

Turbulence and dispersion below and above the interface of the internal and the external boundary layers

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Abstract

This study has looked at the development of the internal boundary layer (IBL) over a block array close to a sharp change in surface roughness and its effect on dispersion from a ground level source for ratios of the downstream distance to the roughness length of less than 300. This was done by comparing a Large-Eddy Simulation (LES) with inflow boundary conditions against a LES with inlet-outlet periodic boundary conditions and data from a wind tunnel experiment. In addition to established methods, an alternative approach based on the vertical Reynolds stress was used to evaluate the depth of the IBL as it developed over the array which enabled the location of the interface to be more clearly defined. **It was confirmed that the IBL growth rate close to the change in surface roughness could be described by a power law profile, similar to the power law formula used in previous studies for a ratio of the downstream distance to the roughness length greater than 1000.** An analysis of mean concentration and turbulent scalar fluxes suggested that the presence of the IBL constrained the vertical development of the plume from a ground level source and so led to trapping of material in the canopy layer.

Keywords: IBL, inflow turbulence, dispersion, urban environments

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1. Introduction

Urban roughness is heterogeneous consisting of different type of surfaces (e.g. Antoniou et al., 2016; King et al., 2017; Vasaturo et al., 2018; Tolias et al., 2018). A change in surface roughness, such as exists at the edge of the city, or at the junction between the central business district (CBD) and an area of surrounding low-rise buildings, leads to a region of transitional flow as the turbulent boundary layer takes time to adapt to the new wall condition (e.g. Smits & Wood, 1985; Cheng & Castro, 2002; Barlow, 2014; Cao & Tamura, 2007; Hanson & Ganapathisubramani, 2016). This transitional flow results from the development of an internal boundary layer (IBL) above the roughness elements. It is challenging to identify the interface of the IBL and the approaching boundary layer. The interface may have a crucial effect on scalar exchange. To gain a deeper understanding of dispersion from a ground level source downstream of a change in surface roughness, it is important to analyse the development of the IBL.

Barlow (2014) analysed a turbulent boundary layer approaching a rural-to-urban transition region (rough-to-very rough surface change) and found that on the city scale an IBL began to form at the junction between the smoother rural and the rougher urban surfaces. However, on the neighbourhood scale, and close to the ground, the flow was continuously adjusting to changes in roughness and that locally generated IBLs were in equilibrium with the underlying surfaces. This meant that multiple changes in roughness could lead to overlapping local IBLs and, as a consequence, the IBL assumed a non-homogeneous 3-dimensional structure extending up to 2 – 5 times the mean building height (Barlow & Coceal, 2008). These findings were supported by those of Hanson & Ganapathisubramani (2016), who analysed boundary layer development across a rougher-to-smoother surface change and identified an IBL with two regions: an energetic region near the wall in which the flow had adapted to the new wall condition and an outer region in which the flow retained characteristics of the upstream condition.

31 In order to investigate the effects of the IBL it is first necessary to define its
 32 outer limit. Some authors (e.g. Cheng & Castro, 2002; Schlichting & Kestin,
 33 1979) have defined the height of the IBL as the point on a log-linear plot where
 34 the velocity reaches 99% of that for upstream roughness at the same position.
 35 However, this definition is difficult to use because of the uncertainty of mea-
 36 suring differences of 1% experimentally or numerically. An alternative method
 37 (Antonia & Luxton, 1972) involves plotting the streamwise velocity profile at
 38 a series of locations against the square-root of the height above ground. The
 39 profiles are then approximated by two straight line segments which correspond
 40 to the external and IBLs, and the intersection of the segments defines the height
 41 of the IBL. The method devised by Efros & Krogstad (2011) is similar, but in-
 42 volves plotting the streamwise Reynolds stress against the height. The depth
 43 of the IBL is again indicated by the intersection of two lines. Both of these
 44 methods are based on the “knee” point technique which might be open to inter-
 45 pretation in situations where the differences between the boundary layer velocity
 46 profiles are small. Nevertheless, they are easy to implement and provide a good
 47 indication of the IBL growth rate.

48 The strength of the step change in roughness between two regions may be
 49 described by the roughness length ratio (z_{01}/z_{02}), where z_{01} and z_{02} are the
 50 upstream and downstream roughness lengths respectively. Despite this, Jackson
 51 (1976) used atmospheric and wind-tunnel data to demonstrate that the growth
 52 rate of the IBL is essentially driven by the rougher surface and is not related
 53 to the roughness length ratio, or to the ratio of boundary-layer thickness to
 54 roughness element height. This conclusion is supported by work conducted by
 55 Townsend (1965) and Schofield (1975), which showed that if $(z_{01}/z_{02}) < 1$ (a
 56 change from smoother to a rougher wall) only z_{02} is important in estimating
 57 the growth of the IBL.

58 Bradley (1968) conducted the first atmospheric experiments on IBL devel-
 59 opment due to an increase in surface roughness. His observations showed that
 60 the growth rate of the IBL was independent of wind speed and described well by
 61 Elliot’s formula (Elliott, 1958) which also indicates that the IBL development

62 is independent of the roughness length ratio:

$$\frac{\delta}{z_{02}} = a \left(\frac{X}{z_{02}} \right)^P \quad (1)$$

63 where X is the distance from the step change, δ is the depth of the IBL, and
64 P and a are the exponent and the coefficient of the power-law formula respec-
65 tively. Elliott (1958) found that the coefficient a varied from 0.6 to 0.9 and that
66 $P=0.8$ for $X/z_{02} > 1000$. His work has been further confirmed by (Wood, 1982;
67 Pendergrass & Arya, 1984). Elliot emphasised that the exponent $P = 0.8$ in
68 Eq. 1 was only valid for $X/z_{02} \geq 1000$ as it relied upon assumptions of constant
69 stress and a logarithmic profile that were only valid downstream of that point.
70 He showed that closer to the roughness transition point the development of the
71 IBL could be fitted with a similar power law relationship, but with a lower
72 exponent P and greater coefficient a .

73 Cheng & Castro (2002) performed an experimental study of the flow field
74 immediately downstream of a roughness transition in which they fitted their
75 experimental results for the IBL at distances of $X/z_{02} < 1000$ by applying
76 Eq. 1 using an exponent $P = 0.33$ and a coefficient $a = 10.56$. This confirmed
77 Elliott’s finding that the exponent P decreased while the coefficient a increased
78 as X/z_{02} was reduced. In their work Cheng & Castro (2002) defined the IBL
79 height as the location where the velocity was 99% of that for upstream roughness
80 at the same height. This led to significant scatter in the derived IBL height due
81 to the difficulty of measuring 1% differences experimentally.

82 Large-Eddy Simulations have demonstrated the capability to model turbu-
83 lence, dispersion and heat transfer in urban environments (Baker et al., 2004;
84 Fuka et al., 2017; Hanna et al., 2002; Kanda et al., 2004; Xie & Castro, 2006).
85 The majority of LES flow and dispersion studies have focussed on the street-
86 scale below and immediately above the canopy and used simple periodic inlet-
87 outlet boundary conditions. Very few numerical studies have analysed the char-
88 acteristics of turbulent flow as it passes over a change in roughness. Two which
89 have are those by Michioka et al. (2011) and Tomas et al. (2017). Both of these
90 applied the LES approach using the inflow boundary condition method to com-

91 pute the flow over arrays of obstacles with various aspect ratios with the aim
 92 of better understanding the dispersion mechanisms. However, their focus was
 93 limited to examination of the advective and turbulent pollutant fluxes around
 94 the array obstacles up to the canopy height, and they did not examine IBL
 95 development. To the authors' knowledge there have been no numerical stud-
 96 ies or experimental works which have specifically addressed the effects of IBL
 97 development on gas dispersion.

98 In this paper we examine LES predictions made using the inflow generator
 99 proposed by Xie & Castro (2008), and then identify how the height of the IBL
 100 evolves over a psuedo rural-to-urban transition region using a similar approach
 101 to those proposed by Efros & Krogstad (2011) and Antonia & Luxton (1972),
 102 but based on using the vertical Reynolds stress. This was done with the objective
 103 of understanding the extent to which the dispersion of a neutrally buoyant gas
 104 from a ground-level point source is influenced by the interaction of the external
 105 boundary layer and IBL. The governing equations are briefly described in Sect. 2.
 106 Details of the numerical settings including geometry, mesh and inflow conditions
 107 are given in Sect. 3. LES predictions for turbulence and dispersion are discussed
 108 in Sect. 4. Finally, the conclusions are summarised in Sect. 5.

109 2. Governing equations

110 In LES the filtered continuity and Navier-Stokes equations are written as
 111 follows:

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0 \quad (2)$$

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial \bar{u}_i \bar{u}_j}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\frac{\tau_{ij}}{\rho} + \nu \frac{\partial \bar{u}_i}{\partial x_j} \right) \quad (3)$$

113 where the filtered velocity and pressure fields are \bar{u}_i and \bar{p} respectively, ν is the
 114 kinematic molecular viscosity and ρ is the density. The standard Smagorinsky
 115 subgrid-scale (SGS) model was applied to determine the isotropic part of the
 116 residual stress tensor τ_{ij} :

$$\tau_{ij} = -2\nu_r \bar{S}_{ij} \quad (4)$$

117 where $\overline{S}_{ij} = \frac{1}{2} \left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right)$ is the filtered rate of strain and ν_r is the SGS
 118 residual viscosity. The SGS residual viscosity ν_r is modelled as:

$$\nu_r = (C_S \Delta)^2 \overline{S} \quad (5)$$

119 where \overline{S} is the characteristic filtered rate of strain, the filter width Δ was taken
 120 as the cube root of the cell volume and the Smagorinsky coefficient as $C_S = 0.1$.
 121 The Van Driest damping function was applied in the near wall region.

122 The Smagorinsky model supplemented with a wall-damping function is known
 123 to be less accurate near a flow-reattachment point or in free-shear layer regions
 124 (Inagaki et al., 2005). However, Castro et al. (2017) compared the performance
 125 of the dynamic mixed time scale sub-grid model (Inagaki et al., 2005) and the
 126 standard Smagorinsky over an identical array of uniform blocks and their results
 127 revealed only small differences in the spatially averaged mean velocities and tur-
 128 bulence stresses. Based on those results the standard model and wall-damping
 129 function were adopted for the simulations reported here.

130 The filtered transport equation for a passive scalar is:

$$\frac{\partial \overline{C}}{\partial t} + \frac{\partial \overline{u}_j \overline{C}}{\partial x_j} = \frac{\partial}{\partial x_j} \left[(K + K_r) \frac{\partial \overline{C}}{\partial x_j} \right] + S \quad (6)$$

131 where \overline{C} is the filtered scalar concentration and S is a source term. The second
 132 term on the left-hand side is the advection term and the first term on the right-
 133 hand side is the diffusion term. K is the molecular diffusivity and K_r is the
 134 SGS turbulent diffusivity computed as:

$$K_r = \frac{\nu_r}{Sc_r} \quad (7)$$

135 where Sc_r is the subgrid Schmidt number. A constant Schmidt number of
 136 $Sc_r = 0.7$ was assumed.

137 **3. Numerical settings**

138 The LES model was implemented within the open-source CFD package
 139 OpenFOAM version 1.7.1. A second-order backward implicit scheme in time and

140 second-order central difference scheme in space were applied for the discretisation of the terms in Eqs. 3 and 6. Flow and turbulence within the domain were
 141 simulated as a half channel. An efficient inflow turbulence generation method
 142 (Xie & Castro, 2008) was used at the inlet, with periodic conditions at the lateral boundaries and a stress-free condition at the top of the domain ($y = 12h$,
 143 where $h = 70mm$ is the uniform height of the array element). The Reynolds
 144 number based on h and the free stream velocity $U_{ref} = 2m/s$ at $y = 12h$ was
 145 approximately 12,000. The averaged CFL (Courant-Friedrichs-Lewy) number
 146 was 0.2, based on a time step resolution of 0.0014s. Flow and second-order
 147 statistics were initialized for 40s and then averaged over 180s (180 flow-passes).
 148
 149

150 3.1. Geometry, mesh and resolution

151 Although computational power is increasing, the simulation of most real
 152 urban scenarios still represents a challenge, especially when large and complex
 153 geometries have to be analysed. In studies to improve the understanding of
 154 building aerodynamics it is therefore usual to represent urban configurations in
 155 their simplest form as an array of cuboids in regular or non-regular patterns
 156 (e.g. Hanna et al., 2002; Xie & Castro, 2006).

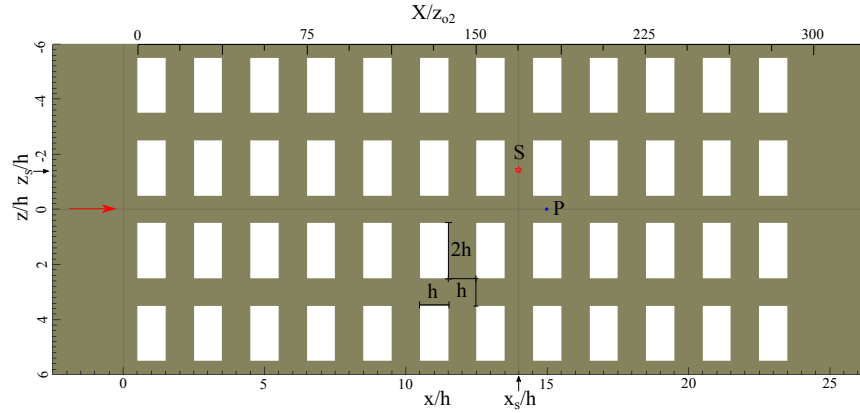


Figure 1: The array configuration: dimensions of buildings and streets, the coordinate system, the flow direction, the distance from the leading edge X/z_{02} , the position x_s and z_s of source S and measurements location P .

157 The array of regular cuboids modelled in this paper represents part of a larger
 158 array used in a wind tunnel experiment designed to simulate a neighbourhood
 159 scale region in which statistical homogeneities should exist. On the basis that
 160 the length of the streets should exceed the building height h , to establish devel-
 161 oped street-canyons flows, Castro et al. (2017) adopted cuboid obstacles with
 162 dimensions $1h(\text{length}) \times 1h(\text{height}) \times 2h(\text{width})$. The section of the array mod-
 163 elled is shown in Fig. 1 where the street units parallel to the x axis are $1h$ long
 164 and referred to as ‘short streets’ hereinafter. Street units parallel to the z axis
 165 are $2h$ long and referred to as ‘long streets’. The rectangular array comprised
 166 48 aligned blocks with h spacing, which considering the single block unit leads
 167 to a plan area density of $\lambda_p = 0.33$.

168 The dimensions of the modelled domain were $29h \times 12h \times 12h$ within a uni-
 169 form Cartesian grid of resolution $\Delta = h/16$. Simulations by Castro et al. (2017)
 170 at this resolution yielded LES results for turbulence that agreed well with higher
 171 resolution Direct Numerical Simulation (DNS) data. **The top boundary was**
 172 **placed at $y = 12$, which is very close to the boundary layer height in**
 173 **the wind tunnel. Castro et al. (2017) performed a sensitivity test of**
 174 **smaller domain heights ($y = 6h, 8h$ or $10h$) and recommended a top**
 175 **domain of at least six canopy heights in order to capture the most**
 176 **important turbulence features.** Computations were made for the 0° wind
 177 direction by assuming that the mean wind flow was perpendicular to the front
 178 face of the cuboid elements as indicated in Fig. 1.

179 3.2. *Scalar source*

180 A passive scalar was released from a ground-level point source within the
 181 array of cuboid elements. The shape and size of the point source were identical
 182 to that reported in Fuka et al. (2017). The source was positioned at the middle
 183 of a long street after the seventh row of buildings (Fig. 1) where the downstream
 184 flow would be fully developed (Hanna et al., 2002). Because the modelling used
 185 a uniform grid, the shape of the source only approximated the source used in the
 186 experiment. The diameter was represented by 4 cells and so measured $0.25h$,

187 while the height was one cell ($h/16$). A constant scalar flux release rate was set
 188 for each cell inside the source volume.

189 3.3. Inflow conditions

190 The simulation of flow over a rural-to-urban transition region requires a
 191 continuous specification of inlet turbulence. This was achieved by using the
 192 inflow turbulence method developed by Xie & Castro (2008) to generate a syn-
 193 thetic turbulent inflow with exponential-form correlations in time and space.
 194 **The used inflow method proved to reconstruct energy-containing re-**
 195 **gion and inertial sublayer of the spectra in high fidelity. Moreover,**
 196 **(Bercin et al., 2018) showed that the use of exponential-form correla-**
 197 **tion functions as a model approximation is more advisable than that**
 198 **of Gaussian-form.**

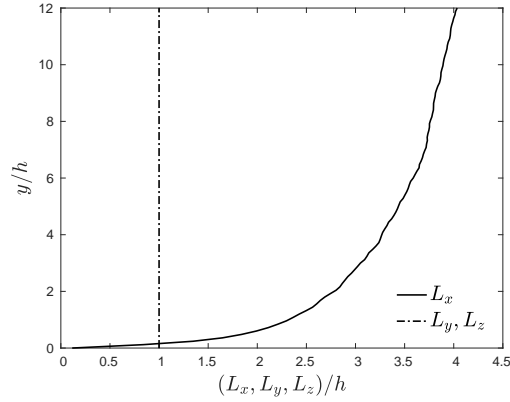


Figure 2: Vertical profiles of prescribed integral length scales at the LES inlet $x = -2.5h$.

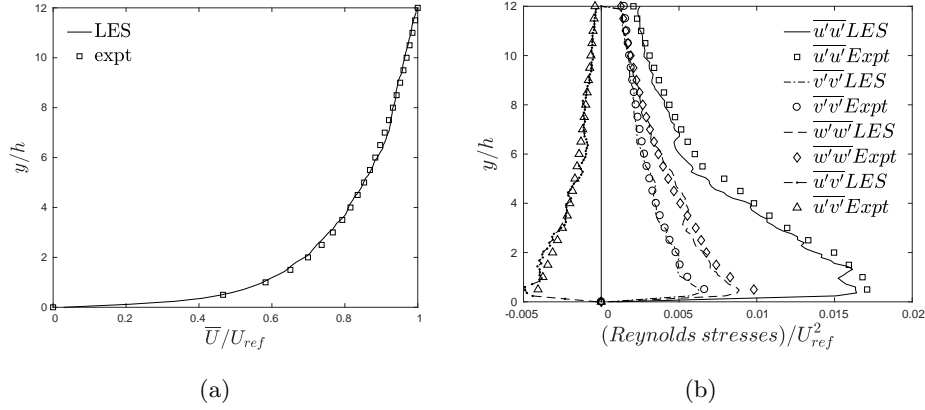


Figure 3: (a) Vertical profiles of laterally averaged mean velocity from LES at inlet and prescribed mean velocity from experiments. (b) Vertical profiles of prescribed Reynolds stresses at the LES inlet and experimental values.

199 The generated turbulence satisfied the prescribed integral length scales and
 200 Reynolds stress-tensor values. The integral length scales L_x, L_y and L_z in the
 201 streamwise, vertical and lateral directions respectively were estimated from data
 202 presented in Castro et al. (2006) and shown in Fig. 2. **Xie & Castro (2008)**
 203 **performed LES for different length scale combinations imposed at**
 204 **inlet (i.e. L_x, L_y and L_z factored by 0.5, 1 or 2). It was found that the**
 205 **results of mean velocity and turbulent stresses within or immediately**
 206 **above the canopy were insensitive to the precise inflow length scales.**

207 The prescribed mean velocity and Reynolds stresses were obtained from the
 208 wind tunnel experiment reported in Castro et al. (2017) by assuming lateral ho-
 209 mogeneity. **Fig. 3a shows the prescribed mean velocity profile. Castro**
 210 **et al. (2017) fitted the profile in the usual log-law form $U = \frac{u^*}{\kappa} \ln \left(\frac{z-d}{z_0} \right)$**
 211 **with $z_{01} = 1.8mm$, $d = 0$ and by assuming $\kappa = 0.41$. They also estimated**
 212 **that the friction velocity u^* is $0.067U_{ref}$ at $7h$ upstream of the array.**
 213 **This is consistent with the peak Reynolds shear stress measured at**
 214 **the same location.**

215 4. Results

216 The turbulence and dispersion predictions produced using the inflow method
217 were compared against LES predictions made using periodic boundary condi-
218 tions at the inlet and outlet and the wind tunnel experiment data reported in
219 Castro et al. (2017). The Reynolds numbers of the flows over the array were
220 similar in all three cases.

221 A representative atmospheric boundary layer profile was generated in the
222 experiment by a set of Irwin spires at the entry of the working section and
223 an array of thin 2D plates (height $\sim 0.3h$) placed upstream of the cuboid ar-
224 ray. **As mentioned, the experimental and LES value of the upstream**
225 **roughness length was $z_{01} = 1.8mm$ whereas the roughness length of the**
226 **array of cuboid elements was $z_{02} = 5.6mm$ as in Castro et al. (2017).**
227 This meant that an IBL was created from the leading edge of the array which
228 developed in the downstream direction.

229 The development of the IBL was captured by the simulation made using
230 the turbulence inflow generation method with prescribed turbulence statistics
231 (§ 3.3), but was not by the simulation based on using periodic boundary con-
232 ditions (PBC) at the inlet and outlet. This was because the PBC simulation
233 effectively modelled the array as a single repeated unit of an infinite domain.
234 One might therefore expect the inflow boundary condition (IBC) simulation to
235 give a more accurate prediction of flow characteristics measured in the exper-
236 iment, not only within the IBL but also above it when compared to the PBC
237 simulations.

238 4.1. Flow and turbulence

239 For a simulation to accurately predict the dispersion of a pollutant it must
240 accurately predict the turbulence statistics of the flow. This was assessed by
241 examining the mean velocity and second-order statistics in the middle of the
242 short streets (e.g. position P of Fig. 1) normalized by the reference velocity.

243 For the IBC case the results were averaged at the four locations equivalent
244 to point P in Fig. 1 after the seventh row of cuboids at $x = 15h$. Whereas the

PBC results produced by Castro et al. (2017) were averaged over all equivalent locations within the array. The experimental data were averaged in time over 3 minutes, but not in space. The wind tunnel errors were assumed to be 2% for \overline{U} , 10% for $\overline{u'u'}$ and 5% for $\overline{v'v'}$ and $\overline{w'w'}$, respectively.

The IBC predictions for mean velocity (Fig. 4a) were found to be in good agreement with the experimental data below the canopy and up to $y = 2h$. Above that height, the IBC results slightly over-predicted while the PBC under-predicted the mean velocity.

Fig. 4b shows that the streamwise Reynolds stress was predicted more accurately by the IBC simulation than the PBC. The peak stress occurred at the canopy height and was successfully captured by the IBC. The Reynolds stress profile above the canopy was also well predicted. The PBC simulation under-predicted the peak streamwise stress at the canopy height, and over-predicted the streamwise stress for $y/h > 3$.

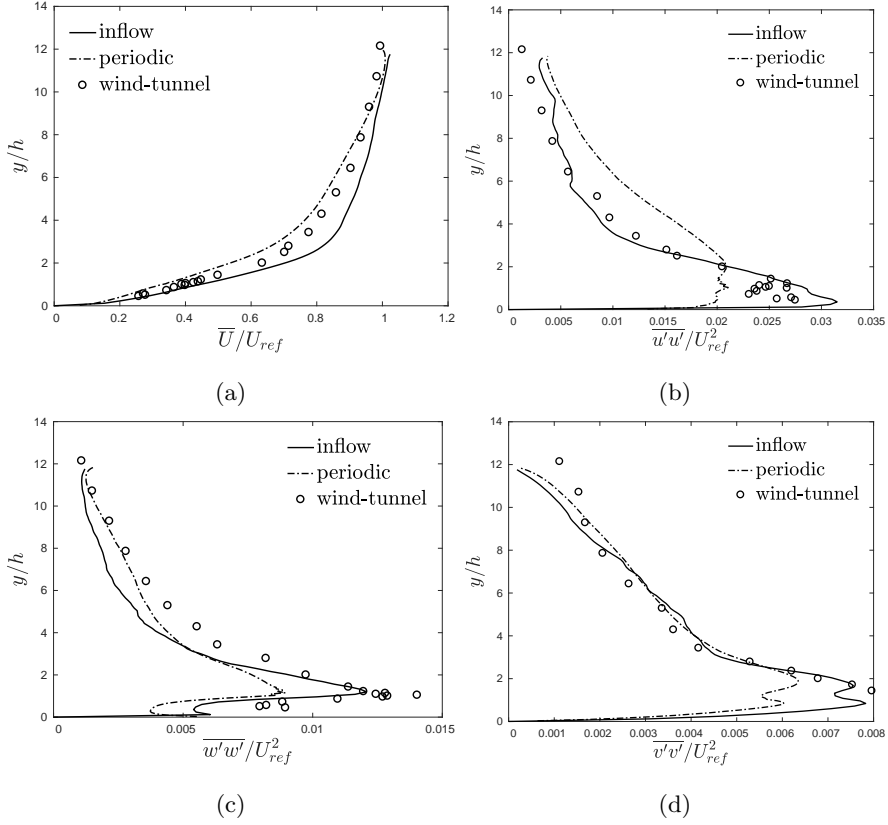


Figure 4: (a) IBC and wind tunnel mean velocity profiles measured at $x = 15h$ and spanwise averaged for position P in Fig. 1. Periodic mean velocity values were averaged at all similar points across the array. Corresponding profiles of streamwise normal stress (b), lateral normal stress (c) and vertical normal stress (d).

259 The lateral Reynolds stress, $\overline{w'w'}$, was well predicted by the IBC below and
 260 immediately above the canopy as shown in Fig. 4c, but at greater heights it
 261 under-predicted the stress compared to the wind tunnel data.

262 The vertical stress (shown in Fig. 4d) was well predicted by both IBC and
 263 PBC simulations. Nevertheless, the inflow method gave more accurate results
 264 immediately above the canopy height. Close to the top of the domain, both LES
 265 computations underestimated the vertical stress because the vertical velocity
 266 gradient was fixed to zero by the symmetric boundary condition.

267 The results show that imposing inflow turbulence using IBC captured the

268 transition from a rough to a very rough wall and led to predicted Reynolds
 269 stresses that were in better agreement with experimental results below and
 270 immediately above the canopy than those obtained from the PBC approach.
 271 This confirmed that the IBC method provided a better approach to predicting
 272 the characteristics of the flow below and immediately above the canopy.

273 *4.2. Growth of the internal boundary layer*

274 The transition from the relatively smooth surface ahead of the array to
 275 the much higher roughness of the array itself causes an IBL to develop from
 276 the leading edge of the obstacles. The IBL increases in depth as it develops
 277 downstream through the array and the flow within it is characterised by having
 278 greater turbulent kinetic energy (TKE) than that in the external boundary
 279 layer above it. As TKE is the primary driver of dispersion, it is expected that
 280 the location of the interface between the internal and external boundary layers
 281 will be have an important influence on the dispersion of material from a source
 282 within the array.

283 Three methods were used to determine the interface between the internal
 284 and external boundary layers along the length of the array in the IBC simula-
 285 tion. Method I was that developed by Antonia & Luxton (1972). Fig. 5 shows
 286 the result of applying method I using normalized velocity profiles obtained by
 287 averaging over 48 lateral positions, for nine streamwise locations (a vertical off-
 288 set is imposed for ease interpretation). The regions related to the internal and
 289 external boundary layers were then linearly fitted to a residual error of less than
 290 2%.

291 The first velocity profile was taken at $x = -2.5h$ ($3h$ upstream of the leading
 292 edge LE of the array in Fig. 1) where the mean velocity profile approaching the
 293 urban array is shown. There is no IBL at that point, and the profile cannot
 294 be linearly fitted. At the second location, at $x = 2h$ ($1.5h$ downstream of the
 295 leading edge) the profile is distinctly different and has two linear fits, whose
 296 intersection identifies the edge of the IBL ($x = 2h$, $y = 1.8h$). Following the
 297 same approach, the edge of the IBL can be identified for a further 7 downstream

298 locations and the evolution of the interface derived.

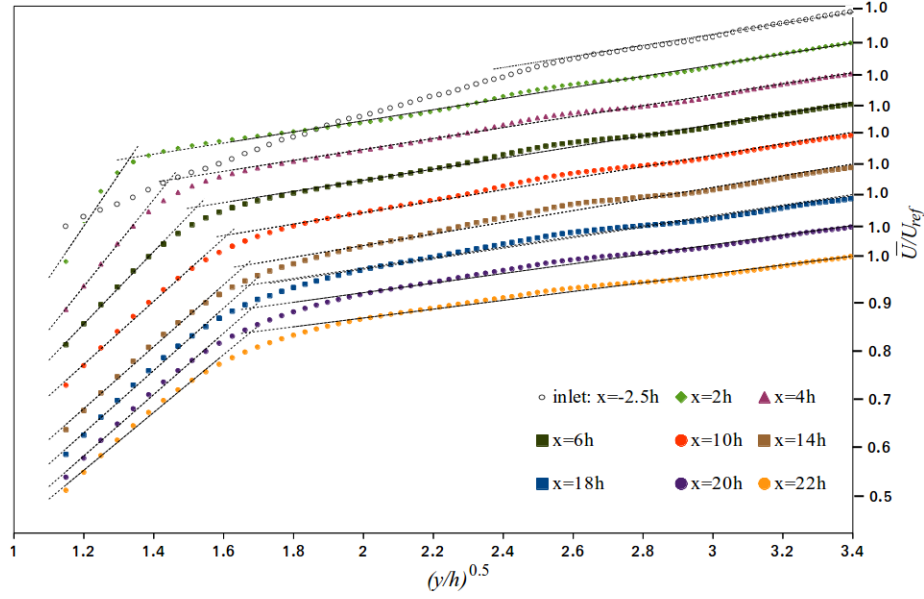


Figure 5: Laterally averaged mean velocity profiles in 9 streamwise locations: 1 upstream and 8 downstream of the leading edge (LE). The velocity profiles are shifted upwards to facilitate interpretation.

299 Method II was that developed by Efros & Krogstad (2011) based on plotting
 300 the streamwise Reynolds stress component normalized by the friction velocity
 301 u^* , i.e. $\overline{u'u'}^+$, against the height normalized by the domain height H . Method II
 302 was applied by calculating the streamwise stress profile at the same x -locations
 303 and averaged over 48 lateral positions as previously. The profiles within the
 304 external and IBL were then linearly fitted to a residual error less than 5%.
 305 The edge of the IBL was again found at each location and its growth with
 306 downstream distance is shown in due course.

307 The flow over an array of cuboid obstacles is a complex, anisotropic 3D
 308 turbulent flow. This complexity means that if the TKE generated upstream of
 309 the leading edge is similar to that produced downstream, then identifying the
 310 interface between the internal and external boundary layers may be difficult.

311 **A more accurate method for defining the edge of the IBL helps to**

analyse flow and dispersion mechanisms over such roughness transition regions, in particular in some specific scenarios such as in stable stratification (e.g. Kanda & Yamao, 2016). A step change over cuboid elements with uniform height, perpendicular to the flow direction, determines a more visible interface. The interface is more well-defined as greater is the difference between the TKE below and above it. Therefore, a more accurate method for defining the edge of the IBL helps to analyse flow and dispersion mechanisms over such roughness transition regions.

Given that the IBL grows in the vertical direction and a laterally homogeneous flow is assumed above the canopy, then it may be hypothesised that the use of a wall-normal parameter may make identifying the interface easier.

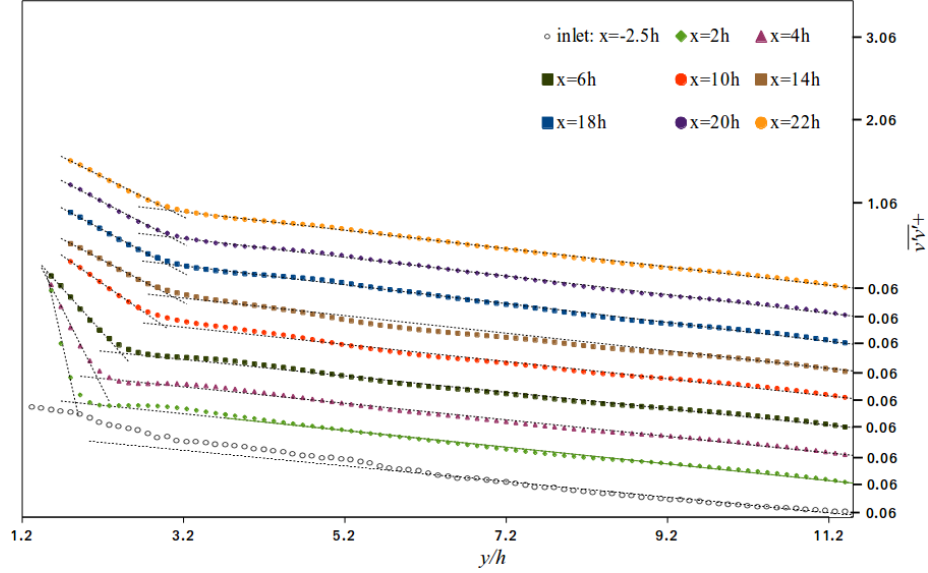


Figure 6: Laterally averaged vertical Reynolds stress profiles at 9 streamwise locations: 1 upstream and 8 downstream of the leading edge (LE). The stress profiles are shifted downwards to facilitate interpretation.

This paper tests a method based on the wall-normal turbulent variance $\overline{v'v'}$, referred to as method III. Fig. 6 shows the vertical Reynolds stress profiles

326 normalized by the friction velocity u^* , i.e. $\overline{v'v'}^+$, plotted against the height
 327 normalised by the domain height H , in a similar way to applying methods I and
 328 II. The Reynolds stress profiles for the external and IBL regions were linearly
 329 fitted to a residual error of less than 1%.

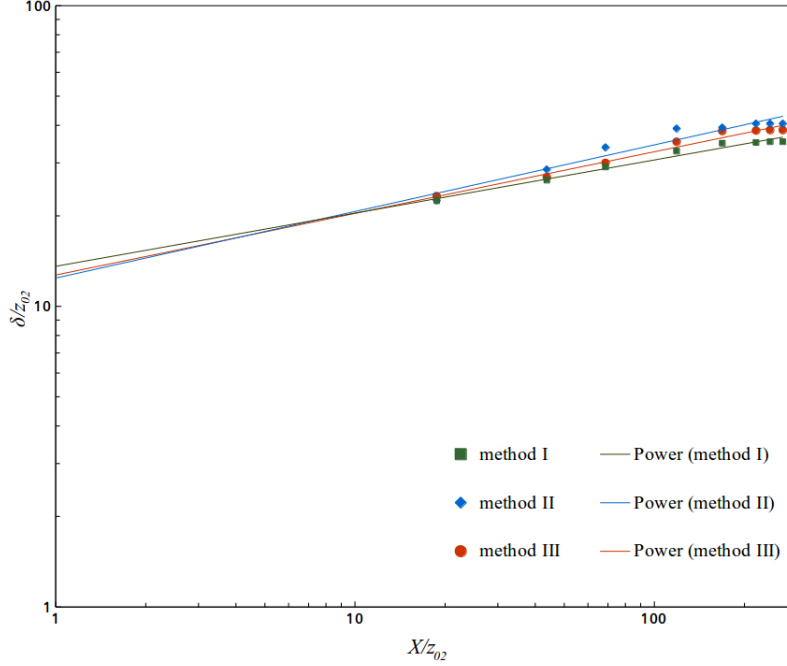


Figure 7: IBL depth δ derived by using the mean velocity \bar{U} (method I, square green), the streamwise stress $\overline{u'u'}$ (method II, diamond blue) and the vertical stress $\overline{v'v'}$ (method III, circle red). These data fit to power-law profiles with lines respectively.

330 Fig. 7 shows the result of fitting the IBL depth data derived from the three
 331 methods to the Elliott (1958) power-law formula (Eq. 1). The residual error of
 332 the power-law fit for method I (\bar{U}) was less than 3% with exponent $P = 0.18$
 333 and coefficient $a = 13.59$:

$$\frac{\delta}{z_{02}} = 13.59 \left(\frac{X}{z_{02}} \right)^{0.18}, \quad (8)$$

334 The residual error of the power-law fit for method II ($\overline{u'u'}$) was less than

335 6% with exponent $P = 0.22$ and coefficient $a = 12.42$:

$$\frac{\delta}{z_{02}} = 12.42 \left(\frac{X}{z_{02}} \right)^{0.22}. \quad (9)$$

336 Lastly, the residual error of the power-law fit for method III ($\overline{v'v'}$) was less
337 than 2.5% with exponent $P = 0.21$ and coefficient $a = 12.71$:

$$\frac{\delta}{z_{02}} = 12.71 \left(\frac{X}{z_{02}} \right)^{0.21}. \quad (10)$$

338 The fitted results (Eqs.8–10) from the three methods all confirmed that near
339 the step change in roughness ($X/z_{02} < 300$) the exponent P of the power-law
340 formula is much lower than the value $P = 0.8$ found in literature for $X/z_{02} >$
341 1000. Moreover, the estimated coefficient a is much higher than the range
342 of values suggested by Elliott (1958). This is perhaps not surprising as the
343 fitted results are dependent on the details of step change in roughness and the
344 characteristics of the roughness elements.

345 The fitted results from the three methods are consistent. Of the three meth-
346 ods analysed here, the IBL heights derived from method III were fitted to the
347 power-law formula with the lowest residual error. The coefficient $a = 12.71$ is
348 not significantly different from $a = 10.56$ obtained in Cheng & Castro (2002),
349 which studied the height of an internal boundary layer over an array of two-
350 dimensional rib-type roughness elements at a range $X/z_{02} < 1000$. Nevertheless,
351 the exponent $P = 0.21$ was significantly different from that $P = 0.33$ found by
352 Cheng & Castro (2002). Again, this is owing to the difference of the roughness
353 elements between the current study and Cheng & Castro (2002). We specu-
354 late that the two-dimensional rib-type elements used in Cheng & Castro (2002)
355 may yield a steeper IBL than that by using the three-dimensional cuboid type
356 elements in the current study.

357 4.3. Point source dispersion

358 The point source dispersion was simulated by a source placed at point ‘S’ in
359 Fig. 1 at $x = 14h$ and $z = -1.5h$. Although the source size and location were

360 similar in the experiment and LES simulations, the source shape was substan-
 361 tially simplified in the LES.

362 The mean scalar concentration \overline{C} was normalized as follows:

$$\overline{C^*} = \overline{C} \frac{U_r L_{ref}^2}{Q} \quad (11)$$

363 where the characteristic length L_{ref} was the building height h and Q was
 364 the emission rate. **Because LES predictions with inlet-outlet periodic**
 365 **boundary conditions differed from the experimental wind profile and**
 366 **turbulence statistics above $y \sim 3h$ (Castro et al., 2017), the mean**
 367 **velocity at $y = 3h$ and $x = -2.5h$ was chosen here as the reference**
 368 **velocity U_r .** Similarly, the scalar variance $\overline{c'c'}$ was normalized as:

$$\overline{c'c'^*} = \left[\frac{\sqrt{\overline{c'c'}} U_r L_{ref}^2}{Q} \right]^2. \quad (12)$$

369 Coceal et al. (2007) defined the near-field as being within a distance of
 370 $2 \sim 3h$ from the source. Within the near-field the results are likely to be affected
 371 by the source shape, size and location, but in the far-field ($> 3h$) turbulent
 372 mixing would be expected to show little memory of the source characteristics
 373 and the results are expected to be insensitive to the shape of the source.

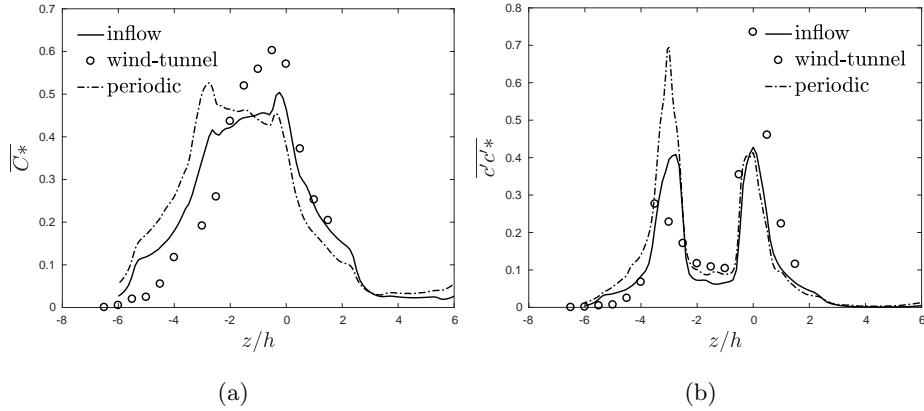


Figure 8: (a) Inflow, periodic and wind tunnel normalized mean concentration values measured at $x = 16h$ and $y = 0.5h$, resulting from a source at $x = 14h$ and $z = -1.5h$. (b) Normalized mean scalar variance measured at $x = 16h$ and $y = 0.5h$.

374 The IBC LES concentration data were compared against the PBC LES and
 375 wind tunnel experiment data reported in Fuka et al. (2017). The first com-
 376 parison was of data taken in the near-field along a lateral line at $x = 16h$ and
 377 $y = 0.5h$. For both sets of LES data the averaging process was long enough
 378 (180 flow-passes) to give fully converged results. The results for the dimension-
 379 less mean concentration and scalar variance are shown in Fig. 8a and Fig. 8b
 380 respectively. The wind tunnel standard error for the mean concentration \overline{C} was
 381 2% .

382 Both PBC and IBC results for mean concentration in the near-field (Fig. 8a)
 383 showed two non-symmetric peaks located in alignment with the corners of the
 384 upwind obstacle. Recalling that the source was located in the centre of the long
 385 ‘street’ (position $z = -1.5h$), the IBC highest peak was located on the right side
 386 of the source and the PBC highest peak on the left (when looking downwind).
 387 In contrast, the experimental data showed a single peak on the right side of the
 388 source at $z = 0h$.

389 The flow around the obstacle downwind of the source determines how the
 390 scalar plume divides into the left and/or right channels. In the experiment and
 391 the IBC case the plume was found to be mainly transported down the right-
 392 hand street, rather than the left. The asymmetry in the experimental results was
 393 suspected to be due to imperfect alignment of the array and/or a small effective
 394 offset in the flow direction. The wind tunnel alignment error is expected to be
 395 of the order of 0.25° (Fuka et al., 2017).

396 The PBC LES simulation had periodic boundary conditions applied to the
 397 lateral sides of the domain, so symmetric results might be expected in the span-
 398 wise direction. That the results were found to be asymmetric was perhaps due
 399 to strong 3-dimensional anisotropic turbulence leading to non-zero spanwise ve-
 400 locity on the lateral boundaries.

401 Whether the peaks matched on either the right or left side close to the source
 402 was considered to be arbitrary, and of little importance to the results of any far-
 403 field analysis. The near-field LES and wind tunnel results were both sensitive
 404 to the local flow details at the 0° wind direction. Except for the peak alignment

discrepancies discussed above, the LES with IBC simulation captured the lateral size of the plume and scalar peak mean values well.

Numerical predictions and measurements of the spanwise scalar variance at a height of $y = 0.5h$ and distance $x = 16h$ are compared in Fig. 8b. The experimental results again show a higher peak to the right of the source position, indicating that the plume drifted to the right, whereas the LES with PBC results show a higher peak to the left of the source. The LES with IBC shows two peaks which are almost symmetric about the source position. These results are consistent with those discussed above. As no standard error data are available for the experimental scalar variance measurements no further conclusions can be drawn.

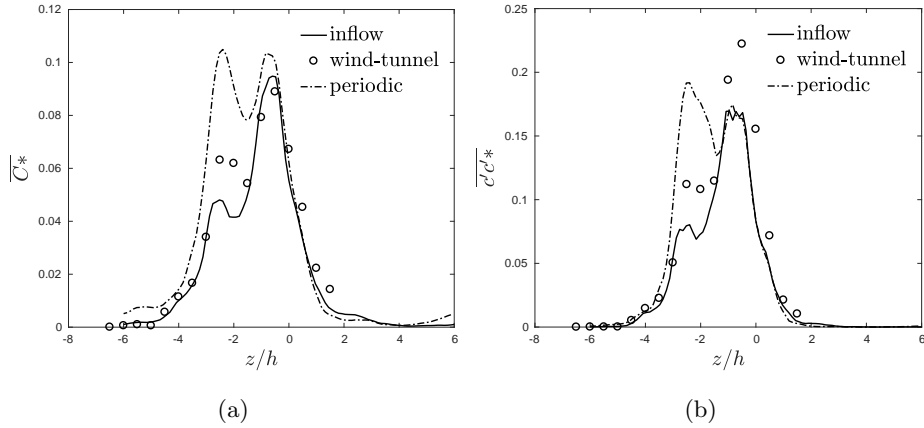


Figure 9: (a) Inflow, periodic and wind tunnel normalized mean concentration data measured above the canopy at $x = 16h$ and $y = 2h$, for a source at $x = 14h$ and $z = -1.5h$. (b) Normalized mean scalar variance measured at $x = 16h$ and $y = 2h$.

Fig. 9a and Fig. 9b show a comparison of the spanwise variation in mean concentration and variance data above the canopy at $y = 2h$ and $x = 16h$. In this case some of the wind tunnel sampling stations might approach or cross the edge of the plume. If this was so, fluctuations in concentration and intermittency would make accurate agreement between modelling and experiment difficult to achieve. Fig. 9a also shows that the mean concentration profiles are not in a

422 Gaussian shape. Nevertheless, the IBC results were found to be in fair agreement
 423 with the wind tunnel measurements, with both the magnitude and the lateral
 424 size of the plume being well predicted.

425 Although the alignment of both the IBC and experimental plumes on the
 426 same side is considered to be fortuitous, the higher peak is well captured and
 427 the lower peak only slightly underestimated. The double peak of the measured
 428 variance was also fairly well predicted by the IBC method. The PBC results
 429 were also in fair agreement with the wind tunnel measurements in terms of
 430 magnitude and the lateral size of the plume. In contrast to the experimental
 431 and IBC LES results, the PBC LES results show almost symmetric double peaks
 432 for the mean concentration, although there is more asymmetry in the variance.
 433 The IBC results were qualitatively closer to the experimental data than the
 434 PBC ones.

435 From the results above, it appears that based on the array geometry and
 436 locations examined, the IBC method leads to a superior prediction of scalar
 437 dispersion than the PBC one, in that it captures the asymmetry observed.
 438 This is believed to result from the better agreement between measurements
 439 of Reynolds stresses and IBC predictions immediately above the canopy § 4.1.

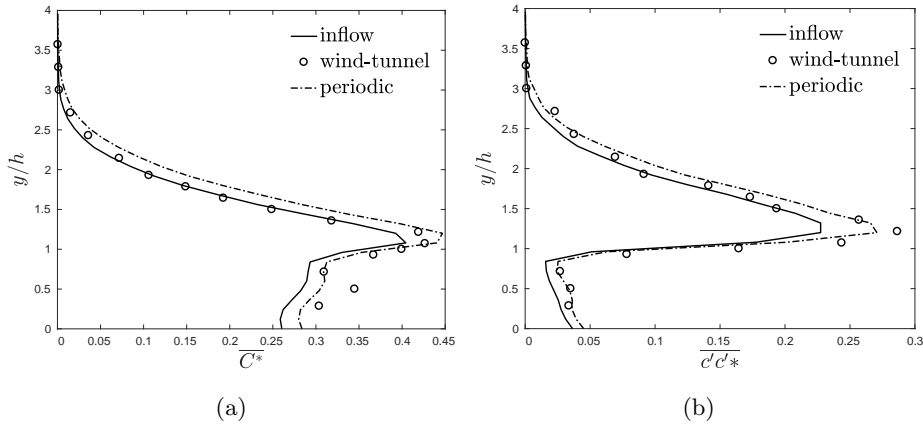


Figure 10: (a) Inflow, periodic and wind tunnel normalized mean concentration measured at $x = 18h$ and $z = -1.5h$, resulting from source at $x = 14h$ and $z = -1.5h$. (b) Normalized mean scalar variance measured at $x = 18h$ and $z = -1.5h$.

Further comparisons were made between simulations and measurements of mean concentration and variance in the far-field along a vertical line at $x = 18h$, $z = -1.5h$ (Fig. 10a and Fig. 10b). Examination of Fig. 10a shows that both LES IBC and PBC predictions for mean concentration and concentration variance are in fair agreement with the experimental results below $y = 1.5h$. However, the IBC predictions are consistently better than the PBC ones above $y = 1.5h$. Given the differences observed in the near-field, the similarity between these IBC and PBC far-field results confirms that beyond two rows downstream of the source, the effect of the difference in size and shape of the source becomes negligible and one can expect more accurate comparisons.

4.4. Interface effects on dispersion

The mechanisms that affect dispersion below and above the urban canopy depend on the position of the source. For example, if the source is placed in the wake of an obstacle in a recirculation zone, the plume is effectively transported upwards either by the mean flow or by the turbulent Reynolds stresses (Fuka et al., 2017; Tomas et al., 2017; Brixey et al., 2009). The dimensionless vertical flux components were defined in Fuka et al. (2017) as follows:

$$\psi_{adv}^{v*} = \overline{V} \overline{C} \frac{h^2}{Q} \quad (13)$$

$$\psi_{turb}^{v*} = \overline{v'c'^*} = (\overline{VC} - \overline{V} \overline{C}) \frac{h^2}{Q} \quad (14)$$

where v' and c' are the vertical velocity fluctuation and the scalar fluctuation respectively and \overline{V} is the mean vertical velocity. It is these fluxes, the advective vertical concentration flux (Eq. 13) and the turbulent vertical concentration flux (Eq. 14), that determine the exchange of pollutants between the canopy flow and the boundary layer above.

In the wakes of obstacles the mean vertical velocity and the vertical velocity fluctuation are not negligible, and both flux components contribute to the upwards transport of the scalar. Above the canopy the mean vertical velocity decreases significantly because the flow is predominantly parallel to the array

467 canopy, nevertheless, the vertical fluctuation component may still remain sig-
 468 nificant. This means though that the vertical turbulent concentration flux may
 469 contribute more than the advective flux to the upwards transport of the plume
 470 above the canopy and close to the IBL interface.

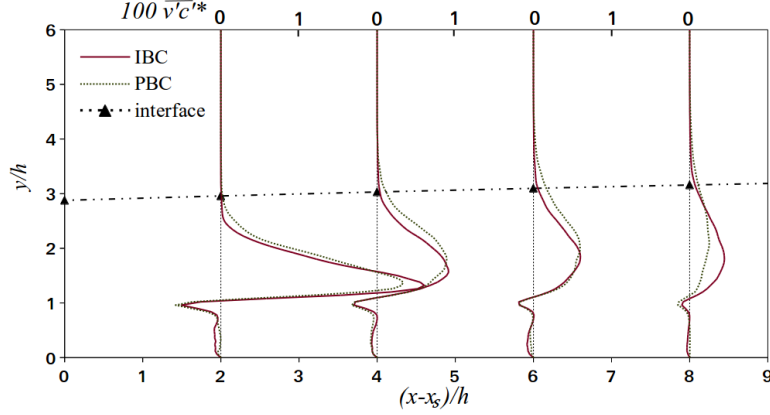


Figure 11: Turbulent vertical flux $\overline{v'c'^*}$ profiles scaled by 100 at four locations downstream of the source position ($x_s = 14h$ and $z_s = -1.5h$, Fig. 1). The black dashed line shows the IBL interface over the block array.

471 In Fig. 11, the vertical turbulent flux profile $\overline{v'c'^*}$ (Eq. 14) calculated by
 472 using LES IBC and LES PBC predictions is shown at four streamwise locations
 473 downstream of the source. The black dashed line represents the interface of
 474 the IBL as calculated in § 4.2 using method III. The vertical profiles in Fig. 11
 475 suggest that the edge of the plume grew from the source and matched the
 476 interface after 2 rows of cuboids, as further downstream both the interface and
 477 the edge of the plume were found to be approximately at the same elevation.

478 The IBC turbulent flux profiles at all the x-locations analysed decayed
 479 sharply when approaching the IBL interface. Looking at the flux profiles at
 480 $(x - x_s) = 2h$, a much sharper decay is observed in the IBC profile as the inter-
 481 face is approached than in the PBC one. Similarly, at positions $(x - x_s) = 4h$
 482 and $(x - x_s) = 6h$ the IBC flux profiles decay more rapidly than the PBC pro-
 483 files when approaching the IBL interface. However, at position $(x - x_s) = 8h$,
 484 the IBC vertical flux was observed to be higher than the PBC flux below the

485 interface, but lower above it. This trend shows that vertical transport of the
 486 scalar between the internal and external boundary layers is being constrained
 487 by the interface. Moreover, because the IBL interface is defined using method
 488 III, the distinct changes in vertical flux profile appear related to similar changes
 489 in the vertical Reynolds stress $\overline{v'v'}$ noted in § 4.2.

490 Dispersion from a ground-level point source is a 3D problem. In order to
 491 understand whether vertical constraint by the IBL interface enhanced the lateral
 492 spreading of the plume, the lateral turbulent fluxes were also analysed. The
 493 turbulent component of the lateral concentration flux was defined as follows:

$$\psi_{turb}^{w*} = \overline{w'c'^*} = (\overline{WC} - \overline{W}\overline{C}) \frac{h^2}{Q} \quad (15)$$

494 where w' and c' are the lateral velocity fluctuations and scalar fluctuations
 495 respectively, and \overline{W} is the mean lateral velocity. The lateral turbulent flux
 496 regulates the diffusion of the plume in positive or negative spanwise directions
 497 and determines the lateral extent of the plume.

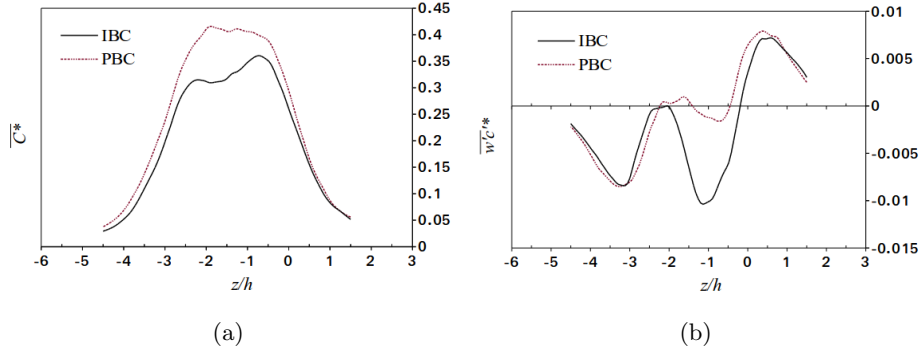


Figure 12: (a) Spanwise normalized mean concentration predictions at $x = 18h$ and $y = 1.5h$.
 (b) Spanwise normalized lateral flux predictions at $x = 18h$ and $y = 1.5h$, resulting from a
 ground level source at $x = 14h$ and $z = -1.5h$.

498 Fig. 12a and 12b show the LES IBC and PBC mean concentration and
 499 lateral flux predictions at $x = 18h$ (i.e. two rows downstream from the source)
 500 and $y = 1.5h$ in the spanwise direction. The spanwise location of the source is
 501 $z = -1.5h$, and the mean concentration is normalized as in Eq. 11.

502 In common with the results at $x = 16h$ and $y = 2h$ shown in Fig. 9a, the
 503 IBC mean concentration in Fig. 12a shows a higher peak located to the right
 504 of the source ($z = -0.5h$) and a lower peak on the left ($z = -2.5h$). Whereas
 505 the PBC mean concentration shows one symmetric peak close to the source's
 506 position. The double peak in the IBC mean concentration means that there are
 507 two zero-crossings of the IBC lateral flux (Fig. 12b). Between $z = -2.5h$ and
 508 $z = -0.5h$, the magnitude of the IBC lateral flux is much greater than that of
 509 the PBC flux. Outside of this range, the fluxes are very close in magnitude.

510 We fitted the mean concentration profiles to Gaussian distributions, and
 511 found that the width of the Gaussian profile for the IBC plume was slightly
 512 greater than that of the PBC. This is interesting given the greater lateral flux
 513 of the IBC. Fig. 4a shows that the mean streamwise velocity immediately above
 514 the canopy in the IBC simulation and the experiment are greater than that of
 515 the PBC, which yields a shorter convection time for the plume to develop. This
 516 might explain why the plume width above the canopy of the IBC is only slightly
 517 greater than that of the PBC.

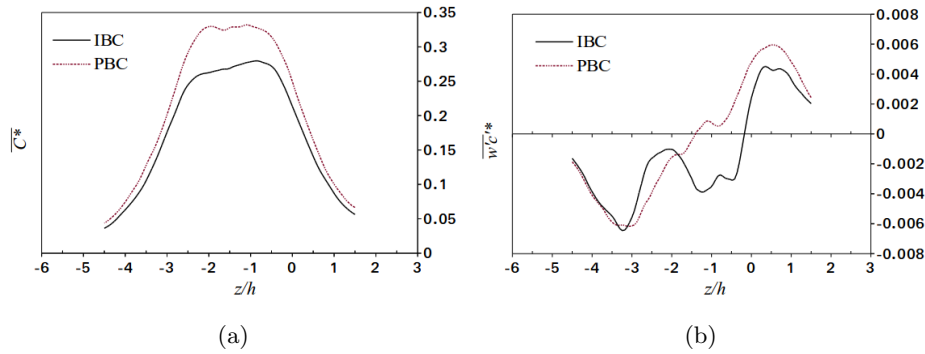


Figure 13: (a) Normalized mean concentration prediction at $x = 20h$ and $y = 1.5h$. (b) Inflow and periodic normalized lateral flux predictions at $x = 20h$ and $y = 1.5h$, resulting from a source at $x = 14h$ and $z = -1.5h$.

518 Following the same approach, the mean concentration and the lateral turbu-
 519 lent flux were analysed at $x = 20h$ (three rows downstream) and $y = 1.5h$ over
 520 the spanwise direction (Fig. 13a and 13b, respectively). The peak PBC mean

concentration in Fig. 13a is again greater than that of the IBC. The magnitude of IBC lateral flux in Fig. 13b is also again greater than the PBC flux near the core of the plume, and the width of the IBC plume was again found to be greater than that of the PBC. These findings are all consistent with those in Figs. 12a and 12b.

The mean concentration and lateral turbulent flux profiles in Figures 12 and 13 suggest that the lateral spreading of the IBC plume is greater than that of the PBC plume. This is consistent with the greater lateral Reynolds stresses observed in the IBC profile than in the PBC profile at $y = 1.5h$ shown in Fig. 4c.

In the IBC simulations vertical transport of the scalar between the internal and external boundary layers is constrained by the lower TKE above the interface. The vertical constraint on the vertical Reynolds stress and the enhancement of the lateral Reynolds stress lead to increased lateral spreading of the IBC plume. This results in the lower mean concentrations observed in the IBC simulation than in the PBC one in Fig. 12a and 13a.

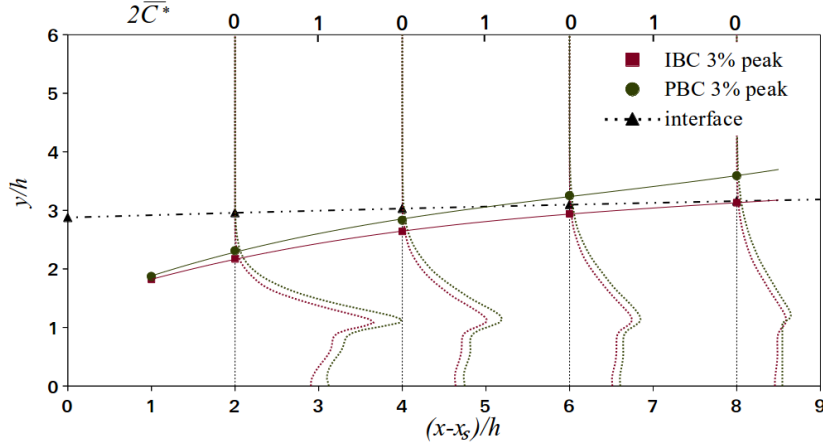


Figure 14: Dimensionless scalar concentration \overline{C}^* scaled by 2 in four locations downstream of the source position ($x_s = 14h$, $z_s = -1.5h$, Fig. 1). The black dashed line shows the IBL interface. The plume edge is taken as 3% of the local peak in both LES simulations.

Finally, in order to determine the position of the edge of the plume compared to the IBL interface, vertical profiles of the dimensionless mean concentration

were taken downstream of the source in several streamwise locations at $z = -1.5h$ (Fig. 14). The results of both PBC and IBC simulations were normalized as in Eq. 11 and compared. The origin of the coordinate system was fixed at the source position.

As far as we are aware, there is no generally accepted definition of the plume's edge. Therefore, the edge of the plume was identified here by considering the 3% value of the local-peak mean concentration measured at the canopy height. The aim here was to evaluate whether or not the predicted development of the plume when using the IBC method differed from that using the PBC. Hence, the choice of the percentage at which to define the plume edge was not critical. Nevertheless, sensitivity tests made using 1%, 5% and 10% values of the local concentration peak all showed similar plume growth rates.

The development of the plume when using IBC was found to be visibly different from the one by using PBC. This is shown in Fig. 14, in which the plume edge in the IBC simulation appears to asymptote to the IBL interface. Whereas when inlet-outlet PBC are used, the roughness boundary layer grows indefinitely up to the top of the domain which allows the plume to continue to expand vertically. This is a result of the interface between the internal and external boundary layers only existing when the inflow method is applied. Within the simulated LES domain, the plume development appears to be influenced by the IBL interface location which leads to trapping of the scalar in the IBL and greater lateral spreading.

5. Conclusions and discussion

LES with prescribed IBC was used to simulate a rural-to-urban transition region where the change in surface roughness generates an IBL at the leading edge of a regular array of cuboids. The LES with IBC was found to provide an accurate simulation of the flow which predicted the TKE to be greater below the interface of the IBL when compared to the TKE obtained from LES with inlet-outlet PBC.

567 To our best knowledge the growth rate of the IBL depth has been evaluated
 568 for the first time by analysing the vertical Reynolds stress profiles in several
 569 streamwise positions. The vertical Reynolds stress method was found to define
 570 the IBL interface more clearly than existing methods based on mean streamwise
 571 velocity and streamwise Reynolds stress. It was further found that the IBL
 572 growth rate derived from the vertical stress method followed the power-law
 573 formula with a similar coefficient a as that derived by Cheng & Castro (2002)
 574 in the near roughness transition region ($X/z_{02} < 1000$), but with a significantly
 575 lower exponent $P = 0.21$ compared to $P = 0.33$ derived by Cheng & Castro
 576 (2002). We speculate this is owing to the difference of characteristics of the
 577 roughness elements within a range $X/z_{02} < 1000$.

578 LES predictions of turbulence and dispersion from a ground-level point
 579 source were compared against wind tunnel measurements reported in Castro
 580 et al. (2017) and Fuka et al. (2017). The impact of the interface between the in-
 581 ternal and external boundary layers on dispersion was then analysed by studying
 582 vertical and lateral profiles of dimensionless mean concentration and turbulent
 583 fluxes downstream of the source. The IBC vertical scalar turbulent flux pro-
 584 files decayed more rapidly than the PBC profiles when approaching the IBL
 585 interface. We speculate that the distinct changes in IBC vertical flux profiles
 586 appear related to similar changes in the vertical Reynolds stress. Furthermore,
 587 the lateral spreading of the IBC plume was found to be greater than that of
 588 the PBC plume, this was found to be correlated with greater values of lateral
 589 turbulent Reynolds stress. These features led to the plume's upper edge in
 590 the IBC simulation differing distinctly from that obtained by using inlet-outlet
 591 PBC. It is concluded that the presence of the IBL constrains vertical spreading,
 592 and so leads to trapping of the scalar. The development of the interface be-
 593 tween the internal and external boundary layers will also be affected by thermal
 594 stratification conditions, and further work should seek to quantify this.

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