,  $[C]_V - [C]_{ext}$ . Figure 3a schematically illustrates the  
 397 flux balance for a street box. Dispersion above the canopy, where the street-network concept  
 398 breaks down, has to be modelled by a different approach, e.g. using a Gaussian plume model.

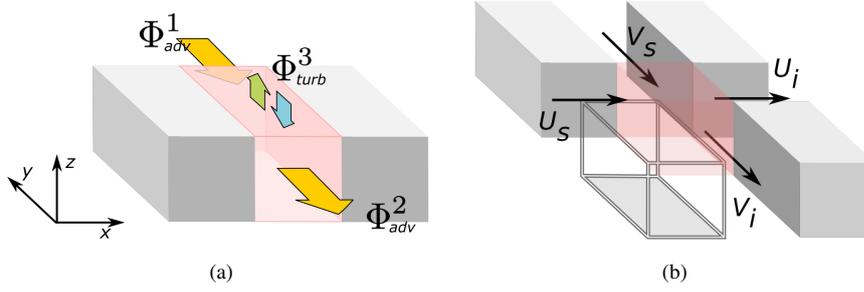


Fig. 3: (a) Flux balance for a street box: Material is transported into the box through facet 1 ( $\Phi_{adv}^1$ ) and out of the box through facet 2 ( $\Phi_{adv}^2$ ). Through the top facet, the box can gain or lose material through turbulent exchange with the external field ( $\Phi_{turb}^3$ ). (b) Horizontal advection velocities defined in the UoR street-network model (UoR-SNM). The index ‘s’ denotes flow coming out of a street, the index ‘i’ is for flow coming out of an intersection.

### 399 3.3.1 UoR-SNM

400 For a general demonstration of the street-network modelling approach, we use the Univer-  
 401 sity of Reading Street-Network Model (UoR-SNM) introduced by [6], where a detailed  
 402 derivation of the model formulation is presented. This model was previously tested against  
 403 DNS dispersion data in a cube-array environment [35,36].

404 In contrast to the fully operational street-network model SIRANE, UoR-SNM does not  
 405 include built-in flow parametrisations. Instead, we use a hybrid approach by deriving from  
 406 an external flow simulation the velocity parameters,  $U_i^k$  and  $E$ , required by the model  
 407 to compute the horizontal and vertical concentration fluxes based on Eqs. (5) and (6). In this  
 408 study, we use the LES data for this purpose. Hence, the main aim of including UoR-SNM  
 409 in the inter-comparison study is to demonstrate the viability of the approach and to highlight  
 410 its strengths and limitations with regard to the representation of dispersion processes.

411 Horizontal advection velocities,  $U_i^k$ , used in Eq. (5) were obtained from the LES in terms  
 412 of facet-averages of the time-mean velocity components along  $x$  and  $y$  streets as shown in  
 413 Fig. 3b. In order to account for upwind transport of scalars, a diffusive transport component  
 414 was added in the UCL together with an additional transport term into sheltered regions (here  
 415 into  $x$  streets) following Hamlyn et al. [38]. The vertical turbulent exchange velocity used in  
 416 Eq. (6) at the top of the canopy layer ( $z/H = 1$ ) was derived from the LES according to

$$E = \frac{\langle c'w' \rangle_{z/H=1}}{[C]_{ucl} - [C]_{ext}} \quad (7)$$

417 where  $[C]_{ucl}$  are LES concentrations averaged over street and intersection volumes within  
 418 the UCL ( $0 \leq z/H \leq 1$ ) and  $[C]_{ext}$  box-averaged concentrations in the external flow over a  
 419 depth of  $1 \leq z/H \leq 2$  [5]. Exchange velocities were computed for  $x$  streets ( $E_x$ ),  $y$  streets  
 420 ( $E_y$ ) and intersections ( $E_i$ ) individually. Dispersion above the canopy was modelled in UoR-  
 421 SNM by a simple advection-diffusion approach using the same box discretisation as in the  
 422 UCL and mean horizontal transport velocities derived from the LES.

### 423 3.3.2 SIRANE

424 The second street-network model is the fully operational model SIRANE [71–73]. Previous  
 425 validation studies using *in-situ* field measurements in Lyon [70] and wind-tunnel experi-  
 426 ments in a model of a part of central London [21] documented the suitability of SIRANE  
 427 for fast and reliable urban dispersion simulations.

428 Unlike UoR-SNM, SIRANE is equipped with a suite of parametrisations to compute  
 429 all necessary flow parameters and only requires the specification of the external wind speed,  
 430 direction and atmospheric stability. A horizontally homogeneous boundary-layer flow above  
 431 the canopy is modelled using Monin-Obukhov similarity theory, where we specified the  
 432 roughness length, displacement height and friction velocity for the DIPLOS geometry based  
 433 on the LES results (see Sect. 2.2.2). The uniform building height was set to  $H = 10$  m.  
 434 Dispersion in the external flow is computed by a Gaussian plume model [71].

435 In SIRANE the vertical exchange velocity is linked to the standard deviation of the  
 436 vertical velocity component,  $\sigma_w$ , through

$$E = \frac{\sigma_w}{\sqrt{2\pi}} \quad (8)$$

437 and  $\sigma_w$  is parametrised for different stability ranges via  $u_*$ . Another difference between  
 438 UoR-SNM and SIRANE is the treatment of dispersion through intersections. In the former,  
 439 the intersection is assumed to be well-mixed and fluxes out of the intersection into downwind  
 440 streets are parametrised through the advection velocities  $U_i$  and  $V_i$  (Fig. 3b). In SIRANE,  
 441 mixing in the intersection and the 2D branching of material is determined by the external  
 442 flow using a model for the volume-flux conservation. This approach takes into account the  
 443 local geometry, the external wind direction and the standard deviation of its fluctuations [68,  
 444 71]. Imbalances are overcome by vertical exchange with the external flow.

445 We ran SIRANE in two modes: (1) with the default flow parametrisations described  
 446 above; (2) with the LES flow information provided as in the case of UoR-SNM. Since  
 447 SIRANE treats intersections purely as nodal points connecting adjacent streets, only the  
 448 vertical exchange velocities in the  $x$  and  $y$  streets need to be parametrised together with the  
 449 horizontal advection velocities along each street,  $U_s$  and  $V_s$ . In order to adjust the external  
 450 flow field to the reference conditions, in both cases the average horizontal wind direction in  
 451 the LES over  $1 \leq z/H \leq 2$  ( $-54^\circ$ ) was prescribed as the forcing direction.

## 452 4 Flow and dispersion characteristics

453 In the following all flow and concentration quantities are presented in a non-dimensional  
 454 framework. Non-dimensional concentrations,  $C^*$ , and concentration fluxes,  $\overline{c'u_i'}$ , are com-  
 455 puted as

$$C^* = \frac{CU_{ref}H^2}{Q} \quad (9)$$

456 and

$$\overline{c'u_i'^*} = \frac{\overline{c'u_i'}H^2}{Q}, \quad (10)$$

457 where  $Q$  is the constant mass emission rate and  $U_{ref}$  is the mean streamwise reference ve-  
 458 locity defined in the approach-flow coordinate system in a height of  $4.5H$ .

## 459 4.1 Flow behaviour

460 The quality of dispersion predictions to a large degree depends on whether the underlying  
461 flow as the main physical driver of advection and mixing processes is adequately repre-  
462 sented. Both SIRANE and the QUIC modelling suite are complete operational systems that  
463 include means of calculating all necessary flow information in the UCL and the external  
464 boundary layer that is required by the dispersion modules. In order to understand the con-  
465 centration output it is therefore crucial to also appraise the adequacy of the flow modelling.

466 QUIC-PLUME requires the most detailed flow information in terms of a full 3D repre-  
467 sentation of the mean flow. Previously, [54] evaluated the performance of QUIC-URB and  
468 QUIC-CFD against wind data measured during the Joint Urban 2003 field campaign in Ok-  
469 lahoma City and found that both wind models performed similarly well. When tested in an  
470 idealised cube-array geometry, which is closer to the DIPLOS set-up regarding the degree  
471 of geometrical abstraction, [65] found that building-induced flow features in QUIC-URB  
472 compared well with wind-tunnel data.

473 Figure 4 shows wind vectors and vertical mean velocities of the LES and the two QUIC  
474 wind models for the DIPLOS case. For  $-45^\circ$  and other model orientations, Castro et al. [23]  
475 previously validated the LES flow against the wind-tunnel measurements and found that the  
476 salient features of the complex UCL flow patterns agree as well as can be expected with the  
477 experiment given the uncertainties described in Sect. 2.2.1.

478 The data is shown in a horizontal plane at  $z/H = 0.5$  in terms of an ensemble-average  
479 over the time-averaged flow in all repeating units of the domain (Fig. 2b). Doubling the  
480 length of one building side introduced a geometrical asymmetry for which the resulting  
481 flow patterns deviate strongly from the corresponding cube-array case with its symmetric  
482 corner vortices and flow convergence in intersections (e.g. Fig. 4 in Coceal et al. [26]).

483 The LES shows a fully developed channelling region along the  $y$  street through the in-  
484 tersection, cutting off most of the outflow from the  $x$  street, where a strong recirculation  
485 pattern is established. This is also reflected in the histogram of LES mean horizontal wind  
486 directions,  $\theta$ , over the entire UCL (Fig. 5), which reveals a strong peak at  $-90^\circ$  (flow in  
487  $-y$  direction) and only a small plateau between  $0^\circ$  and  $90^\circ$ . The intersection shows a highly  
488 three-dimensional flow structure. Alternating regions of up-drafts and down-drafts in both  
489 streets indicate recirculation patterns in the vertical plane. In combination with the observed  
490 along-street channelling this results in a helical recirculation [29] along the  $y$ -street canyon,  
491 which extends well into the intersection. Channelling in the long streets was also observed  
492 in the MUST geometry at a similar inflow angle [28], but the larger street width resulted  
493 in weaker flow deflection and also in less well-established flow recirculation in the short  
494 street. Unlike the LES, the histograms of both QUIC wind models show peaks at the forc-  
495 ing direction of  $-45^\circ$  (Fig. 5). In the case of QUIC-CFD, this is mainly due to the flow  
496 behaviour in the intersections and the flow entering the long streets, which has a stronger  
497  $u$ -component compared to the LES. The general patterns of updraft regions protruding from  
498 the leeward building sides well into the intersection and downdraft regions on the wind-  
499 ward sides are very similar in the LES and QUIC-CFD. In contrast to that, in QUIC-URB  
500 the helical flow does not extend into the intersection but is confined to the long street. In  
501 both QUIC flow models, the recirculation zone in the short street is much larger and less  
502 confined compared to the LES. Here, QUIC-URB shows a strong flow reversal into  $-x$  di-  
503 rection (peak at  $\pm 180^\circ$  in Fig. 5) and also predicts a stronger negative  $u$ -component in the  
504  $y$ -street compared to the two prognostic flow simulations (peak at about  $-110^\circ$ ). Whereas  
505 in the LES and QUIC-CFD, the flow pattern in the intersection is determined by the chan-  
506 nelling in the long street, in QUIC-URB the outflow from the long streets is entering the

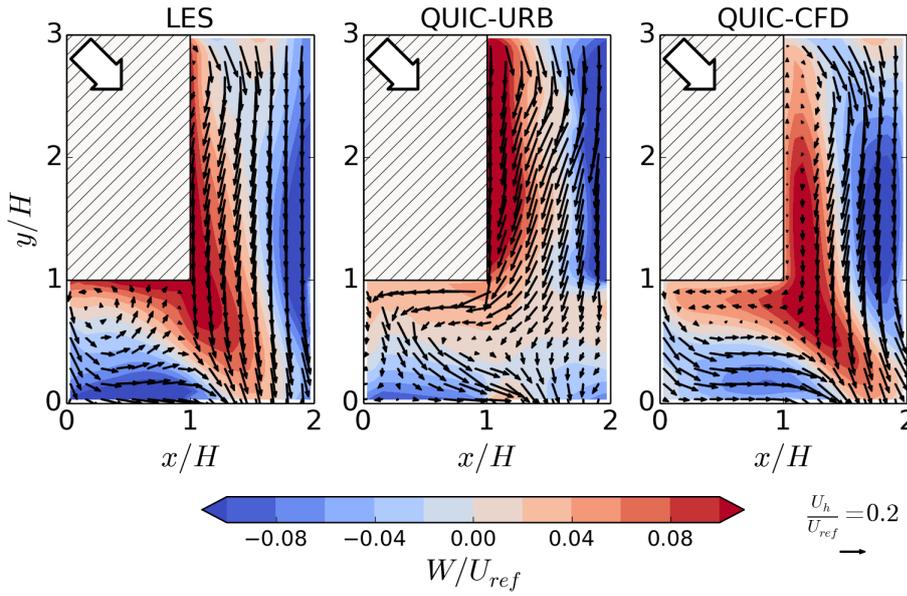


Fig. 4: Horizontal cross-sections at  $z/H = 0.5$  showing mean horizontal velocity vectors and vertical velocities of the LES (left), QUIC-URB (centre) and QUIC-CFD (right). The data represent ensemble averages over all repeating units of the array (see Fig. 2b). The length of the vectors scales with the mean wind speed  $U_h = \sqrt{U^2 + V^2}$ . Note that only every fourth vector is shown. Large arrows indicate the forcing wind direction.

507 upwind short street and the intersection flow largely reflects the recirculating flow pattern.  
 508 These differences are expected to have an influence on the topological dispersion behaviour  
 509 through the street network.

#### 510 4.1.1 Horizontal advection velocities

511 Mean horizontal advection velocities as defined in Fig. 3b were computed from the LES in  
 512 terms of facet-averaged mean velocities at the four interfaces between street and intersection  
 513 boxes. This resulted in values of  $\langle U_i \rangle = 0.22 \text{ m s}^{-1}$  and  $\langle V_i \rangle = -0.71 \text{ m s}^{-1}$  for flow out of  
 514 the intersection into the downwind  $x$  and  $y$  streets, respectively, and  $\langle U_s \rangle = 0.23 \text{ m s}^{-1}$  and  
 515  $\langle V_s \rangle = -0.77 \text{ m s}^{-1}$  for flow from the streets into the intersections (for  $U_{ref}$  of  $3 \text{ m s}^{-1}$  at  
 516  $z_{ref} = 4.5H$ ). As a result of the flow channelling along the  $y$  streets (Fig. 4), the magnitudes  
 517 of advection velocities along the  $y$ -axis,  $\langle V \rangle$ , exceed those along the  $x$ -axis,  $\langle U \rangle$ , by more  
 518 than a factor of 3. Similar ratios are observed in the experiment, with the important caveat  
 519 that here we compare point values measured at the interfaces in heights of  $z/H = 0.5$  and not  
 520 averages over the entire facets from the ground to roof level. Based on the same reference  
 521 velocity as in the LES, from the wind-tunnel flow measurements we obtain:  $U_i = 0.21 \text{ m s}^{-1}$ ,  
 522  $V_i = -0.51 \text{ m s}^{-1}$ ,  $U_s = 0.18 \text{ m s}^{-1}$  and  $V_s = -0.58 \text{ m s}^{-1}$ . Note that here we used flow data  
 523 measured on a much denser grid in a small region of the array compared to the relatively  
 524 coarse mapping grid shown in Fig. 2c.

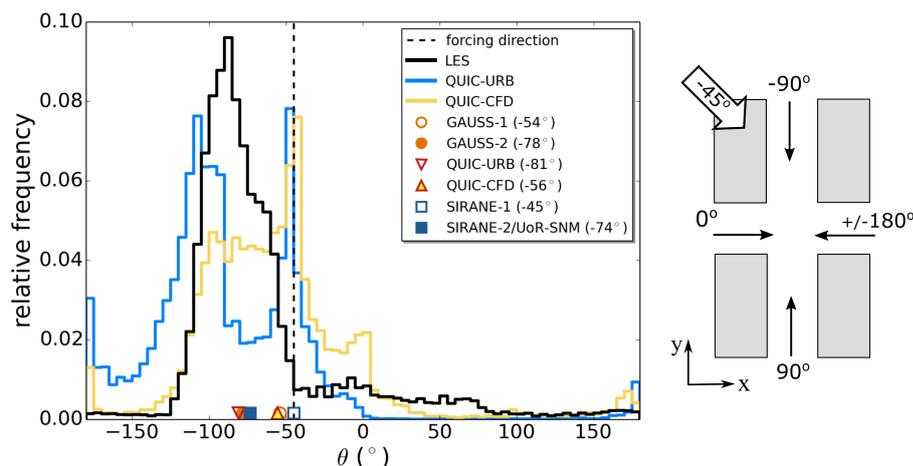


Fig. 5: Histograms of horizontal wind directions,  $\theta$ , in the UCL ( $0 \leq z/H \leq 1$ ) derived from LES, QUIC-URB and QUIC-CFD mean flow fields at a forcing wind direction of  $-45^\circ$ . A wind direction of  $-90^\circ$  represents flow into negative  $y$  direction;  $0^\circ$  flow into positive  $x$  direction as indicated in the schematic on the right. The plume directions for the Gaussian model runs are shown together with the canopy-layer plume direction derived from the bulk horizontal advection velocities in the Lagrangian and street-network models (see Tab. 3).

525 Table 3 contrasts these results with the advection velocities modelled in SIRANE-1  
 526 and the equivalents from both QUIC wind models. Unlike the LES, the parametrisation in  
 527 SIRANE-1 produces the same velocity magnitudes for  $\langle U_s \rangle$  and  $\langle V_s \rangle$ . As a result, the dis-  
 528 persion module will be unaware of the strong change in flow direction within the canopy  
 529 layer and resulting pollutant channelling effects. The transport velocity along the short  $x$   
 530 street is significantly over-predicted compared to the LES, yet a much better agreement is  
 531 found for  $\langle V_s \rangle$  along the longer  $y$  streets. Currently the SIRANE velocity model formulation  
 532 does not take into account effects of the street length, but instead assumes a fully developed  
 533 flow as through an ‘infinite’ street. The shorter the street, the less applicable this assumption  
 534 becomes. However, a mere factor-of-2 increase of the  $y$ -street lengths compared to the  $x$   
 535 streets in the DIPLOS array already resulted in a good agreement with the LES. The ad-  
 536 vection velocities derived from the QUIC wind models support the previous assessments.  
 537 In QUIC-CFD the channelling in  $y$  direction and through large parts of the intersections  
 538 resulted in an exceedance of magnitudes of  $\langle V \rangle$  compared to  $\langle U \rangle$  by about a factor of 1.4,  
 539 which is less than half of the factor in the LES and also much lower compared to the ex-  
 540 periment. For QUIC-URB, on the other hand, there is more than a factor of 6 difference  
 541 between the outflow from the long and the short streets, i.e. twice the factor seen in the LES.  
 542 Here, the low value of  $\langle U_s \rangle$  results from the flow reversal along the facet triggered by the  
 543 recirculation regime;  $\langle U_i \rangle$  is similarly small as there is less outflow from the intersection  
 544 into the downwind short street compared to the LES and QUIC-CFD. The different flow ori-  
 545 entations based on the advection velocities listed in Tab. 3 are summarised in Fig. 5 together  
 546 with the prescribed values for the two Gaussian model runs.

Table 3: Horizontal advection velocities and vertical turbulent exchange velocities derived from the LES together with modelled parameters from SIRANE-1. Velocity parameters derived from the LES are used in UoR-SNM and SIRANE-2. Corresponding advection velocities from both QUIC wind models are included for comparison. All velocities have units of  $\text{m s}^{-1}$  and correspond to a reference velocity  $U_{ref}$  of  $3 \text{ m s}^{-1}$  at  $z_{ref} = 4.5H$ .

Model	$\langle U_s \rangle$	$\langle V_s \rangle$	$\langle U_i \rangle$	$\langle V_i \rangle$	$E_x$	$E_y$	$E_i$
LES	0.23	-0.77	0.22	-0.71	0.10	0.15	0.12
SIRANE-1	0.84	-0.84	—	—	0.09	0.09	—
QUIC-URB	0.10	-0.63	0.12	-0.68	—	—	—
QUIC-CFD	0.42	-0.61	0.40	-0.55	—	—	—

## 547 4.2 Dispersion behaviour

548 Before discussing the results of the model inter-comparison study in Sect. 5, in the following  
549 paragraphs some general features of the dispersion scenario are presented based on the LES  
550 and wind-tunnel data.

### 551 4.2.1 Plume characteristics

552 Figure 6 shows the 3D LES plume in terms of a concentration iso-surface at  $C^* = 0.01$ . The  
553 overall plume shape is strongly non-Gaussian and the material is distributed asymmetrically  
554 about the forcing wind direction of  $-45^\circ$ . Vertically the plume extends up to approximately  
555  $z/H = 5$  in the region covered by the simulation. The plume shape implies that within the  
556 building array, material is transported along the  $y$  direction downwind of the source, where  
557 there is significant detrainment of material out of the UCL. Above the array pollutant path-  
558 ways adjust to the forcing wind direction. Differences in concentration distributions within  
559 and above the UCL are further illustrated in Fig. 7, showing LES mean concentrations in the  
560  $(x, y)$  plane together with corresponding point-wise wind-tunnel measurements at  $z/H = 0.5$   
561 and 1.5. The agreement between LES and experiment regarding the shape of the plume  
562 footprints and the local concentration levels is satisfactory. The extent of the plumes in  $+x$   
563 direction agrees very well, also with regard to the level of upwind spread of material from  
564 the source street. Both LES and experiment show strong channelling of the plume down the  
565 source street, which overall leads to an asymmetric plume footprint. Some differences in  
566 the plume shapes and concentration levels farther away from the source can be determined.  
567 Some of these could be attributable to positional uncertainties of the wind-tunnel data in any  
568 horizontal plane as discussed in Sect. 2.2.1, which can be as large as  $0.06H$  in the vertical.  
569 However, there seems to be a slight systematic difference in the orientation of the plumes in  
570 the UCL, which becomes more effective further downwind of the source. Here we note that  
571 the lowest two rows of measurements (around  $y/H = -15$ ) were taken only one block away  
572 from the edge of the model (see Fig. 2a) and there is an increase in uncertainties attached  
573 to the concentration measured far downwind of the source. For further discussions of the  
574 general comparison between experiment and LES see Fuka et al. [32].

575 The LES plume centreline in the canopy, here defined as the line of maximum concen-  
576 tration downwind of the source, proceeds along the  $y$  axis ( $x/H = 0$ ) and thus is offset by  
577  $45^\circ$  to the external flow as a result of the flow channelling in the long streets. The near-field  
578 behaviour of the plume is similar to the MUST case reported by Dejoan et al. [28] for a sim-  
579 ilar scenario. However, due to the narrower streets in the DIPLOS array, channelling effects

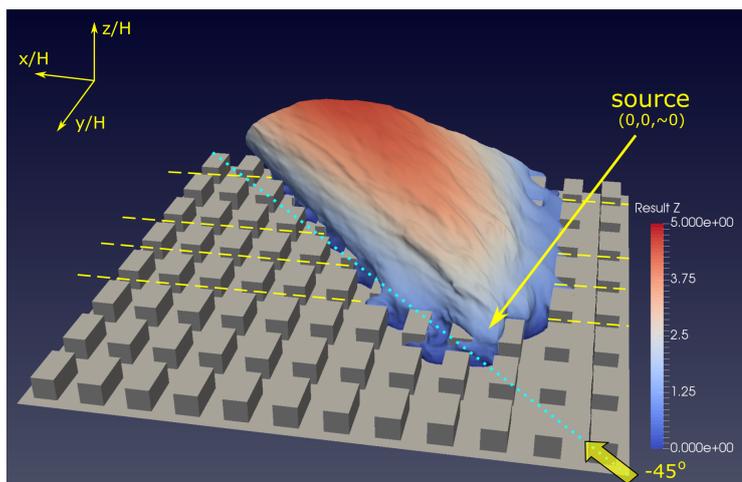


Fig. 6:  $C^* = 0.01$  iso-surface of the LES plume looking into downwind direction. Colour contours on the plume indicate the height above ground,  $z/H$ . The position of the ground source and the forcing wind direction are indicated (large arrow; dotted line along  $-45^\circ$ ). Dashed lines show the locations of the  $(x, z)$  cross sections discussed in Fig. 8.

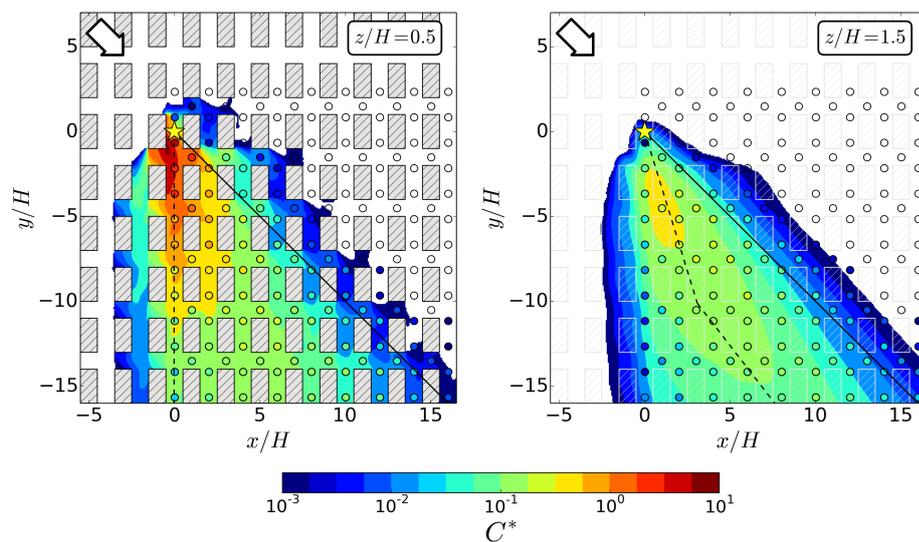


Fig. 7: Mean concentrations in the horizontal plane at  $z/H = 0.5$  (left) and  $z/H = 1.5$  (right). Contours represent the LES data and circles the point-wise wind-tunnel measurements. Empty circles for the wind tunnel show measurement sites where the  $C^*$  was less than  $10^{-3}$  and the experimental data can be subject to large uncertainties. Solid black lines show the forcing wind direction; dashed black lines indicate the approximated LES plume direction based on the maximum mean concentration in the horizontal plane. In this and all following figures, arrows indicate the forcing direction and stars the source location.

580 are much stronger and comparable to observations in other idealised street networks [33]  
 581 or realistic urban centres [82]. As the flow above the canopy re-adjusts back to the forcing  
 582 direction, the offset of the plume centreline decreases. This is particularly the case in the  
 583 downwind regions of the plume, where less material is detrained from the canopy (Fig. 7).  
 584 A similar shift can also be seen in the wind-tunnel data.

#### 585 4.2.2 Vertical exchange

586 The vertical transport of pollutants out of and back into the canopy layer plays a defining  
 587 role in the dispersion scenario investigated here. Concentration distributions and turbulent  
 588 exchange characteristics in the vertical  $(x, z)$  plane are shown in Fig. 8 for four fixed  $y/H$   
 589 positions downstream of the source as indicated in Fig. 6. While in the UCL the concentration  
 590 maxima are located at  $x/H = 0$  over the entire  $y$  extent of the plume, above the buildings the  
 591 plume is advected into  $+x$  direction with the re-adjusting flow. Due to the higher velocities  
 592 here, the material is transported much faster horizontally than in the canopy layer. Already  
 593 at a distance from the source of  $4.5H$  in  $-y$  direction, a significant part of the plume is  
 594 located outside of the UCL. The corresponding fields of the vertical turbulent momentum  
 595 flux,  $\overline{c'w'^*}$ , show that the detrainment of material out of the UCL is strongest close to the  
 596 source as seen in the slices at  $y/H = -1.5$  and  $-4.5$ , while in the far-field of the plume the  
 597 exchange is directed back into the canopy and is strongest in the shear layer just above roof-  
 598 level ( $y/H = -13.5$ ). The cross section at  $y/H = -7.5$  indicates an intermediate regime.  
 599 This agrees with previous findings by Carpentieri et al. [19] and Goulart et al. [36].

600 Following Eq. (7) the vertical exchange velocity is defined at the top of each network-  
 601 model box in the UCL. Figure 9a shows a map of  $\langle \overline{c'w'^*} \rangle_{z/H=1}$  as derived from the LES by  
 602 facet-averaging the high-resolution concentration flux output at the top of each street and  
 603 intersection box. In the horizontal plane, distinct regions of detrainment and re-entrainment  
 604 are evident. In the near-field of the source and along the plume centreline at  $x/H = 0$   
 605 on average the vertical turbulent concentration flux is directed out of the canopy layer at  
 606 roof-level ( $\langle \overline{w'c'^*} \rangle_{z/H=1} > 0$ ). Transport of pollutants back into the street system is domi-  
 607 nant away from the plume centreline in lateral  $+x$  direction. The regions of re-entrainment  
 608 ( $\langle \overline{w'c'^*} \rangle_{z/H=1} < 0$ ) coincide with regions where  $[C^*]_{ucl} - [C^*]_{ext} < 0$  (not shown), i.e. where  
 609 concentrations are higher in the external layer than in the canopy. This positive vertical con-  
 610 centration gradient is a result of the advection of material above the array that was detrained  
 611 from streets along the plume centreline (see Figs. 6 and 8).

612 The spatial extent of the detrainment and re-entrainment regions respectively reflect  
 613 the footprints of the main parts of the plume within and above the canopy. Figure 9a im-  
 614 plies that surface concentrations are not exclusively governed by processes in the street  
 615 network, but in certain circumstances can be controlled, locally, by the dispersion above  
 616 the canopy. This is particularly important at some intermediate distance from the source,  
 617 where tests with UoR-SNM for this case suggest that re-entrainment can increase street-  
 618 level concentrations by a factor greater than 10. In both street-network models, the vertical  
 619 transfer is parametrised assuming a linear relationship between the local turbulent vertical  
 620 scalar flux (facet-averaged) and the vertical concentration gradient (volume-averaged), with  
 621 the exchange velocity  $E$  determining the slope. The LES data for this test case supports this  
 622 assumption and we find a strong positive correlation between these quantities. We also find  
 623 that differences between the exchange velocities associated with upward (detrainment) and  
 624 downward (re-entrainment) motions are comparable to variations in exchange efficiency for  
 625 different street types. We note that the two network models used here differ in their treat-  
 626 ment of dispersion above the canopy. In SIRANE above-roof dispersion is implemented as

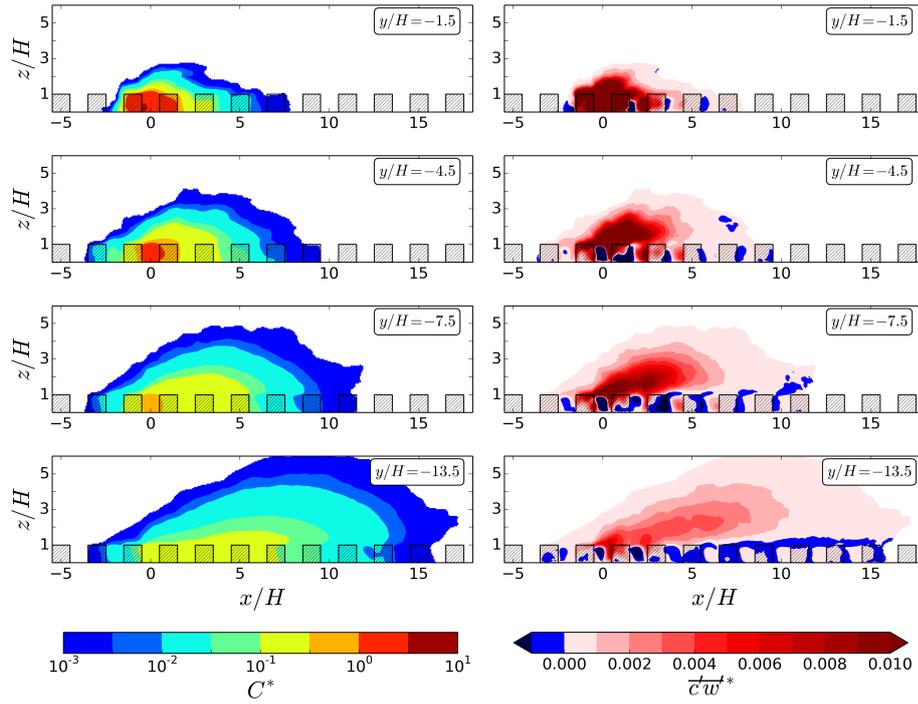


Fig. 8: Vertical ( $x, z$ ) cross sections of mean scalar concentrations (*left*) and vertical turbulent concentration fluxes (*right*) at four  $y/H$  locations downwind of the source as indicated in Fig. 6. The source is located at  $x/H = 0$ .

627 a series of point sources giving rise to Gaussian plumes that are then superimposed [71]. In  
 628 UoR-SNM mean and turbulent horizontal fluxes are separately parametrised using advection  
 629 velocities and diffusion coefficients in the discretised advection-diffusion equation [36].

630 Figure 9b compares height profiles of the LES and wind tunnel vertical concentration  
 631 flux taken in a region of the plume where there is a transition between predominantly upward  
 632 or downward-oriented turbulent transport (sites indicated in Fig. 9a). In both data sets, in  
 633 the  $x$  street (P1) and the intersection (P2) scalar fluxes are positive over all heights, while  
 634 in the centre of the  $y$  street (P3) the exchange around roof-level and below is negative.  
 635 The quantitative agreement between LES and experiment around roof-level is very good.  
 636 However, there is approximately a factor of two difference in the peak values observed at  
 637 about  $z/H \simeq 1.6$ . Larger differences can also be observed at site P2 below roof-level, where  
 638 the LES and experiment show opposite trends. Several reasons can explain these differences.  
 639 The sites are located in a region of large spatial concentration gradients as can be seen in the  
 640  $y/H = -4.5$  cross section in Fig. 8, which coincides with sites P1 and P2. The limited (but  
 641 comparable) averaging times in the simulation and the experiment will cause much higher  
 642 levels of uncertainty this close to the source and towards the plume edge, especially in the  
 643 fluxes, where spatial concentration gradients are large and temporal signal intermittency  
 644 is high compared to more well-mixed plume regions. Further uncertainties are introduced  
 645 by the inevitable spatial offset between the LDA and FFID (constant downwind shift) as  
 646 discussed in Sect.2.2.1. Further aspects are the slight difference in the plume orientation

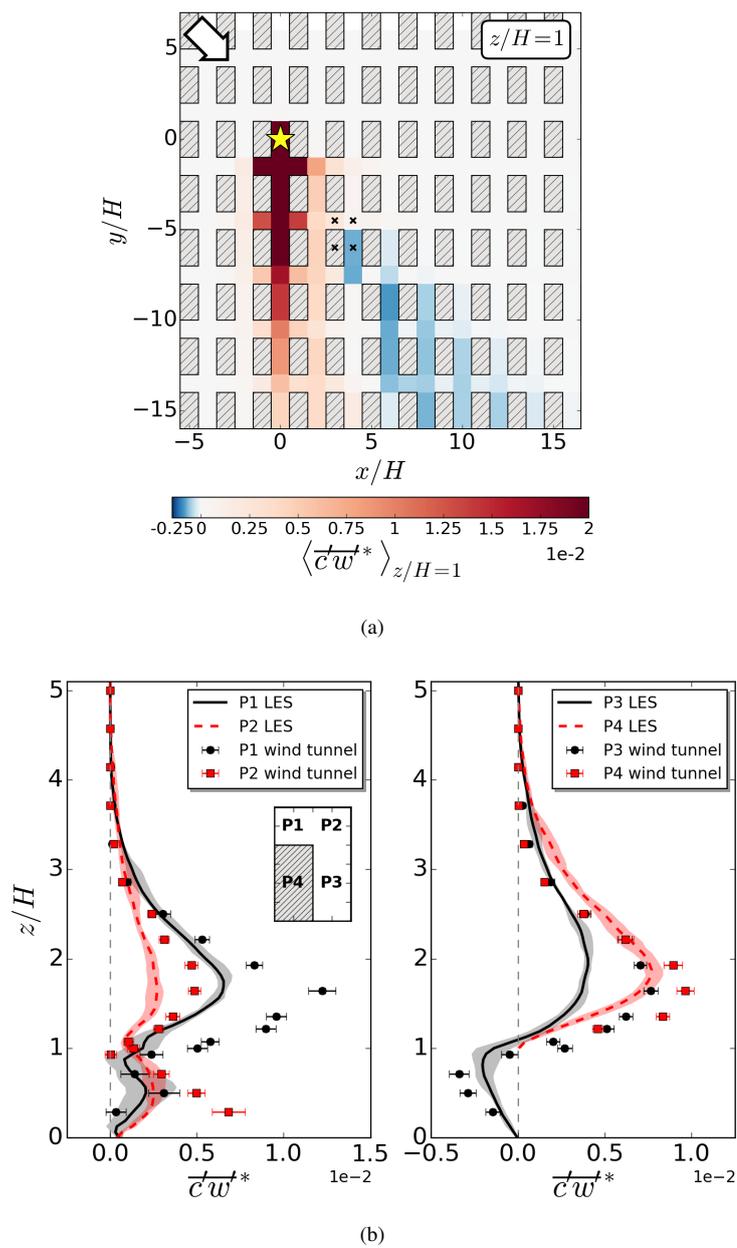


Fig. 9: (a) Facet-averaged vertical turbulent concentration flux at  $z/H = 1$ . Crosses indicate the locations of vertical profiles measured in the wind-tunnel experiment. (b) Comparison of experimental and LES height profiles of the vertical turbulent concentration flux. Lines for the LES data represent ensemble averages and the shaded areas indicate the corresponding value range among the four ensemble members.

647 in the LES and the experiment and the effects of the difference of the inflow boundary  
 648 conditions in the wind tunnel (constant-direction boundary layer profile) as opposed to the  
 649 fully developed periodic boundary conditions in the LES.

650 As discussed above, the patterns seen in Fig. 9a support the gradient-approach taken to  
 651 derive the vertical exchange velocities for the UoR-SNM network model (Eq. 7). Further-  
 652 more, it was found that the turbulent component of the vertical exchange,  $\langle c'w'^* \rangle_{z/H=1}$ , on  
 653 average is dominant compared to the advective transport,  $\langle (CW)^* \rangle_{z/H=1}$ , for this scenario in  
 654 agreement with Belcher et al. [6]. Vertical exchange velocities for UoR-SNM and SIRANE-  
 655 2 were determined from the LES by ensemble-averaging individual results obtained in re-  
 656 gions of significantly high flux magnitudes, resulting in  $E_x = 0.1 \text{ m s}^{-1}$ ,  $E_y = 0.15 \text{ m s}^{-1}$   
 657 and  $E_z = 0.12 \text{ m s}^{-1}$  for  $x$  streets,  $y$  streets and intersections, respectively.  $E_x$  is about 30 %  
 658 lower than  $E_y$ , indicating that the recirculating flow in the short street reduces the potential  
 659 for vertical exchange. Applying the SIRANE parametrisation given in Eq. (8) together with  
 660 the facet-averaged LES value of  $\langle \sigma_w \rangle_{z/H=1}$  at the UCL top resulted in exchange velocities  
 661 of  $E_x = 0.07 \text{ m s}^{-1}$  and  $E_y = 0.08 \text{ m s}^{-1}$ . These agree well with  $E_x = E_y = 0.09 \text{ m s}^{-1}$   
 662 that were obtained via the parametrisation for  $\sigma_w$  based on  $u_*$  that is used in SIRANE-1.  
 663 However, compared to  $E_y = 0.15 \text{ m s}^{-1}$  derived from Eq. (7) the SIRANE-1 value of  $E_y$  is  
 664 40 % lower. During the model run, both network models determine the direction of vertical  
 665 transport for a certain street via the local vertical concentration gradient between UCL and  
 666 above-roof concentrations. A summary of all exchange velocities is given in Tab. 3.

### 667 4.2.3 Mixing conditions

668 The flux parametrisations in the street-network modelling framework (Eqs. 5 and 6) are  
 669 based on the assumption that pollutants are well-mixed within each box, i.e. spatial gra-  
 670 dients within individual streets are small [6]. The appropriateness of this approximation is  
 671 examined on the basis of the high-resolution LES data. Figure 10 shows the distribution  
 672 of spatial root-mean-square (r.m.s) values of concentrations in each network-model box as  
 673 a fraction of box-averaged concentrations for two layers:  $0 \leq z/H \leq 1$  and  $1 \leq z/H \leq 2$ .  
 674 The smaller the value of this ratio, the better the mixing within the volume. Not surpris-  
 675 ingly, upwind of the source and at the lateral edges of the plume, the well-mixed condition  
 676 is not satisfied and spatial concentration fluctuations are of the same order or greater than  
 677 the volume average. Particularly strong gradients are found in and around the source street,  
 678 whereas only a few streets downwind the pollutants had enough time to become well mixed.  
 679 Hence, in those plume regions where significant levels of concentrations are encountered  
 680 (Fig. 7) the street-network dispersion models can be expected to perform best.

681 Within the UCL, two interesting patterns can be observed: On the one hand, the inter-  
 682 section boxes tend to be less well mixed than the neighbouring street boxes, whereas the  
 683 short  $x$  streets, on the other hand, tend to be better mixed than the surrounding boxes. Both  
 684 features become more apparent at the plume edges. The patterns can be related to the typical  
 685 flow behaviour observed in the DIPLOS array as discussed in Sect. 4.1 (see Fig. 4). In the  
 686  $x$  streets pollutants are trapped within the prevalent recirculating flow and hence become  
 687 better distributed over the street volume. The intersection flow is strongly three-dimensional  
 688 and thus more prone to the mixing-in of 'clean' ambient air, which becomes increasingly  
 689 relevant at the edges of the plume.

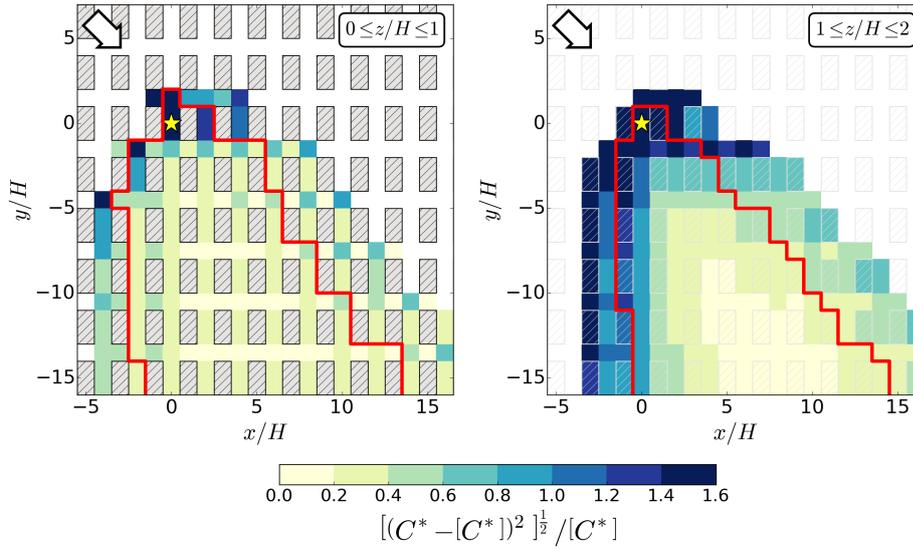


Fig. 10: Spatial r.m.s. values of concentrations in each network-model box as a fraction of box-averaged concentrations within the UCL (left;  $0 \leq z/H \leq 1$ ) and in the external layer just above the buildings (right;  $1 \leq z/H \leq 2$ ) derived from the LES. Statistics are shown for boxes where  $[C^*] \geq 1 \cdot 10^{-4}$ . The thick red lines border the part of the plume where the volume-averaged concentrations are  $\geq 1 \cdot 10^{-2}$ .

## 690 5 Dispersion model evaluation

691 The above analyses showed that the DIPLOS geometry represents an interesting test envi-  
 692 ronment for the dispersion models. While still being a strongly idealised setting, the geomet-  
 693 ric asymmetry together with the existence of a mixture of different flow regimes can pose  
 694 challenges to fast dispersion models.

695 In the following, the plume predictions from the different dispersion models intro-  
 696 duced in Sect. 3 (Tab. 1) are inter-compared. To provide a suitable benchmark for the inter-  
 697 comparison, concentration data from the LES are used as a reference. The wind-tunnel data  
 698 are not spatially extensive enough to be used directly for this purpose, but can instead be  
 699 employed to validate the LES. Indeed, comparison with the statistics from the wind-tunnel  
 700 model in this study and in previous validation exercises carried out in DIPLOS [23,32]  
 701 showed that the LES overall represents the salient dispersion features well for this test case,  
 702 given the uncertainties associated with the simulation and the experiment. While most of  
 703 the following quantitative comparisons are between the LES and the dispersion models, the  
 704 experimental data presented in Sect. 4.2 will be revisited for a qualitative appraisal. As we  
 705 set out in this study to evaluate the street-network modelling approach in comparison to  
 706 the more established model categories, we need to compare the model results in a common  
 707 framework. For that, the space-resolved output from the LES, the Gaussian and Lagrangian  
 708 models is converted into volume-averaged concentrations in boxes covering streets and in-  
 709 tersections within the UCL as in the street-network representation. Although this means  
 710 sacrificing spatial resolution, the assessment of danger zones based on street-integrated con-

711 concentrations is more practical in emergency-response contexts. Hence, the space-resolution  
712 limitation of the street-network modelling is no detriment for this type of application.

### 713 5.1 Qualitative model inter-comparison

714 A qualitative inter-comparison of model performances is presented below in terms of con-  
715 centration footprints and plume characteristics in the DIPLOS canopy. A quantitative as-  
716 sessment of model spreads and biases is given in Sect. 5.2.

#### 717 5.1.1 Plume footprints

718 Figure 11 compares volume-averaged UCL concentrations,  $[C^*]$ , from all dispersion models  
719 with the LES output. A quantitative comparison of these results is shown in Fig. 12 in  
720 terms of horizontal transects of volume-averaged concentrations along  $x$  ('lateral') and  $y$   
721 ('longitudinal') directions and corresponding transects of point-wise concentrations from  
722 the experiment in a height of  $z/H = 0.5$ . Due to the different nature of wind-tunnel data  
723 compared to the volume averages, these are meant to supplement the *qualitative* appraisal  
724 of the plume patterns.

725 The decisive difference between the Gaussian models concerns the added plume deflec-  
726 tion, either based on the above-rooftop flow (GAUSS-1; plume centreline along  $-54^\circ$ ) or  
727 on the representative UCL wind direction (GAUSS-2;  $-78^\circ$ ). The latter clearly resulted in  
728 a better agreement with the LES and also with the footprint in the wind tunnel at half the  
729 building height (Fig. 7). The strong lateral plume spread is governed by the enhancement  
730 term for  $\sigma_y$  (Eq. 2) for light-wind situations. Not considering this modification of the classic  
731 Briggs formulation results in too narrow plumes and a significantly poorer agreement with  
732 the LES (not shown). Naturally, the Gaussian models do not capture topological dispersion  
733 effects like the strong pollutant channelling into  $-y$  direction and the uneven splitting in in-  
734 tersections, which resulted in the asymmetric plume shape. The symmetry constraint leads to  
735 too strong upwind spread into  $-x$  direction in GAUSS-2 and hence a much broader plume  
736 in the far-field ( $\Delta x \simeq 22H$ ) compared to the LES ( $\Delta x \simeq 18H$ ) at  $y/H = -13.5$  (Fig. 12).  
737 The best quantitative agreement with the LES is found farther away from the source in those  
738 downwind regions of the plume where material is well-mixed within and above the canopy  
739 (Fig. 10) and where the magnitude of vertical concentration fluxes at the canopy top is small  
740 (Fig. 9a).

741 A much better overall agreement with the plume shape of the LES and the wind tunnel  
742 is found in the outputs of the Lagrangian model. Some differences can be observed in the  
743 runs based on the two native QUIC flow modules, QUIC (URB) and QUIC (CFD). In the  
744 former, a strong lateral spread of the plume into  $-x$  streets is observed, which close to the  
745 source is comparable to GAUSS-2 (see  $y/H = -4.5$  transect in Fig. 12). This behaviour  
746 can be attributed to the stronger negative  $u$ -component of the horizontal flow observed in  
747 the QUIC-URB wind fields (see Figs. 4 and 5), which leads to a redistribution of material  
748 from the intersections into the upwind short streets, there entering the large recirculation  
749 zone. It is noted that there are no data available from the wind-tunnel campaign to further  
750 investigate the spread of the plume into  $-x$  direction. The downstream extent ( $+x$ ) of the  
751 plume and the distribution of scalars along the  $x/H = 0$  transects through the source street,  
752 however, agree well with the reference data.

753 Although the flow field from the RANS model used in QUIC (CFD) in large part showed  
754 a flow channelling along the  $y$  streets and through the intersections similar to the turbulence-

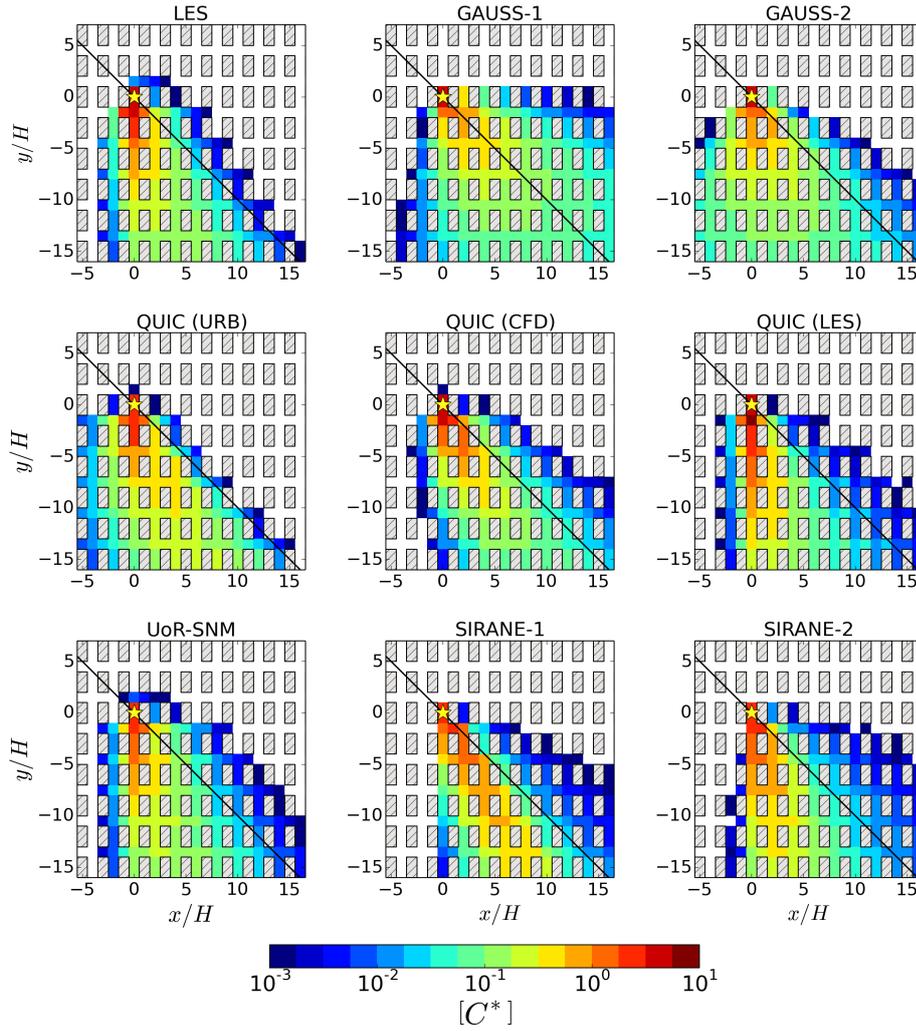


Fig. 11: Volume-averaged concentrations in streets and intersections within the canopy layer ( $0 \leq z/H \leq 1$ ) for the LES reference data and the different dispersion models. The solid black line indicates the forcing wind direction of  $-45^\circ$ .

755 resolving LES, the resulting plume orientations are somewhat different. QUIC (CFD) has  
 756 stronger transport of material into  $+x$  direction than the LES as a result of the stronger out-  
 757 flow from the intersections into the downwind short streets (Fig. 4, Tab. 3). The qualitative  
 758 comparison with the point-wise concentrations from the wind tunnel also shows an under-  
 759 prediction along the  $x/H = 0$  transect, but a better agreement at some distance away from  
 760 the source ( $y/H = -13.5$ ). QUIC-PLUME was also run on turbulence fields provided di-  
 761 rectly by the RANS turbulence model. This resulted in similar results to the QUIC (CFD)  
 762 output presented here, but with a slightly reduced lateral plume spread (not shown).

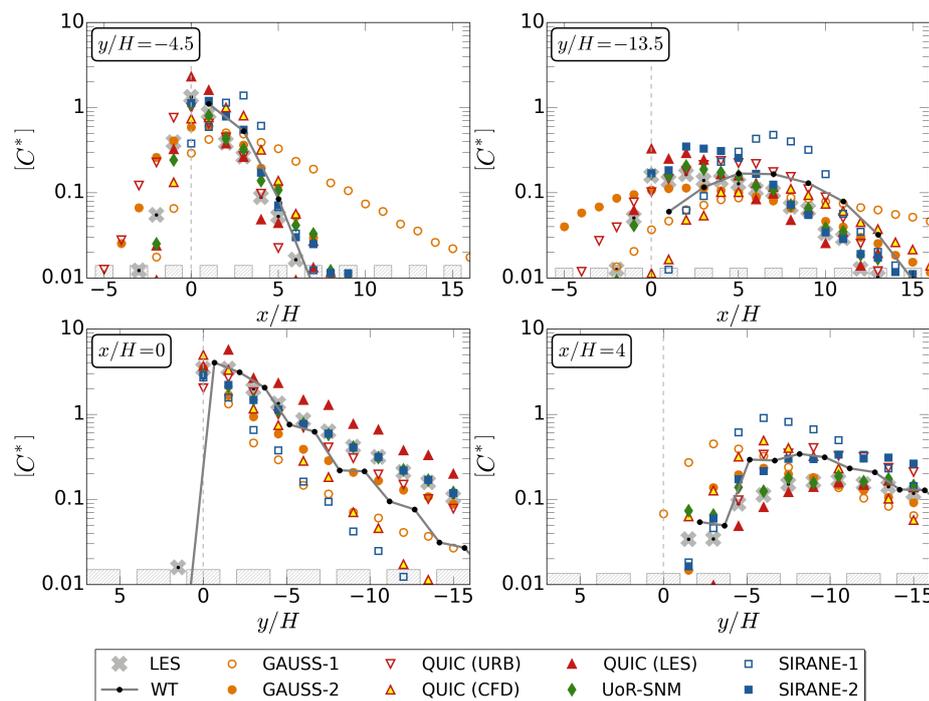


Fig. 12: Comparison of horizontal transects of volume-averaged concentration along the  $x$ -axis (*top*) and along the  $y$ -axis (*bottom*) in the canopy layer. Single-point measurements from the wind tunnel (WT) at a height of  $z/H = 0.5$  are shown as well for the sake of completeness. The source position of  $x/H = y/H = 0$  is indicated by a dashed vertical line.

763 Not surprisingly, the best QUIC–PLUME agreement with the LES is found for the QUIC  
 764 (LES) set-up. Differences apparent here are only attributable to the Lagrangian dispersion  
 765 modelling component, which in this case demonstrates the suitability of the QUIC–PLUME  
 766 urban dispersion algorithms. The largest deviations are apparent along the plume centreline,  
 767 where the model over-predicts concentration levels as seen in the longitudinal transect at  
 768  $x/H = 0$  in Fig. 12 compared to the Eulerian solution from the LES and the experimental  
 769 data. This is paralleled by a slightly larger lateral spread ( $+x$ ) of the plume compared to  
 770 QUIC (URB) and QUIC (CFD). We also observe that QUIC (LES) is the only model where  
 771 the maximum volume-averaged concentration is not located in the source street, but in the  
 772 first downwind intersection box.

773 As expected, the street-network model UoR–SNM run on LES velocity parameters  
 774 matches the longitudinal and lateral concentration profiles computed by the LES extremely  
 775 well. This demonstrates that, despite the minimal flow specifications needed, the simple flux-  
 776 balance methodology is suitable for capturing important features of canopy-layer dispersion.  
 777 This is largely attributable to the fact that the model formulation explicitly represents the  
 778 street topology and directly accounts for associated topological dispersion effects. Running  
 779 UoR–SNM with the re-entrainment term switched on and off is helpful to reveal the sig-  
 780 nificance of adequately representing the vertical pollutant fluxes. This analysis showed that  
 781 in regions where re-entrainment dominates (see Fig. 9a), volume-averaged UCL concen-

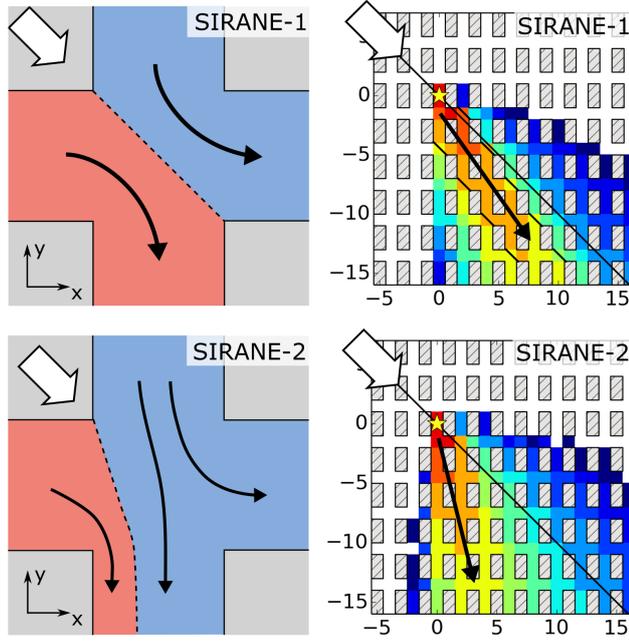


Fig. 13: Schematic of the flux distribution in the intersections for SIRANE-1 with  $\langle U_s \rangle = \langle V_s \rangle$  predicted by the SIRANE flow model (*top left*), and SIRANE-2 with  $\langle U_s \rangle \simeq 0.3 \langle V_s \rangle$  based on the LES information (*bottom left*) together with the corresponding canopy-layer plume footprints and the mean plume advection direction. The forcing wind direction is indicated by thick arrows.

782 trations can be enhanced by an order of magnitude or more (not shown). As evident from  
 783 comparing Figs. 9a and 11, the re-entrainment regions in the LES feature non-negligible  
 784 concentration levels in agreement with the experiment (Fig. 7). The strongest deviations be-  
 785 tween the demonstration model UoR-SNM and the LES occur very close to the source and  
 786 at the plume edges, where the well mixed-condition breaks down.

787 SIRANE-1, which was run in operational mode with parametrisations for horizontal ad-  
 788 vection and vertical exchange velocities, predicts a plume orientation that is much closer to  
 789 the  $-45^\circ$  forcing wind direction than any of the other models. As anticipated in Sect. 4.1.1,  
 790 the larger  $\langle U_s \rangle$  computed the SIRANE-1 flow model resulted in enhanced advection along  
 791 the short  $x$  streets as compared to the LES, which also affected the distribution of material  
 792 from the intersection into the downwind streets. Overall, the plume is less well diluted far-  
 793 ther away from the source than in the LES or in the experiment ( $y/H = -13.5$  and  $x/H = 4$   
 794 transects in Fig. 12). Unlike SIRANE-2, for which  $\langle U_s \rangle < \langle V_s \rangle$  resulted in an uneven branch-  
 795 ing of the plume in the intersection, in SIRANE-1 the material is uniformly distributed into  
 796 the downwind streets since  $\langle U_s \rangle = \langle V_s \rangle$ . The observed deviation from the  $-45^\circ$  forcing di-  
 797 rection is induced by the rectangular shape of the buildings.

798 This behaviour is schematically illustrated in Fig. 13. As a consequence the models pre-  
 799 dict considerably different plume orientations. The even plume splitting in the intersections  
 800 in SIRANE-1 also led to a reduced lateral spread of pollutants. This spatial confinement  
 801 of material together with the reduced vertical exchange velocities compared to SIRANE-2

(Tab 3) is responsible for the significant over-prediction of concentration levels compared to the volume-averaged LES and the point-wise wind-tunnel data. SIRANE-2, which was provided with representative velocities and hence accounts for the dominance of pollutant flux down the y streets from the intersections, shows a high level of agreement with the LES.

## 5.2 Quantitative model inter-comparison

In order to quantify the differences between the dispersion models and the LES, we use a set of well-established dimensionless validation metrics [24, 13, 40]. These are the factor of two of observations (FAC2), the fractional bias (FB), the normalised root mean square error (NMSE), the geometric mean bias (MG), geometric variance (VG) and the correlation coefficients (R) as defined in Eqs. 11–16. As for the qualitative comparison, the quantification of differences between the LES,  $C_o$ , and the model predictions,  $C_p$ , is conducted in terms of a data-pairing of non-dimensionalised, box-averaged UCL concentrations,  $[C^*]$ . Curly brackets,  $\{\dots\}$ , indicate the average over the entire data sample of  $N$  box-averaged concentrations and  $\sigma_C$  are the corresponding sample standard deviations.

Factor of two:

$$\text{FAC2} = \frac{1}{N} \sum_i F_i \quad \text{with} \quad F_i = \begin{cases} 1, & \text{if } \frac{1}{2} \leq \frac{C_{p,i}}{C_{o,i}} \leq 2 \\ 0, & \text{otherwise} \end{cases} \quad (11)$$

Fractional bias:

$$\text{FB} = 2 \frac{(\{C_o\} - \{C_p\})}{(\{C_o\} + \{C_p\})} \quad (12)$$

Normalised mean square error:

$$\text{NMSE} = \frac{\{(C_o - C_p)^2\}}{\{C_o\}\{C_p\}} \quad (13)$$

Geometric mean bias:

$$\text{MG} = \exp(\{\ln C_o\} - \{\ln C_p\}) \quad (14)$$

Geometric variance:

$$\text{VG} = \exp\left(\{(\ln C_o - \ln C_p)^2\}\right) \quad (15)$$

Correlation coefficient:

$$\text{R} = \frac{\{(C_o - \{C_o\})(C_p - \{C_p\})\}}{\sigma_{C_o} \sigma_{C_p}} \quad (16)$$

Fig. 14 shows the underlying scatter plots for the LES and the dispersion models, as well as a comparison of point-values at  $z/H = 0.5$  from the LES and the wind tunnel to complement the earlier qualitative comparison in Fig. 7. Here we used a nearest-neighbour approach to match the LES data to the exact measurement locations and heights of individual wind-tunnel data points.

As discussed in detail by Chang and Hanna [24], in order to obtain a comprehensive picture about the model, different validation metrics should be consulted together. While FB and MG measure the systematic bias of the model and can be influenced by cancelling errors, NMSE and VG measure the mean relative scatter between the data pairs and include systematic and random errors. By using a logarithmic framework, MG and VG are

less susceptible to infrequently occurring very high or low concentrations than their ‘linear’ counterparts, FB or NMSE. This is beneficial in test cases such as the one in this study, where results are compared over several decades of concentrations. R is not a reliable indicator of model accuracy since it is dominated by the fact that concentrations will generally decrease with distance from the source [24]. However, it provides information about the level of common variation in both data sets and can be useful in combination with the other metrics. FAC2 and FAC5 provide the most robust measure with regard to the influence of isolated events of very good or bad agreement between data pairs.

FAC2, FAC5, FB, NMSE and R were obtained from data pairs for which either the LES or the model output was  $\geq 1 \cdot 10^{-3}$  so that misses and false positives are reflected in the metrics. This is not as easy for the MG and VG metrics as these can be overly affected by very low concentration values and are undefined for zero concentrations (plume misses a street completely). For these metrics we follow the recommendation by Chang and Hanna [24] and impose a minimum threshold of  $[C^*] = 1 \cdot 10^{-3}$  on all data.

Table 4 lists the metrics together with the target values for a model that perfectly matches the LES. As a point of reference for the assessment of urban dispersion models, Chang and Hanna [24] and later Hanna and Chang [40] have proposed the following acceptance criteria for a ‘good’ model performance:  $FAC2 > 0.3$  (or  $> 0.5$  based on earlier assessments),  $|FB| < 0.67$ ,  $NMSE < 6$ ,  $0.7 < MG < 1.3$  and  $VG < 1.6$ . In other words, the mean model bias as measured by FB and MG should be within 30 % of the mean and the mean relative scatter (NMSE and VG) within approximately a factor of 2 of the mean. It has to be noted that these acceptance thresholds were originally proposed for arc-maximum concentrations, but meanwhile are also commonly applied to assess the model performance over the entire extent of the plume. In general, however, it is important to highlight that such thresholds should be understood as being strongly case-specific and linked to the margins of error that are acceptable in the scenario under investigation. In the absence of such constraints in this study, we revert to the criteria proposed by Hanna and Chang [40].

Only GAUSS-2, QUIC (URB), QUIC (LES) and UoR-SNM are within a factor of 2 of the LES more than 30 % of the time. Of these, QUIC (URB) is the only model that was not provided with information from the LES flow. Only QUIC (LES) and UoR-SNM meet the less stringent FAC5 criterion more than 75 % of the time. For both FAC2 and FAC5, SIRANE-1 persistently shows the lowest values. In contrast to that, the overall low FB indicates only small systematic bias in all models. Inspecting the corresponding scatter plots in Fig. 14, however, shows that in some cases this is a result of error cancellation of over and under-predictions. This is particularly apparent in the plots for QUIC (CFD) and SIRANE-1, where data pairs group symmetrically about the 1-to-1 line. According to the MG metric, all models except for QUIC (LES) which is closest to the ideal value of 1.0, have a tendency to over-predict mean concentrations (positive bias). The strongest deviations from the LES reference are associated with approximately a factor of 2 mean over-prediction as seen for the Gaussian models ( $MG \simeq 0.5$ ). The VG metric shows the highest relative scatter with almost a factor of 7 of the mean for GAUSS-1 as a result of the largest mismatch of plume footprints. QUIC (CFD) and SIRANE-1, which showed a similar tendency in the plume centreline although associated with different concentration levels, have comparable VG values indicating a relative scatter of about a factor of 4. QUIC (URB), QUIC (LES) and UoR-SNM exhibit the smallest scatter. This is also reflected in very high correlation coefficients compared to GAUSS-1 and SIRANE-1.

Parts of the above results are visually summarised in a Taylor diagram [76] in Fig. 15, based on the normalised standard deviation,  $\sigma_{C_p}/\sigma_{C_o}$ , the normalised relative root-mean-

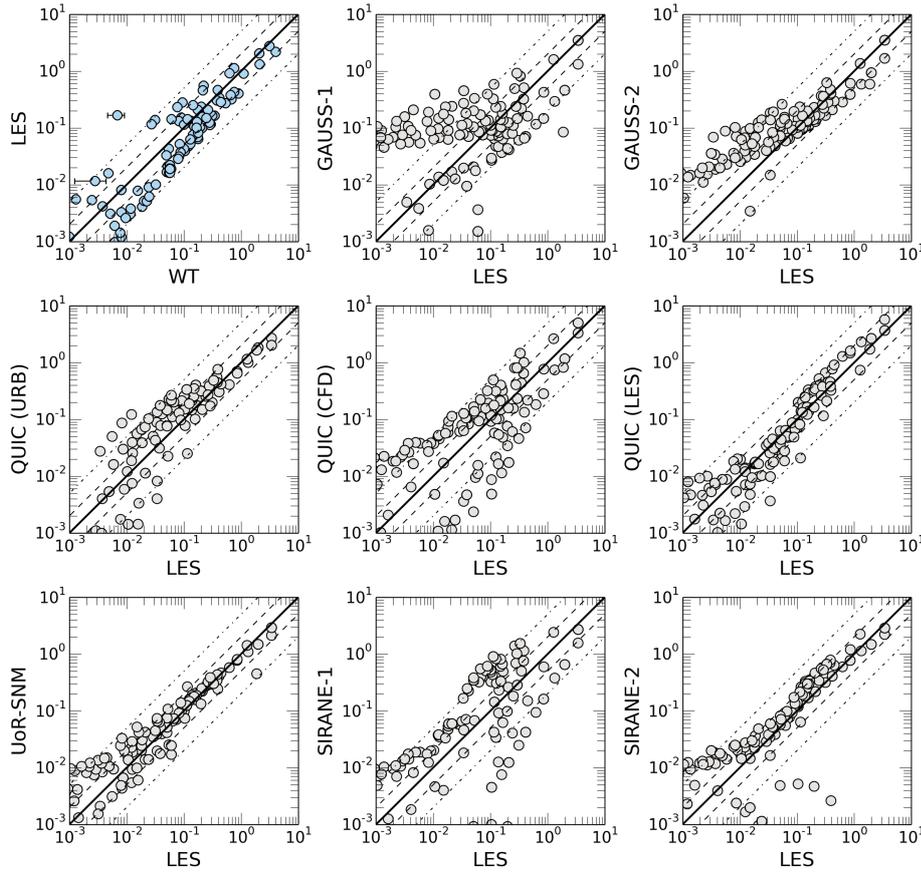


Fig. 14: Scatter plots of model predictions versus the LES based on volume-averaged UCL concentrations  $[C]^*$ . In contrast to that, the upper left plot shows LES and wind-tunnel single-point data pairs at a nominal height of  $z/H = 0.5$  (see plumes in Fig. 7). Thick solid lines indicate the ideal 1-to-1 relationship; dashed and dashed-dotted lines show the factor-of-2 and factor-of-5 margins, respectively.

880 square error and the correlation coefficient, which all measure the random (non-systematic)  
 881 scatter are related to each other through the law of cosines [24].

882 The diagram shows a cluster of models that have a high level of agreement with the  
 883 LES (GAUSS-2, QUIC (URB), SIRANE-2 and UoR-SNM) with comparably low root-  
 884 mean-square errors ( $\sim 0.4$ ) and high correlation (0.9–0.96), but overall smaller variability  
 885 compared to the LES reference ( $\sigma_{C_p}/\sigma_{C_o} < 1$ ). SIRANE-1 and GAUSS-1 show compar-  
 886 able metrics with larger random errors than the other models. Only the output from the  
 887 Lagrangian dispersion runs based on the CFD-RANS and LES wind fields overall exhibit a  
 888 larger variability than the LES, which could be related to the fact that the material is diluted  
 889 over a larger lateral region than in the LES or QUIC (URB). An interesting observation is  
 890 that QUIC (URB) agrees better with the LES than QUIC (LES), although the latter is run on  
 891 the LES mean flow fields that showed some significant differences to the flow pattern from

Table 4: Evaluation metrics for all models in comparison to the LES reference data. All metrics were computed from box-averaged concentrations  $[C^*]$  within the UCL. The target values in the sense of a perfect agreement with the LES are given together with the maximum box-averaged concentrations in the domain,  $[C^*]_{\max}$ , from all data sets.

Model	$[C^*]_{\max}$	FAC2	FAC5	FB	NMSE	MG	VG	R
Target value	—	1.0	1.0	0.0	0.0	1.0	1.0	1.0
LES	3.42	—	—	—	—	—	—	—
GAUSS-1	3.47	0.21	0.42	0.07	4.11	0.54	38.44	0.76
GAUSS-2	3.49	0.37	0.60	0.13	1.89	0.56	3.70	0.90
QUIC (URB)	2.69	0.44	0.71	-0.06	0.71	0.73	2.46	0.96
QUIC (CFD)	4.99	0.23	0.55	-0.11	1.95	0.85	7.92	0.89
QUIC (LES)	5.71	0.58	0.86	-0.26	1.46	1.02	1.66	0.96
UoR-SNM	2.91	0.60	0.83	0.12	1.06	0.80	1.60	0.96
SIRANE-1	2.70	0.11	0.34	-0.27	5.10	0.61	7.27	0.65
SIRANE-2	2.87	0.29	0.42	-0.23	2.41	0.74	3.79	0.86

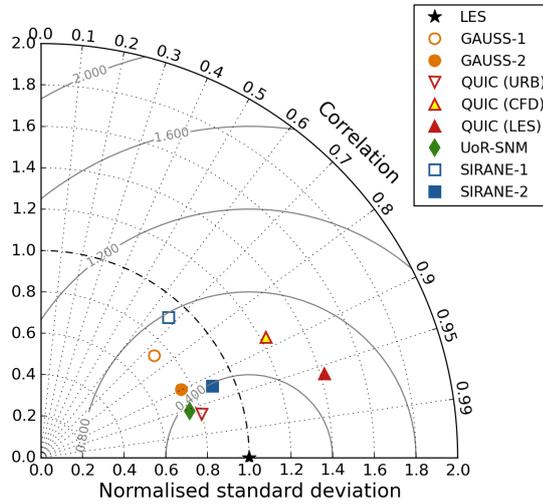


Fig. 15: Taylor diagram based on the normalised standard deviation (dotted arcs), the normalised relative root-mean-square error (solid arcs) and the correlation coefficient  $R$  (cosine of the angle to the horizontal axis; dotted lines). The thick dashed arc indicates  $\sigma_{C_p}/\sigma_{C_o} = 1$ . The star symbol shows the LES reference.

892 QUIC-URB (Fig. 4). Given the differences in the concentration fields, this implies that in  
 893 QUIC (URB) the component of flow reversal ( $-x$ ) counteracts the tendency of the dispersion  
 894 module to produce a stronger downwind spread ( $+x$ ) of the plume. Interestingly, among the  
 895 well-informed models, the performance is not directly correlated with the amount of flow  
 896 information provided. Although QUIC (LES) was run on data of the entire high-resolution  
 897 LES mean flow, the Lagrangian model did not outperform the much simpler Gaussian and  
 898 street-network models that were only provided with few velocity parameters.

## 899 **6 Further discussions and conclusions**

900 We presented a process-based evaluation of different methods for fast urban dispersion mod-  
901 elling for emergency-response applications. The focus was put on the comparison of UCL  
902 concentration footprints resulting from the continuous release of pollutants from a ground  
903 source. Representatives across the hierarchy of dispersion modelling approaches were evalu-  
904 ated: (i) Gaussian and (ii) Lagrangian models and the comparatively new (iii) street-network  
905 modelling. The urban test bed, albeit with geometric simplicity, induced complex mean flow  
906 patterns that resulted in a strong plume asymmetry. Capturing the resulting topological dis-  
907 persion features proved to be a challenge for the models tested.

908 Running the models in different configurations with respect to the detail of flow in-  
909 formation provided, resulted in large differences in performance when compared to data  
910 from high-resolution LES. The strongest effect was seen in the two simplest modelling cat-  
911 egories: the Gaussian and the street-network models. The simple baseline Gaussian plume  
912 model used in this study improved significantly after some degree of building-awareness  
913 was added by means of a plume deflection in the UCL. However, the geometry-induced  
914 asymmetry of the plume and other topological dispersion features cannot be captured as  
915 there is no explicit awareness of the urban morphology in this model class. It is empha-  
916 sised, however, that more advanced Gaussian dispersion models are available as outlined in  
917 Sect. 1.2, some of which have added capabilities to take into account bulk effects of typical  
918 street-canyon flow and validation studies of such Gaussian plume or puff models can be  
919 found in the literature, e.g. [16, 60].

920 Running the street-network model UoR-SNM on flow parameters completely derived  
921 from the reference LES provided a demonstration of the suitability of the street-network  
922 methodology for canopy-layer dispersion modelling, and showed that the main relevant  
923 dispersion processes were captured. Advective transport mechanisms like pollutant chan-  
924 nelling along streets and plume splitting in intersections were adequately represented by  
925 flux-balance parametrisations, just as the vertical turbulent transfer of pollutants between  
926 UCL and external boundary layer. Naturally, detailed flow information is not usually avail-  
927 able in an emergency event. Hence, operational urban dispersion models have to rely on  
928 suitable parametrisations of relevant building-induced flow features.

929 Lagrangian models require the largest amount of input information in terms of 3D mean  
930 flow fields that need to be provided by an external module. Running QUIC-PLUME offline  
931 on flow fields from three different building-resolving simulations (diagnostic, CFD-RANS  
932 and LES) highlighted the strong dependence of the dispersion pattern on the underlying  
933 flow structure. The work also highlighted the benefits of conducting basic process studies  
934 like this in idealised geometries. In the DIPLOS array processes are complex enough to  
935 be challenging for models, while it is still possible to understand causalities. Initial runs  
936 with the diagnostic QUIC-URB model for this study, for example, revealed bugs in the flow  
937 module, which had a strong effect on the plume dispersion behaviour. Once identified, these  
938 bugs were easily corrected by the developers. Such errors would have been much harder to  
939 detect in more complex geometrical settings where it can be difficult to distinguish genuine  
940 features from artefacts.

### 941 **6.1 Run-speed requirements**

942 Regarding computing times, the two street-network dispersion models and the Gaussian  
943 model performed comparably with run speeds of  $\mathcal{O}(1 \text{ min})$  on a typical desktop computer.

We ran all QUIC simulations in parallel on two cores on a Windows computer with an Intel Core i5 3.3 GHz processor. This resulted in run times for the QUIC-URB flow module of approx. 1 min and of  $\sim 1$  h for the QUIC-CFD RANS model. Additional computing times from the Lagrangian stochastic model also were in the order of 1 h. However, it is emphasized that the QUIC-PLUME set-up used in this study was designed for the purpose of an evaluation exercise and not for operational use. Much faster computing times in complex urban environments of  $\mathcal{O}(1 \text{ min})$  to  $\mathcal{O}(10 \text{ min})$  can be achieved with QUIC-PLUME in general and for the DIPLOS geometry in particular by running on more cores and using an optimised combination of fewer particles, larger model time steps and shorter averaging periods [M. Brown, pers.comm.]. Current advancements of the QUIC system focus on the optimisation of computational speed by running on graphics processors [66, 64]. Based on these studies, it is likely that the new GPU-PLUME model can run up to 180 times faster than QUIC-PLUME for typical urban dispersion scenarios.

## 6.2 Strengths and limitations of the street-network approach

One aim of this study was to assess the performance of street-network models against more established methods based on an idealised test case with a building packing density representative of city centres. While requiring much fewer velocity input parameters, in the idealised-geometry scenario investigated here the simple street-network models performed equally well or better compared to the more complex Lagrangian dispersion model run on full 3D wind fields, when compared to data from the high-resolution, turbulence-resolving LES. At the same time, computational costs and computing times associated with the network approach are low. Unlike the similarly inexpensive Gaussian plume models, street-network models directly account for building-induced dispersion effects. We showed that the conceptual design of models like SIRANE and UoR-SNM enables to represent the dominant processes affecting pollutant dispersion in the DIPLOS canopy: topological dispersion effects like channelling along streets and branching at intersections as well as pollutant exchange with the external flow.

The basic rationale behind the approach is to study urban dispersion at the scales of interest for emergency-response applications: entire street canyons and intersections. For the regular, equal-height DIPLOS geometry, we could show that such a volume-averaged representation of concentrations becomes representative after a short distance from the source and particularly in those regions of the plume where concentration levels are non-negligible. However, the spatial variability of the mean concentration patterns is expected to be enhanced in the case of non-stationary wind forcing as encountered in the natural atmosphere. Naturally this model formulation is also associated with uncertainties regarding the exact location of emission sources and receptors within a street segment. The location of the source with regard to the surrounding buildings and the prevailing flow patterns can have a strong influence on the near-field dispersion behaviour. In scenarios involving very long streets a too coarse resolution has to be avoided by subdividing into shorter segments.

The study highlighted the importance of flow-field modelling in all types of operational dispersion models. Whether or not the driving flow is representative of the encountered scenario to a large degree determines the prediction quality that can be achieved with the dispersion model. An evaluation of the flow parametrisations in SIRANE showed a dependence of the accuracy of modelled horizontal advection velocities on the length of the street. In short streets the modelling assumption of a fully developed flow field does not apply, which resulted in an over-prediction of along-street velocities in the current test case. This

990 had knock-down effects on the way in which material is redistributed from the intersection  
991 into the downwind streets. Not capturing the uneven branching in the intersections of the  
992 DIPLOS array resulted in significant differences between plume centrelines in SIRANE-1  
993 and the LES. Related to the advection characteristics in the UCL is the representation of  
994 deviations from the forcing wind direction in the roughness sublayer above the buildings.  
995 The current SIRANE parametrisation of the vertical turbulent exchange velocity based on  
996  $u_*$  does not account for local mixing effects in the roughness sublayer above the buildings  
997 and hence is not a complete way of representing this process.

998 Further limitations of the street-network approach are expected to result from the fact  
999 that SIRANE and UoR-SNM were developed for street-canyon dispersion in urban environ-  
1000 ments with high packing density, where there is a sufficient degree of decoupling between  
1001 UCL and the external boundary layer. On the city-scale, however, urban environments are  
1002 comprised of areas with vastly different morphological characteristics, for some of which  
1003 the street-network modelling framework breaks down. For dispersion through ‘open’ ar-  
1004 eas like parks or squares, through very wide streets (wake interference or isolated roughness  
1005 regimes) or streets only partially bordered by buildings different processes need to be consid-  
1006 ered and parametrised. Additionally, the need to account for environments with a significant  
1007 heterogeneity of building heights is an area of ongoing model development. Furthermore,  
1008 studying effects of atmospheric stratification (stable, unstable) on urban dispersion and their  
1009 parametrisation in street-network models have become a priority for further experimental  
1010 and computational work.

## 1011 Acknowledgements

1012 The DIPLOS project is funded by the UK’s Engineering and Physical Sciences Research  
1013 Council grants EP/K04060X/1 (Southampton), EP/K040731/1 (Surrey) and EP/K040707/1  
1014 (Reading). The EnFlo wind tunnel is an NCAS facility and we gratefully acknowledge on-  
1015 going NCAS support. We are grateful for comments and ongoing discussions with other  
1016 colleagues at Surrey, Southampton and elsewhere. We thank Michael Brown and Eric Pardy-  
1017 jak for providing access to the QUIC dispersion modelling system and helpful discus-  
1018 sions throughout this study. Stephen Belcher and Elisa Goulart are gratefully acknowl-  
1019 edged for their development of and support with the University of Reading Street-Network  
1020 Model (UoR-SNM). The wind-tunnel data measured in the DIPLOS project are avail-  
1021 able from the University of Surrey (DOI: <https://doi.org/10.6084/m9.figshare.5297245>). The  
1022 LES data analysed in this study can be obtained from the University of Southampton (DOI:  
1023 <https://doi.org/10.5258/SOTON/D0314>).

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