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Turbulence Kinetic Energy Budget in the Urban-like Boundary Layer using Large-Eddy Simulation

Geng Tian^{1,2} · Boris Conan^{1,2} · Isabelle Calmet^{1,2}

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Abstract This work aims to describe and understand the turbulent processes at play in the lower part of the urban boundary layer through performing a large-eddy simulation of the flow over an urban-like canopy. This canopy is composed of a staggered array of cubes with a packing density of 25%, while the simulation models neutral thermal conditions at a Reynolds number (based on both velocity at the top of the domain and the domain height) of $Re = 50,000$. A dynamic Smagorinsky model is implemented in order to allow for energy backscattering from sub-grid scales. A wall refinement of the grid allows resolving the viscous sublayer. Turbulent statistics up to the third order, as well as each term of the turbulence kinetic energy budget, are computed individually everywhere in the domain. Results are discussed in relation to experimental and numerical data from the literature in order to describe the turbulent energy transfers occurring in the roughness sublayer. The fine grid resolution close to surfaces serves to analyze in depth the three-dimensional distribution of turbulence production inside the urban canopy layer. This analysis in turn leads to discovering areas, never previously documented in an urban-like canopy, of highly positive and highly negative production close to the surface, away from the well-known high production area in the shear layer. Furthermore, evidence of a close link between high and low production areas near the surfaces and singular points in the mean flow is presented, thus laying the groundwork for a simple pre-diagnostic tool to detect TKE production areas near surfaces.

Keywords Large-eddy simulation · OpenFOAM · Turbulence kinetic energy budget · Turbulence production · Urban canopy layer · Wall-bounded flow

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1 Introduction

In the context of rapid urbanization, an understanding and accurate modeling of turbulent flow in the urban boundary layer (UBL) is of great importance in evaluating the influence of urban design on air quality and urban climate. The roughness sublayer (RSL) is the lowest part of the UBL (Oke, 1997) and where high momentum, heat and mass exchanges between the urban canopy layer (UCL) and the atmosphere take place (Rotach, 1999). The RSL extends from the ground surface up to 2 to 5 times the average building height, depending on the geometric arrangement of the element (Raupach et al., 1991; Cheng et al., 2007). The presence of roughness elements gives rise to complex flows consisting of vortical structures and low-momentum regions (Coceal et al., 2007b). The UCL is the lowest part of the RSL, lying below the average building height, where the flow is directly influenced by ground obstacles.

Over the past few decades, a number of field experiments (Christen et al., 2009; Inagaki and Kanda, 2010; Roth et al., 2015; Perret et al., 2016) and wind tunnel experiments (Macdonald, 2000; Cheng and Castro, 2002; Kastner-Klein and Rotach, 2004; Castro et al., 2006; Blackman and Perret, 2016; Blackman et al., 2017; Herpin et al., 2018; Monnier et al., 2018) have been conducted to investigate the nature of turbulence over urban-like canopies. These studies have extended the understanding of turbulent flow characteristics by determining the mean flow and main turbulent processes occurring within the RSL as a function of obstacle density, arrangement and height. Unsteady urban-like canopy flows have also been studied by means of Computational Fluid Dynamics (CFD) simulations using Direct Numerical Simulation (DNS) (Coceal et al., 2006, 2007a,b; Leonardi and Castro, 2010) and Large-Eddy Simulation (LES) (Kanda et al., 2004; Xie and Castro, 2006; Bou-Zeid et al., 2009; Kono et al., 2010; Tomas et al., 2016). Numerical studies show good agreement on both mean flow and turbulence statistics compared to the wind tunnel results. Since LES explicitly resolves the large flow-scales and introduces a subgrid-scale (SGS) model to parameterize the small-scale processes, it is considered as a powerful tool for simulating 3D unsteady flow more effectively than DNS when dealing with high Reynolds number flows. Numerical studies have made it possible to investigate non-neutral conditions and yielded a spatial description of the mean flow and standard turbulent characteristics (Tomas et al., 2016; Coceal et al., 2007a). More recently, several combined experimental/numerical studies have also been performed on cuboidal arrays (Tomas et al., 2017; Castro et al., 2017).

The turbulent mechanisms responsible for energy transfers both within and above the RSL can be investigated using the turbulence kinetic energy (TKE) budget. This method, based on an analysis of TKE sources and sinks in a fully-developed turbulent flow, serves to analyze TKE transfers. Over a flat and homogeneous surface, TKE production, an unsteady phenomenon by its very nature, is partially driven by hairpin-like turbulent structures near the ground (Adrian, 2007). The TKE budget terms only vary in the direction perpendicular to the surface and, far enough from the surface, a balance between

76 production and dissipation is observed (Kim et al., 1987; Lyons et al., 1989;
77 Brooke and Hanratty, 1993). This property characterizes the energy transfer
78 between scales in the inertial subrange and is the basis for several turbulence
79 models and wall boundary conditions (Hudson et al., 1996).

80 The presence of obstacles inside an urban canopy layer is expected to de-
81 stroy the homogeneity of the time-averaged TKE budget terms of a flat plate.
82 Indeed, over a single wall-mounted cube, Yakhot et al. (2006) observed the dis-
83 tribution of production and enlighten negative production areas close to the
84 foot of a cube and on its front face. They describe negative production regions
85 by discussing the sign and magnitude of each production term. They suggest
86 that "the flow dynamics in front of a cube is strongly affected by the negative
87 energy production" and underline their proximity with stagnation lines.

88 In their experimental work on an urban-like arrangement of cubes, Castro
89 et al. (2006) computed vertical profiles of the TKE budget at several locations
90 upstream and downstream of a cube featuring a staggered arrangement. TKE
91 dissipation was estimated from power spectral density measurements, and the
92 pressure transport of TKE was deduced as the residual term needed to balance
93 the TKE budget. These authors showed that TKE production is highest after
94 the cube, where the shear stress (and vertical gradient of the velocity) is sig-
95 nificant. They also observed that production is nearly balanced by dissipation
96 above the RSL (greater than 4 times the obstacle height) and moreover that
97 turbulent transport is an energy sink within the shear layer, i.e. just above
98 the canopy. Blackman et al. (2017) investigated the TKE budget using Par-
99 ticle Image Velocimetry (PIV) over a 2D plane. In this work, the dissipation
100 rate was evaluated using a Large-Eddy PIV (LE-PIV) model, based on use
101 of a SGS model according to the methodology applied in LES. Despite some
102 interesting findings, experimental restrictions tended to prevent capturing the
103 three-dimensional flow field that often limits analysis of the TKE budget to
104 one or two spatial dimensions, requiring researchers reconstitute the missing
105 information (spatial gradients, dissipation) based on theoretical simplifications
106 or modeling (Castro et al., 2006; Blackman et al., 2017). In addition, experi-
107 mental constraints often prevent measuring turbulence very close to the wall.
108 As opposed to plant canopy flows (Dwyer et al., 1997; Finnigan, 2000; Yue
109 et al., 2008), very few numerical studies have analyzed in detail all TKE bud-
110 get terms in an urban-like canopy. Giometto et al. (2016) computed the TKE
111 budget over a realistic urban model and found that pressure transport is sig-
112 nificant in the near-wall regions, while turbulent transport transfers the TKE
113 produced above the canopy downwards into the urban canopy. Tomas et al.
114 (2016) explicitly computed all TKE budget terms in order to study the effect
115 of thermal stratification on the various terms, with an emphasis on the upper
116 part of the RSL and the inertial layer.

117 As reported in the aforementioned literature, the TKE budget is very different
118 around the obstacles of an urban-like boundary layer flow, as compared to a
119 flat plate boundary layer flow. However, existing studies are mostly focused on
120 the upper part of the RSL and leave open questions regarding TKE processes
121 inside the urban canopy layer, namely:

- 122 – What is the relative contribution of the TKE budget terms at different
 123 locations inside an idealized UCL?
 124 – How is TKE production spatially distributed in the UCL to maintain the
 125 boundary layer? To what extent does it differ from that of a flat plate or
 126 a single wall-mounted cube?
 127 – Can TKE production within the urban canopy layer be correlated with
 128 mean flow distinctive features?

129 This article proposes tackling these questions by setting up and running a
 130 fine-scale LES over an urban-like canopy in order to directly compute each
 131 term of the TKE budget inside and outside the UCL without the need for any
 132 theoretical assumptions or further modeling beyond those of an LES. Results
 133 reveal areas never before documented of strong positive and negative turbu-
 134 lence production inside the UCL, in addition to improving the understanding
 135 of the main turbulent mechanisms in the RSL.

136 This study focuses on the fully-developed neutral turbulent flow over an
 137 array of staggered cubes with a 25% packing density, representing an idealized
 138 infinite city. This choice has been made to enable analyzing highly-converged
 139 statistics. The LES described in Sect. 2 is applied in a $16h \times 12h \times 8h$ com-
 140 putational domain, where cubical obstacles of dimension h are explicitly rep-
 141 resented and where the mesh is refined close to the walls so as to resolve the
 142 viscous sublayer. A dynamic Smagorinsky SGS model (Germano et al., 1991) is
 143 specifically implemented in OpenFOAM to allow the model coefficient to vary
 144 within this highly heterogeneous flow. In Sect. 3, LES results are discussed and
 145 compared to literature data, including mean profiles up to the second-order
 146 momentum and turbulent spectra. Among the wind tunnel data, recent exper-
 147 iments performed in the LHEEA wind tunnel (Centrale Nantes Laboratory)
 148 provide a new dataset for assessing numerical simulations. Section 4 evaluates
 149 the TKE budget through a joint analysis with the wind tunnel measurements
 150 recorded by Blackman et al. (2017); also, a detailed analysis of TKE produc-
 151 tion is proposed via an in-depth description of its 3D organization. The final
 152 section collates the main outcomes and findings of this work.

153 2 Numerical Approach

154 2.1 The Governing Equations

155 The present LES is performed using the filtered Navier-Stokes equations for
 156 incompressible flows, as defined by the continuity equation:

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

157 and the conservation of momentum equation:

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

158 where \tilde{u}_i (for $i = 1, 2, 3$) are the filtered velocity components; \tilde{p} is the filtered
 159 pressure, ρ the reference density, ν the kinematic viscosity, and $\tau_{ij} =$
 160 $\tilde{u}_i\tilde{u}_j - \tilde{u}_i\tilde{u}_j$ the SGS stress tensor. The LES is carried out by means of a
 161 finite-volume method within the framework of the open-source C++ library
 162 OpenFOAM[®] 2.4.0 using MPI for interprocessor communication. The equa-
 163 tions are solved in space according to a second-order central scheme, while
 164 the temporal integration is performed by a second-order backward implicit
 165 scheme.

166 2.2 The Dynamic Smagorinsky Subgrid-scale Model

167 LES results are known to be sensitive to the choice of SGS model, especially in
 168 the vicinity of walls where small-scale structures are prevalent. The well-known
 169 Smagorinsky (1963) model, widely employed in atmospheric flow research (Xie
 170 et al., 2008; Boppana et al., 2010), assumes a local equilibrium of turbulence
 171 at small scales where shear production and dissipation are in balance. In this
 172 model, the deviatoric part of the SGS stress tensor is defined as:

$$\tau_{ij} - \frac{1}{3}\tau_{kk}\delta_{ij} = -2\nu_{sgs}\tilde{S}_{ij}, \quad (3)$$

173 where:

$$\tilde{S}_{ij} = \frac{1}{2} \left(\frac{\partial\tilde{u}_i}{\partial x_j} + \frac{\partial\tilde{u}_j}{\partial x_i} \right) \quad (4)$$

174 is the resolved strain rate tensor and the SGS kinetic viscosity ν_{sgs} is modeled
 175 as:

$$\nu_{sgs} = (C_S\tilde{\Delta})^2|\tilde{S}_{ij}|, \quad (5)$$

176 where $\tilde{\Delta} = \sqrt[3]{\Delta x\Delta y\Delta z}$ is the grid-filter width, C_S the model coefficient, and
 177 $|\tilde{S}_{ij}| = \sqrt{2\tilde{S}_{ij}\tilde{S}_{ij}}$. According to the Smagorinsky model, the isotropic part of
 178 the SGS stress tensor, which corresponds to the SGS energy, is not modeled
 179 but instead included in the pressure term of Eq. 1 so-called modified pressure
 180 (Calmet and Magnaudet, 1997; Tomas et al., 2016). In the flow regions where
 181 the SGS energy is strong, this modified pressure may vary significantly from
 182 the original pressure. In the following, the modified pressure values at the walls
 183 will be used to compute the drag force (Sect. 2.3). These values are expected
 184 to be close to the pressure values since the SGS energy is weak in the viscous
 185 sublayer. The modified pressure also serves to evaluate pressure transport in
 186 the TKE budget (Eq. 9), which involves the fluctuating part of the modified
 187 pressure. No evidence suggests that the SGS energy fluctuations would be
 188 negligible compared to the pressure fluctuations; nonetheless, we expect that
 189 this approximation will not exert undue influence on the statistical results.

190 The model coefficient C_S is typically prescribed to be a constant of a value
 191 ranging from 0.1 to 0.2 depending on the flow type. This *ad hoc* value, com-
 192 bined with the formulation of ν_{sgs} , prevents the model from simulating energy
 193 backscatter and results in an overestimation of modeled near-wall viscosity

194 if no damping is applied. To overcome this drawback, Germano et al. (1991)
 195 proposed a dynamic procedure allowing for the model coefficient to be locally
 196 computed. In this approach, a test-filter $\widehat{\widehat{G}} = \widehat{G} \widetilde{G}$ is defined with a charac-
 197 teristic width of $\widehat{\widehat{\Delta}} = a \times \widetilde{\Delta}$. The momentum equation (Eq. 2) filtered with $\widehat{\widehat{G}}$
 198 introduces a new SGS stress tensor, $T_{ij} = \widehat{\widehat{u_i u_j}} - \widehat{\widehat{u_i}} \widehat{\widehat{u_j}}$, which is an unknown
 199 as well as τ_{ij} . In the dynamic Smagorinsky model the deviatoric part of the
 200 SGS stress tensors at both the grid- and test-filter scales is modeled similarly
 201 to Eqs. 3 and 5, in assuming that model coefficient C remains independent of
 202 the filter scale:

$$\tau_{ij} - \frac{1}{3} \tau_{kk} \delta_{ij} = -2C \widetilde{\Delta}^2 |\widetilde{S}_{ij}| \widetilde{S}_{ij}, \quad (6)$$

203 and

$$T_{ij} - \frac{1}{3} T_{kk} \delta_{ij} = -2C \widehat{\widehat{\Delta}}^2 |\widehat{\widehat{S}}_{ij}| \widehat{\widehat{S}}_{ij}. \quad (7)$$

204 The algebraic identity of Germano et al. (1991) defines the tensor \mathcal{L}_{ij} as:

$$\mathcal{L}_{ij} = T_{ij} - \widehat{\widehat{\tau}}_{ij} = \widehat{\widehat{u_i u_j}} - \widehat{\widehat{u_i}} \widehat{\widehat{u_j}}, \quad (8)$$

205 which can be calculated explicitly by applying the filter $\widehat{\widehat{G}}$ to the resolved
 206 velocity field. From Eqs. 6, 7, and 8, the following can be written:

$$\mathcal{L}_{ij} - \frac{1}{3} \mathcal{L}_{kk} \delta_{ij} = CM_{ij},$$

207 where $M_{ij} = -2 \widetilde{\Delta}^2 (a^2 |\widehat{\widehat{S}}_{ij}| \widehat{\widehat{S}}_{ij} - |\widehat{\widehat{S}}_{ij}| \widehat{\widehat{S}}_{ij})$ with $a = 2$ in the present study.
 208 As suggested by Lilly (1992), the dynamic coefficient C is computed at each
 209 time step and at each computational cell using a least-squares method, through
 210 the relation:

$$C = \frac{\mathcal{L}_{ij} M_{ij}}{M_{ij} M_{ij}}.$$

211 An appropriate SGS model is necessary to ensure an accurate numeri-
 212 cal simulation, especially when analyzing flow close to a solid boundary. The
 213 dynamic approach has been successfully used for simple flows such as plane
 214 channel flows or recirculating flows (Calmet and Magnaudet, 1997; Zang et al.,
 215 1993). It is unquestioned that the advantage of the dynamic Smagorinsky
 216 model lies in its ability to consider the local change in model coefficient as il-
 217 lustrated in Fig. 1. However, this dynamic procedure may locally induce large
 218 negative values of the model coefficient C , giving rise to numerical instabili-
 219 ties. In order to avoid this problem, total viscosity ($\nu + \nu_{sgs}$) is forced to be
 220 locally a non-negative value. This method, called "clipping", can be found in
 221 Calmet and Magnaudet (1997) and Ferziger et al. (2002).

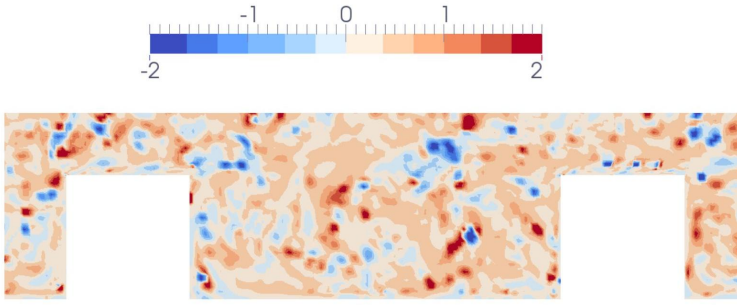


Fig. 1 Snapshot of the normalized dynamic Smagorinsky variable C/C_S^2 in a vertical plane with $C_S = 0.175$.

2.3 Simulation Set-up

Figure 2 shows the computational domain of dimension $16h \times 12h \times 8h$ in the streamwise (x), spanwise (y) and vertical (z) directions, respectively. This domain was chosen with reference to Coceal et al. (2007b) who successfully performed a DNS of the flow over an urban-like canopy. The floor is covered by a staggered array of cubes of uniform height (h) and a packing density of $\lambda_p = 25\%$.

Free-slip conditions are set at the top boundary of the domain, while no-slip conditions are prescribed at the floor and on all obstacle surfaces. Periodic boundary conditions are imposed in the spanwise and streamwise directions to simulate an infinite array of cubes. The flow is driven by a longitudinal pressure gradient adjusted at each time step to maintain a flow rate speed of 3.5 m s^{-1} . The Reynolds number (Re), based on both the velocity at the top of the domain and the domain height ($8h$), equals about $Re = 50,000$ and the friction Reynolds number, based on friction velocity u_τ and h is $Re_\tau = u_\tau h / \nu = 500$. The friction velocity u_τ is derived from the time-averaged total drag force (F) through the relation $u_\tau = \sqrt{\tau / \rho}$, with $\tau = F/A$ and $A = 16h \times 12h$, the total plane area. The total drag force is the sum of the pressure drag on the cubes, friction drag on the cubes and friction drag on the ground, with these contributions representing approximately 95%, 3.8% and 1.2 % of the total drag, respectively. The simulation details are summarized in Tab. 1.

Table 1 Main simulation parameters.

Array type	λ_p	$L_x \times L_y \times L_z$	h	u_τ	z_0	d	Re_τ	Re
Staggered	0.25	$16h \times 12h \times 8h$	0.02 m	0.40 m s^{-1}	$0.07h$	$0.74h$	500	50,000

Mesh size is an important parameter since, along with the considered Reynolds number, it determines both the size of the resolved eddies and the

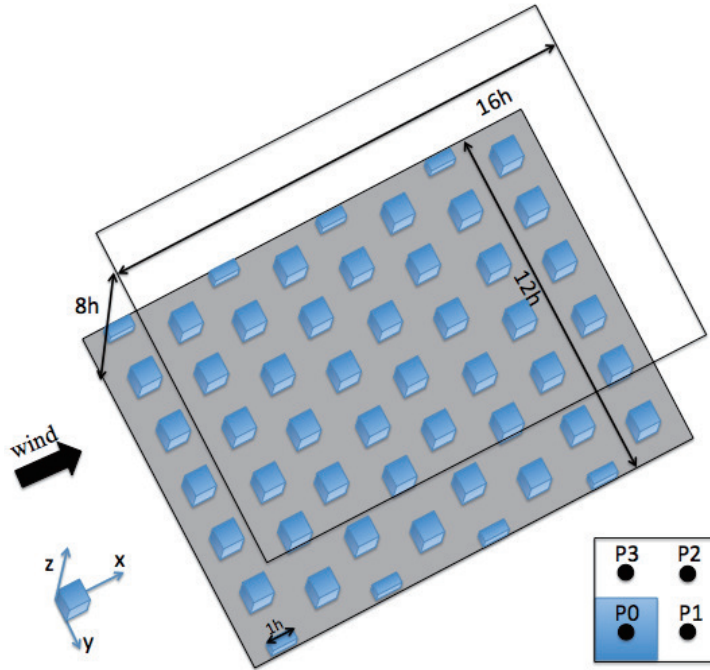


Fig. 2 View of the computational domain, where h is the cube height.

245 ability to account for large velocity gradients occurring near the walls. In comparing
 246 the numerical results they obtained with a grid spacing of $\Delta = h/32$
 247 and $\Delta = h/64$, Coceal et al. (2006) concluded that simulations over a cubic
 248 geometry are generally resolved quite well with $\Delta = h/32$. Xie and Castro
 249 (2006) also pointed out that an LES using $\Delta = h/32$ was able to capture
 250 the vertical gradient of the vertical velocity fluctuations near the top of the
 251 canopy. In their DNS, using a grid spacing of $\Delta = h/32$ Coceal et al. (2007b)
 252 also obtained results in good agreement with wind-tunnel data (Cheng and
 253 Castro, 2002). In the present configuration, a sensitivity analysis (not pre-
 254 sented here) indicated that a grid spacing of $\Delta = h/32$ fails to resolve the
 255 flow gradients that occur within the viscous sublayer near surfaces, especially
 256 at the top of the cubes. Tomas et al. (2016) suggested using a vertical grid
 257 spacing of $\Delta = h/100$ in this region. Here, in the absence of a wall model,
 258 a vertical grid spacing of $h/128$ at the top of the cubes makes it possible for
 259 three mesh layers to be below $z^+ = \frac{zu_*}{\nu} = 5$ (with u_* the local friction velocity
 260 above a cube, determined in the viscous sublayer by $u_*^2 = \nu \frac{\partial \bar{u}}{\partial z}$). This set-up
 261 is sufficient to resolve the viscous sublayer in this region which proves to be
 262 important for developing the shear layer downstream of the cube.
 263 The final mesh configuration is based on a homogeneous $\Delta = h/32$ mesh spac-
 264 ing below $z = 1.5h$ with a refinement of $h/64$ on all surfaces and down to
 265 $h/128$ at the top of the cubes. Above $z = 1.5h$, the mesh keeps the same size

266 in the horizontal directions but gradually stretches in the vertical direction.
 267 The average vertical mesh size is $h/10$ in the region $1.5 < z/h < 5$ and $h/2$
 268 in the region $5 < z/h < 8$ with a maximum value of $2h/3$ at the top of the
 269 domain. The final mesh is non-uniform and contains roughly 28 million cells.
 270 The approximate number of cells in the streamwise, spanwise and vertical di-
 271 rections is $N_x = 520$, $N_y = 410$, and $N_z = 110$, respectively.
 272 The simulation is performed with a constant time step of $\Delta t = 0.00076T$ where
 273 $T = h/u_\tau$ can be interpreted as "the eddy turnover time for the largest eddies
 274 shed by the cube" (Coceal et al., 2006). An initial simulation is run on a period
 275 of $300T$ in order to reach a statistical steady state; this time period is longer
 276 than the duration reported in previous studies (Coceal et al., 2006). The sim-
 277 ulation is then pursued for $200T$ in order to compute the high-order statistics
 278 necessary to determine the TKE budget terms. Xie and Castro (2006) argued
 279 that $80T$ is sufficient for statistical convergence and even observed that the
 280 variation in statistical data throughout the RSL was generally rather small
 281 after an averaging duration in excess of $20T$. Coceal et al. (2007a) and Co-
 282 ceal et al. (2007b) chose $100T$ for their simulation in the same computational
 283 domain as for the present work. In more recent studies, Tomas et al. (2016)
 284 opted for $56T$ yet used inlet/outlet conditions instead of periodic boundary
 285 conditions, while Castro et al. (2017) settled on $710T$ for the statistics collec-
 286 tion step. In the present study, the statistics obtained over a duration of $200T$
 287 are observed to converge at least up to the third-order moments.
 288 In the following discussion, time averaging of the resolved fields will be denoted
 289 by an over-bar ($\bar{\cdot}$). Fluctuation with respect to this average will be denoted by
 290 a prime symbol such that the resolved velocity component can be decomposed
 291 as $\tilde{u}_i = \bar{u}_i + u'_i$. Hereafter, u , v and w denote the streamwise, spanwise and
 292 vertical velocity components, respectively.

293 3 Assessment of the Numerical Approach

294 The mean vertical profiles of both the longitudinal velocity and the Reynolds
 295 shear stress components are investigated at four locations ($P0$, $P1$, $P2$ and $P3$,
 296 as indicated in Fig. 2) to be compared to various experimental and numerical
 297 data in the literature. The experimental work of Castro et al. (2006) has been
 298 used to draw comparisons and enriched by recent experimental datasets from
 299 the LHEEA atmospheric wind tunnel (Nantes, France), i.e.: the Laser Doppler
 300 Velocimetry (LDV) dataset from Herpin et al. (2018), and two datasets gener-
 301 ated from Particle Image Velocimetry (PIV) by Blackman and Perret (2016)
 302 and by Blackman et al. (2017). Note that in order to be directly compared
 303 with numerical results, PIV datasets must undergo two modifications relative
 304 to what has been reported in the cited papers: 1) vertical profiles are extracted
 305 here at points $P1$, $P2$ and $P3$ without spatial averaging, and 2) experimen-
 306 tal data are normalized here by the friction velocity obtained from drag force
 307 measurements (see Sect. 2.3 above and Herpin et al. (2018): viscous drag was
 308 not measured during this experiment). This was the alternative used instead

309 of the Reynolds shear stress values in the region where it remains nearly constant.
 310 constant. Results are also compared to the direct numerical simulations (DNS)
 311 by Coceal et al. (2007b).

312 3.1 Mean Streamwise Velocity

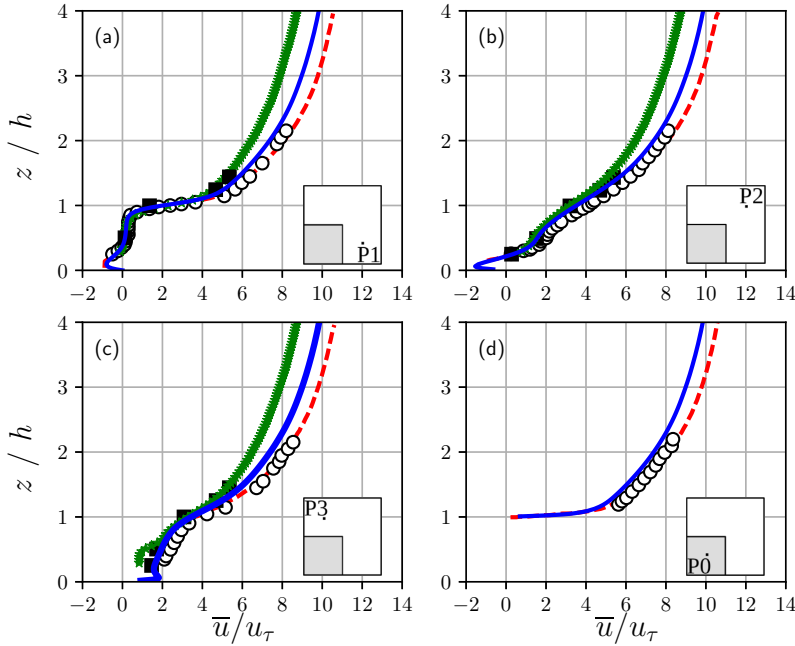


Fig. 3 Vertical profiles of the mean streamwise velocity at locations *P1* (a), *P2* (b), *P3* (c), *P0* (d). Blue solid line: LES computations; Red dashed line: DNS data from Coceal et al. (2007b); Circles: wind-tunnel data from Castro et al. (2006); Squares: wind-tunnel data from Herpin et al. (2018); Stars: PIV data from Blackman et al. (2017).

313 Figure 3 shows the vertical profiles of the mean streamwise velocity component
 314 normalized by the friction velocity (u_τ). LES results (in blue in Fig.
 315 3) are in good agreement with both DNS data from Coceal et al. (2007b) and
 316 wind-tunnel measurements performed by Castro et al. (2006) at the four loca-
 317 tions presented. This observation is equally valid inside the canopy and up
 318 to $z/h = 4$.
 319 Inside the canopy and in the vicinity of the cubes ($z/h \leq 1.25$) results are
 320 also in good agreement with the wind-tunnel output from Herpin et al. (2018)

using LDV and from Blackman et al. (2017) using PIV. Let's note that in the present case, like in Coceal et al. (2007b), the cube height to boundary-layer height ratio equals $h/\delta = 12.5\%$ which is close to the configuration by Castro et al. (2006), i.e. $h/\delta = 13\%$. This ratio however differs by a factor of 2.75 times higher than in both Herpin et al. (2018) and Blackman et al. (2017), for whom $h/\delta = 4.5\%$. The widening differences with increasing height may be attributed to differences in the relative boundary layer height.

The variety of mean velocity profiles observed at different locations inside the canopy illustrates the inhomogeneity of the flow induced by the presence of cubes. The mean reverse flow observed in the numerical results in the lower part of the canopy downstream of a cube at $P1$ (Fig. 3b) and upstream of a cube at $P2$ (Fig. 3a) demonstrates the presence of time-averaged recirculation structures on both the windward (upstream recirculation) and leeward (wake recirculation) sides of the cube. The presence of strong local velocity gradients at $z = h$ (see Figs. 3a-c) indicates a strong shear layer.

3.2 Reynolds Stress Components

Figures 4 and 5 show the turbulent characteristics of the flow normalized by u_τ at locations $P1$, $P2$ and $P3$. These results display the resolved contribution, except for the Figs. 4a, c, e, in which the SGS contribution has been added to the resolved Reynolds shear stress, in this case, accounting for up to 3% or 4% of the total.

The turbulent shear stress ($-\overline{u'w'}$) above the canopy and down to $z/h = 0.2$ at $P1$ and $P2$ corresponds fairly well to both the DNS of Coceal et al. (2007b) and wind-tunnel data (Figs. 4a, c). Upstream of the cube ($P2$), a local maximum is observed in our LES results at $z/h = 0.1$ (Fig. 4c). Xie and Castro (2006) recorded the same observation and suggested as a cause the viscous sublayer which had been well resolved close to the wall at this position. However, at $P2$ for $z/h = 0.1$, a reverse flow is observed in Fig. 3b. A peak is also identified in the standard deviation of the longitudinal velocity component σ_u (Fig. 5c). This peak is more likely to be correlated with the upstream recirculation area located upwind of the cube (more details about this area are given in Sect. 4, see also Fig. 11a).

For the positions presented, the maximum Reynolds shear stress is located near the cube height in both simulations and experiments. In the wake of the cube (at $P1$) the numerical simulations underestimate this maximum in comparison to experimental data of Castro et al. (2006) while the PIV results by Blackman and Perret (2016) yield the lowest maximum (Fig. 4a). Discrepancies are also found for the standard deviation of the vertical velocity component σ_w : the peak of σ_w obtained with numerical simulations lies between the experimental results (Fig. 4b). Similar observations were recorded by Reynolds and Castro (2008) who pointed out two main reasons explaining

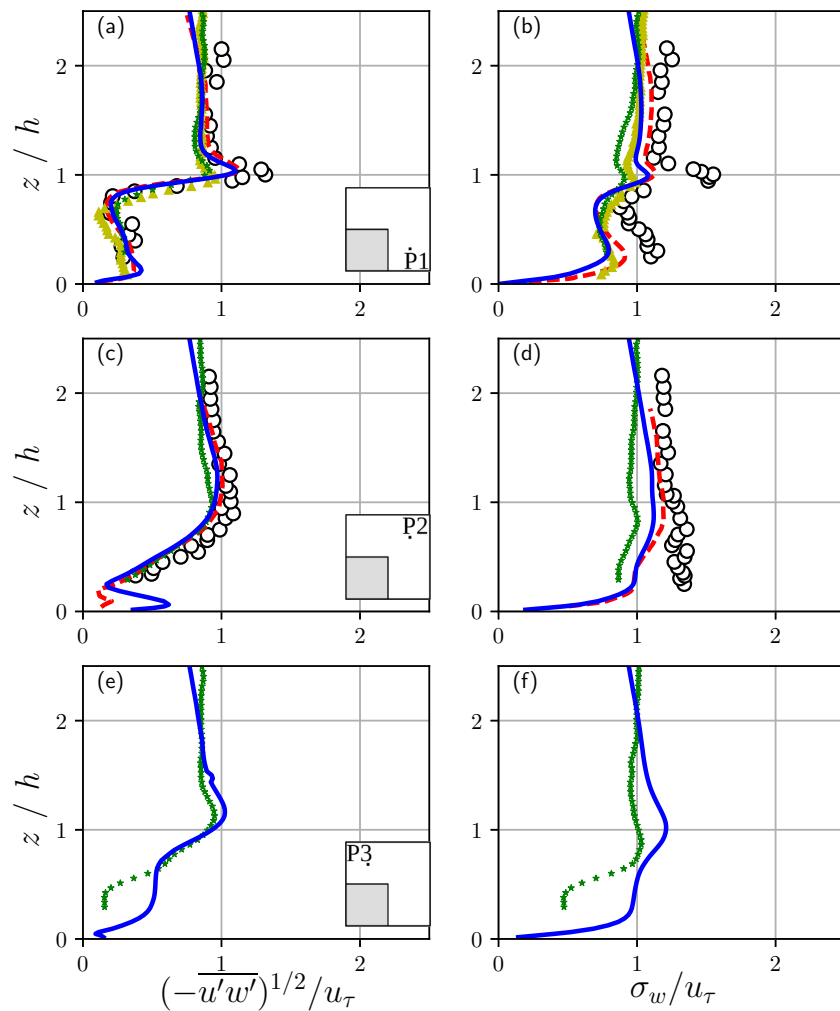


Fig. 4 Vertical profiles of normalized Reynolds shear stress and vertical velocity standard deviation at $P1$ (a, b), $P2$ (c,d) and $P3$ (e, f). Solid line: LES; Dashed line: DNS from Coceal et al. (2007b); Circles: wind-tunnel data from Castro et al. (2006); Triangles: wind-tunnel data from Blackman and Perret (2016); Stars: wind-tunnel data from Blackman et al. (2017).

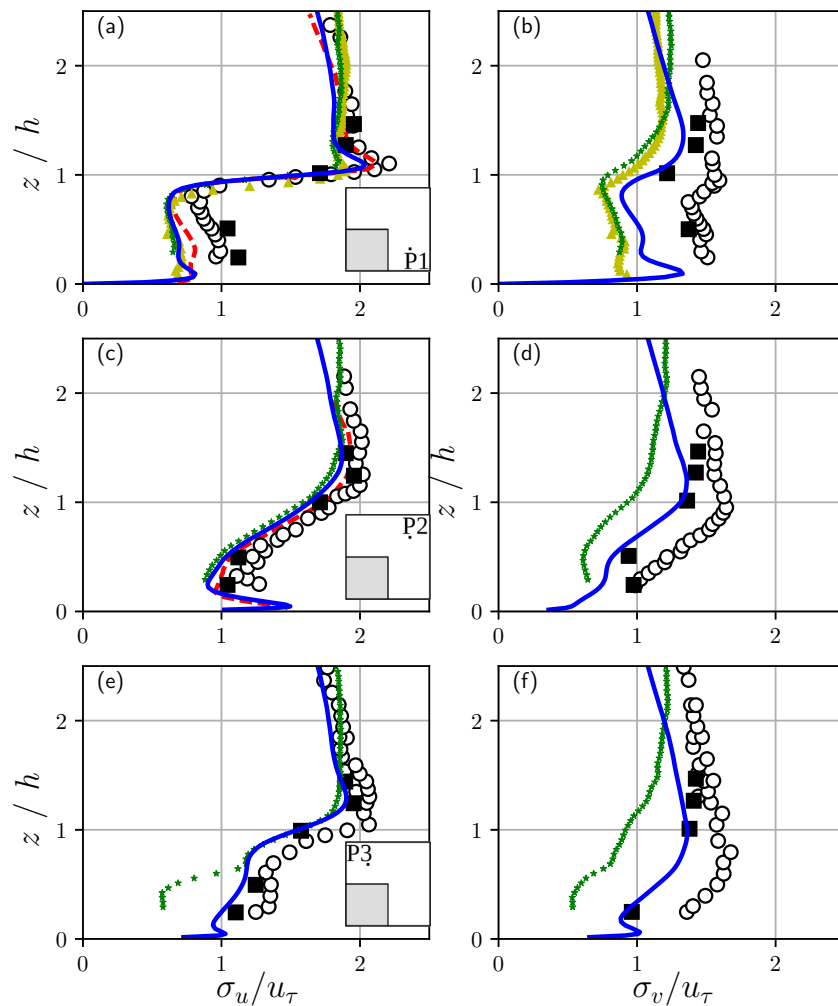


Fig. 5 Vertical profiles of the standard deviation of the streamwise and spanwise velocity components at $P1$ (a, b), $P2$ (c, d) and $P3$ (e, f). Solid line: LES; Dashed line: DNS from Coceal et al. (2007b); Circles: wind-tunnel data from Castro et al. (2006); Squares: wind-tunnel data from Herpin et al. (2018); Triangles: wind-tunnel data from Blackman and Perret (2016); Stars: wind-tunnel data from Blackman et al. (2017).

the differences in the peaks of $(-\overline{u'w'})$ and σ_w . The first is based on the h/δ ratio. These authors found that for $h/\delta < 10\%$, the Reynolds stresses reach a minimum asymptotic value, which means that the greater the h/δ value, the higher the shear stress peaks. This finding is replicated here in Fig. 4, where the datasets contain very different values of h/δ (see Sect. 3.1). The second reason is tied to resolution, whereby a coarser resolution tends to smooth the peak value (Scarano and Riethmuller, 2000). LDV measurements conducted by Castro et al. (2006) have a vertical resolution of approximately $0.015h$, while the PIV resolution by Blackman et al. (2017) is around $0.038h$. PIV is therefore expected to smooth the local peaks of shear components as compared to LDV data. According to a method introduced by Tomas et al. (2016), a rough evaluation of the ratio of shear stress effectively resolved by PIV to total shear stress has been derived; it is based on the work of Scarano and Riethmuller (2000), wherein the percentage of resolved velocity is estimated as a function of the ratio between PIV interrogation window size and the integral length scale. When applied to the works of Blackman and Perret (2016) and Blackman et al. (2017), at $P1$, for $z = h$, the PIV resolved part is estimated at 94% and 90%, respectively. These results are to be treated with caution since the work of Scarano and Riethmuller (2000) is based on idealized PIV images. In LES, the resolution near $z = h$ is approximately $0.031h$, which is indeed finer than PIV but still twice as large as the LDV measurements. This explanation, also proposed by Eisma et al. (2018) is correlated with the observations depicted in Figs. 4a, b.

At point $P2$, the experimental data from Castro et al. (2006) and Blackman et al. (2017) are also available for comparison with the numerical results of σ_w (Fig. 4d). Both DNS and LES values of σ_w fall between the two experimental datasets.

At point $P3$, the vertical profiles of $(-\overline{u'w'})$ and σ_w are rarely reported in the literature. The LES shear stress profile is in rather good agreement with PIV data above the canopy and down to $z/h = 0.6$. Below this level, large discrepancies are observed between LES results and PIV data (Fig. 4f). The vertical profile of σ_w shows large discrepancies at all heights (Fig. 4f), but no experimental data other than Blackman et al. (2017) are available for comparison.

The standard deviation of streamwise (σ_u) and spanwise (σ_v) velocity components are presented in Fig. 5. LES results indicate that the accuracy in simulating σ_u is close to that of the DNS (Coceal et al., 2007b) at $P1$ and $P2$. At $P1$, below $z/h = 1$, numerical data are in good agreement with PIV data (Fig. 5a) yet significantly lower than results from use of the LDV technique. In such a wake region, the lack of spatial resolution probably explains these differences. At $P2$ and $P3$ (Figs. 5c, e) numerical results closely match the LDV data from Herpin et al. (2018).

The standard deviation of the spanwise velocity (σ_v) is undoubtedly the most difficult Reynolds stress-tensor component to measure and simulate. In stereo-PIV measurements, the spanwise velocity component is reconstructed

410 from the in-plane displacement; consequently, the attenuation of velocity fluc-
 411 tuations is expected to be greater than for the streamwise and vertical velocity
 412 components. Large discrepancies can be observed when comparing the results
 413 obtained in the various experiments (Figs. 5b, d, e). The LES however seems
 414 to provide the right trend in the profile of σ_v and is in quite good agreement
 415 with the wind-tunnel data from Herpin et al. (2018) at $P2$ and $P3$, as well as
 416 at $P1$ above and inside the canopy.

417 From this analysis, it is clear that an assessment of the numerical method
 418 cannot be based on a single experimental dataset. The detailed reason why the
 419 various experimental approaches lead to different results lies beyond the scope
 420 of the present work. Nonetheless, the comparisons presented in this section do
 421 demonstrate that the overall agreement between our LES results and available
 422 data, including DNS, is highly satisfactory for both the first- and second-order
 423 moments.

424 3.3 Energy Spectrum

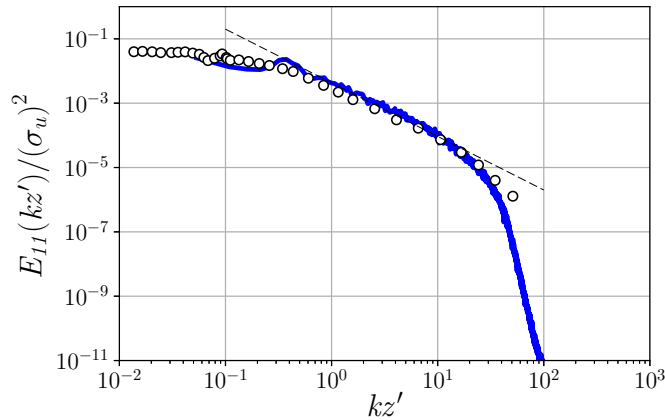


Fig. 6 Turbulent spectra of the axial velocity component $E_{11}(kz')$ at $P2$ for $z/h = 1.62$ from LES (solid blue line), compared with wind-tunnel data (circles) from Castro et al. (2006). The black dashed line represents the $-5/3$ slope.

425 In Fig. 6, the temporal spectrum $E_{11}(kz')$ of the streamwise velocity compo-
 426 nent above the cubes ($z/h = 1.62$) is shown at $P2$ and compared with
 427 wind-tunnel data from Castro et al. (2006). This spectrum has been com-
 428 puted from six time series of the longitudinal velocity fluctuation lasting $45T$
 429 and sampled at $2 kHz$. The wave-number k is defined as $k = 2\pi f/\bar{u}$, with f
 430 being the frequency. The variable z' is defined as $z' = z - d$, with d denoting
 431 the zero-plane displacement estimated as the height at which the total drag

432 is acting. According to the method derived by Jackson (1981), d is computed
433 by:

$$d = \frac{\int_0^h z D(z) dz}{\int_0^h D(z) dz},$$

434 where $D(z)$ is the total drag force profile including pressure and viscous forces
435 within the canopy (See Sect. 2.3). This method has been widely debated be-
436 cause fitting the logarithmic profile with the resulting value of d implies large
437 discrepancies in the value of the von Kármán's constant κ (Coceal et al.,
438 2007b). In our simulation however, this method generally yields acceptable
439 values of $d = 0.74h$ and $\kappa = 0.4$.

440 Assuming that the smallest resolved eddies in the streamwise direction are
441 sized 4Δ , $k_{max}z' = \frac{2H}{4\Delta}z' \approx 44$ can be defined as the highest relevant wave
442 number. Due to a sampling frequency of $2 kHz$, values above $k_{max}z'$ exist
443 but are irrelevant when considering the mesh resolution. Given that the size
444 of the largest structures resolved in the simulation are of the order of the long-
445 itudinal length scale (L_x), $k_{min}z' = \frac{2H}{L_x}z' \approx 0.34$ provides the lower limit of
446 safe interpretation of the turbulent spectra. Data below k_{min} exist because
447 the spectra have been computed from time series lasting $45T$, more than the
448 turnover time under periodic conditions.

449 The simulated energy spectrum (Fig. 6) closely matches with the wind-tunnel
450 data, and the inertial subrange is accurately captured ($-5/3$ slope, dashed
451 line). The cutoff wave number of the LES ($k_{max}z'$) seems to lie at the bound-
452 ary of the inertial subrange, meaning that at this location, the LES solves
453 all the inertial subrange. The SGS dissipation of the dynamic Smagorinsky
454 model should then be small, which will be confirmed in Sect. 4. As expected,
455 for wave numbers greater than $k_{max}z'$, the energy of the small scales starts to
456 drop faster in the simulation than in the experiment. For low wave numbers,
457 the limited size of the LES domain is expected to lead to a poor simulation
458 of the large structures, yet the energy deficit for $kz' < k_{min}z'$ is quite limited
459 compared to wind-tunnel data.

460 4 Turbulence Kinetic Energy Budget

461 In order to further investigate the dynamics of turbulent flow in both the RSL
462 and UCL, the budget of the TKE (defined as $\frac{1}{2}\overline{u'_i u'_i}$) is studied. From LES
463 equations (Eqs. 1, 2, 4 and 6), and in assuming that the turbulent flow has
464 reached a fully steady state, the TKE budget can be written as follows:

$$\begin{aligned}
0 = & \underbrace{-\overline{u_j} \frac{\partial}{\partial x_j} \left(\frac{1}{2} \overline{u'_i u'_i} \right)}_A - \underbrace{\overline{u'_i u'_j} S_{ij}}_P - \underbrace{\frac{1}{2} \frac{\partial}{\partial x_j} \left(\overline{u'_i u'_i u'_j} \right)}_{T_r} - \underbrace{\frac{1}{\rho} \frac{\partial}{\partial x_i} \left(\overline{u'_i p'} \right)}_{T_p} \\
& + \underbrace{\frac{\partial}{\partial x_j} \left(2\nu \overline{u'_i S'_{ij}} \right)}_{D_\nu} - \underbrace{2\nu \overline{S'_{ij} S'_{ij}}}_{\epsilon_r} - \underbrace{\frac{\partial}{\partial x_j} \left(\overline{u'_i \tau'_{ij}} \right)}_{T_{sgs}} + \underbrace{\overline{\tau'_{ij} S'_{ij}}}_{\epsilon_{sgs}},
\end{aligned} \tag{9}$$

465 where A denotes advection by the mean flow, P production by shear, T_r tur-
466 bulent transport by resolved velocity fluctuations, T_p transport by pressure
467 fluctuations, D_ν viscous diffusion, ϵ_r resolved dissipation, T_{sgs} SGS trans-
468 port, ϵ_{sgs} SGS dissipation, which represents the transfer of energy between
469 the resolved-scale and the subgrid-scale through the cutoff, and $\tau'_{ij} = \tau_{ij} - \overline{\tau_{ij}}$.
470 Hereafter, the terms of the TKE budget normalized by u_r^3/h will be provided
471 for comparison and analysis. All contributions to the TKE budget are directly
472 and individually computed during the simulation. A residual term is defined
473 as the value needed on the r.h.s. of Eq. 9 to balance the TKE budget. This
474 residual term (normalized by u_r^3/h) is approximately -1 at $z = h$ and asymp-
475 totically tends to zero for $z > h$. For $z < h$, the residual lies in the range
476 $[-2 : 0]$ (Fig. 8). Since the residual is always negative, this suggests that a
477 destructive TKE term is missing in Eq. 9; this problem may be partially at-
478 tributed to numerical approximation (second-order schemes in Navier-Stokes
479 equation, linear interpolation applied to compute TKE terms at the cell center
480 and computation of gradients in Eq. 9) that tend to smooth velocity gradients.

481 4.1 The Turbulence Kinetic Energy Budget in the Vicinity of a 482 Cube

483 Figure 7 depicts all contributions to the TKE budget at positions $P0-3$. Note
484 that D_ν is not represented because it remains very small at high Reynolds
485 number flows.

486 At all locations, above the height $z/h = 1.5$, the shear production (P) and
487 dissipation terms ($\epsilon = \epsilon_{sgs} + \epsilon_r$) are the major contributors to the TKE
488 budget and tend to balance each other out with increasing height. At $P1$, P
489 reaches a maximum just above the cubes (Fig. 7a), where shear stress is the
490 highest (Fig. 4). The sharp peak then rapidly decreases both above and below
491 $z/h = 1$. With the downwind distance from $P3$ to $P2$, the production peak
492 decreases in intensity as the shear layer develops, becomes thicker and shifts
493 slightly above $z/h = 1$ (see Fig. 7b, c).

494 Dissipation generally acts in mirror with production, at lower absolute values.
495 The maximum $|P|/|\epsilon|$ ratios are found between $z/h = 1$ and $z/h = 2$, reaching
496 1.6, 6, 2.4, and 2.25 for $P0$ to $P3$, respectively. This trend indicates a strong
497 contribution from other TKE budget terms in the area: turbulent transport,
498 advection, and pressure transport. Extending higher above the cubes, the ratio

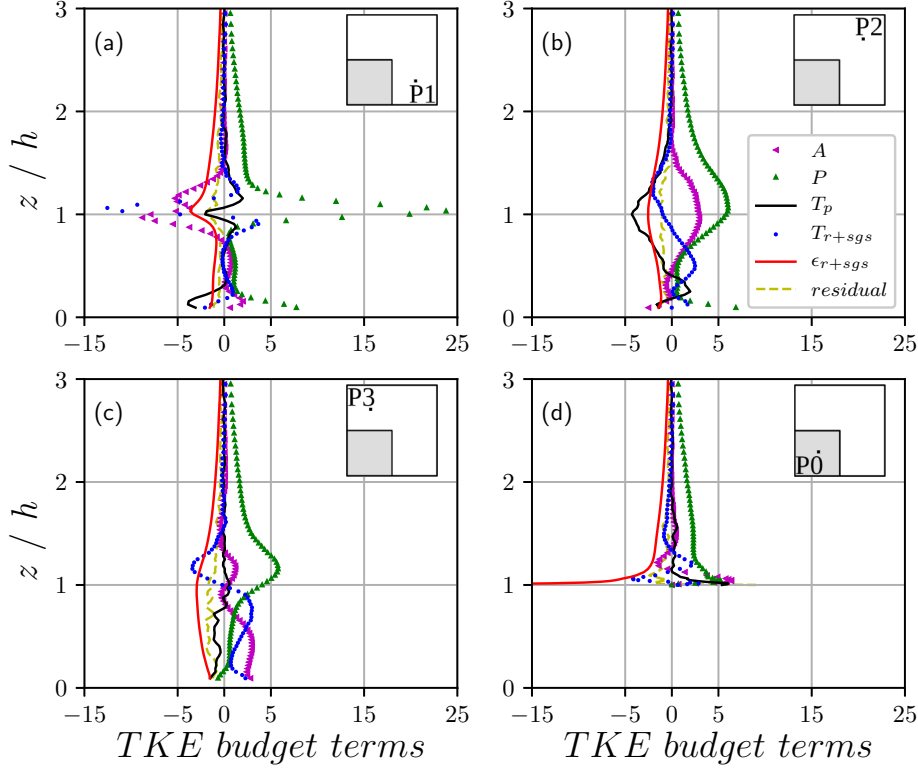


Fig. 7 Vertical profiles of TKE budget terms at locations (a) $P1$, (b) $P2$, (c) $P3$ and (d) $P0$, with all terms being normalized by u^2/h .

499 decreases slowly and stabilizes at a quasi-equilibrium ($|P|/|\epsilon| = 1.1$). The two
 500 locations where dissipation is clearly greater than production are inside the
 501 canopy at $P3$ ($z/h < 1$) and at $P2$ ($0.6 < z/h < 0.2$).

502 In the simulation, the turbulent transport term of the TKE budget ($T_r +$
 503 T_{sgs}) is mostly resolved, as $T_{sgs}/(T_r + T_{sgs}) < 1\%$. At $P1$, turbulent transport
 504 is the major energy sink in the shear layer: $T_r + T_{sgs} < 0$ around $z/h = 1.05$.
 505 Just below and just above, turbulent transport is an energy source ($T_r +$
 506 $T_{sgs} > 0$ around $z/h = 0.9$ and $z/h = 1.2$). Turbulence transport transfers
 507 energy from the thin shear layer downwards inside the canopy and upwards
 508 into the roughness sublayer. Moving downwind, from $P3$ to $P2$, the region
 509 where turbulent transport acts as an energy sink is shifted to a higher altitude
 510 and broadens in agreement with the shear layer thickening. Just upstream of
 511 the cube (at $P2$), this region expands from $z/h = 1.5$ down to $z/h = 0.9$. At
 512 $P1$, turbulent transport acts with the same strength upwards and downwards

513 but, further downwind ($P3$ and $P2$), the energy transfer is clearly oriented
 514 downwards.

515 The transport by pressure fluctuations (T_p) acts similarly to the turbulent
 516 transport in front of the cube (Fig. 7a), by transferring energy both upwards
 517 and downwards. However, the contribution of T_p is much more significant
 518 in front of a cube (at $P2$) than behind (at $P1$). At $P2$, this contribution
 519 constitutes a major energy sink in the region between $z/h = 0.5$ and $z/h = 1.7$.
 520 The advection term (A) has a significant negative contribution in the shear
 521 layer downwind of the cube ($z/h = 1$, $P1$), where the mean flow is transferring
 522 TKE from $P1$ downwind. Further downwind, ($P2$ at $z/h = 1$), A is a TKE
 523 source, the mean flow brings TKE from the upstream. Inside the canopy, the
 524 contribution of advection is normally low, except at $P3$, where A is the major
 525 TKE source, and where TKE is transferred from the high TKE region situated
 526 between the two leading edges of the cubes downstream.

527 4.2 Turbulence Kinetic Energy Budget Comparison

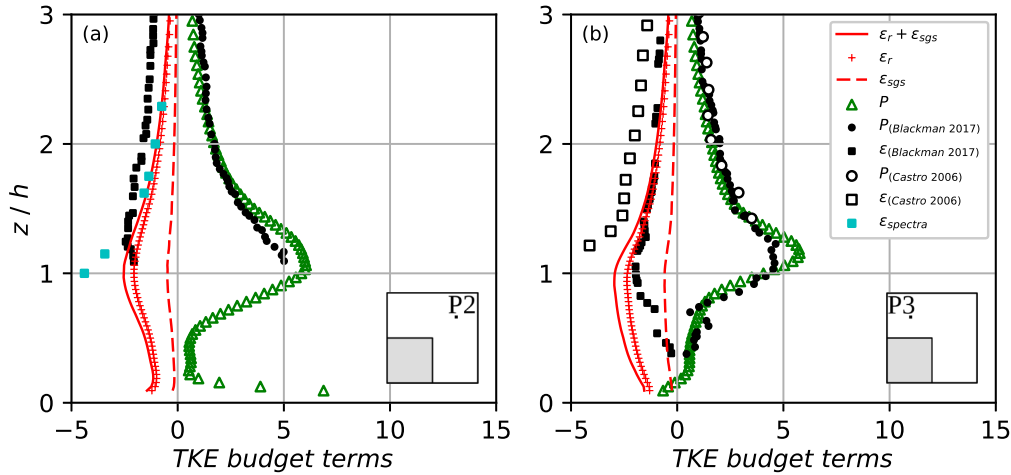


Fig. 8 Production and dissipation terms of the TKE budget vs. wind-tunnel data from Castro et al. (2006) and Blackman et al. (2017) at locations $P2$ (a) and $P3$ (b). All terms are normalized by u_τ^3/h .

528 Figure 8a shows the TKE budget computed from LES at locations $P2$ and
 529 $P3$ compared to the only two (to the best of the author's knowledge) experi-
 530 mental databases available for the TKE budget, i.e. PIV data from Blackman
 531 et al. (2017) and LDV data from Castro et al. (2006). For the sake of clarity,
 532 only production and dissipation are shown here.

533 The production profiles computed in this work are in very good agreement
 534 with experimental datasets both above and below $z = h$. However, at $z = h$,
 535 the computed P is higher than in the measurements found in Blackman et al.
 536 (2017) and displays a sharper peak (the production peak is not available in
 537 Castro et al. (2006)). The attenuation of velocity gradients by the PIV inter-
 538 rogration windows, as discussed in Sect. 3.2, offers a likely explanation. At both
 539 locations, for $z > h$, the total dissipation ($\epsilon_r + \epsilon_{sgs}$) modeled in the present
 540 work is slightly less than in the experimental datasets.

541 At position $P2$, assuming isotropic turbulence, the dissipation can be ob-
 542 tained from integrating of the turbulent spectra by computing:

$$\epsilon_{spectrum} = 15\nu \int_0^\infty k_1^2 E_{11}(k_1) dk_1,$$

543 where k_1 is the wave number and $E_{11}(k_1)$ the one-dimensional wave number
 544 spectra (Perry et al., 1986). Above $z/h = 1.5$, $\epsilon_{spectrum}$ compares well with the
 545 resolved dissipation rate ϵ_r calculated from Eq. 9, thus meaning that the grid
 546 is fine enough to resolve the local velocity gradients. In the shear layer, near
 547 $z/h = 1$, the isotropic turbulence hypothesis fails (see Figs. 4 and 5). Conse-
 548 quently, the calculation of $\epsilon_{spectrum}$ is invalid, and lead to an overestimation of
 549 ϵ_r .

550 Inside the canopy, at $P3$ the computed total dissipation ($\epsilon_r + \epsilon_{sgs}$) is observed
 551 to be higher than in the experimental datasets of Blackman et al. (2017) for
 552 which dissipation rate may also depend on the way it was estimated (SGS
 553 model applied to PIV data).

554 4.3 Production of Turbulence Kinetic Energy in the Vicinity of the 555 Canopy

556 The local TKE budget terms in Fig. 7 displayed great inhomogeneity in both
 557 the UCL and RSL. This section aims to both describe the spatial distribution
 558 of turbulence production P and interpret three-dimensional results from the
 559 LES calculation by showing 3D iso-contours (Fig. 9) and extracting 2D planes
 560 (Figs. 10 and 11). In the following, close to solid surfaces, two kinds of sin-
 561 gular points are used for the description of the flow: saddles points (**S**) are
 562 where streamlines are converging/diverging denoting separation regions and
 563 node points or node lines (**N**) where streamlines are converging. Nodes are
 564 also called attachment points/lines or repelling points/lines.

565
 566 Near the ground, three main areas produce TKE. The first (called P_1^+) is
 567 located at around $h/2$ upstream of a cube, near location $P2$ (as also observed
 568 in Fig. 8a). It is a crosswind-elongated ellipsoid with a length of approximately
 569 h where $P > 10$. This ellipsoid is visible in Figs. 10a and 11a. From Fig. 11a,
 570 it is clearly not horizontally oriented but rather tilted with its upwind part
 571 raised and its downwind part touching the ground. In examining the mean

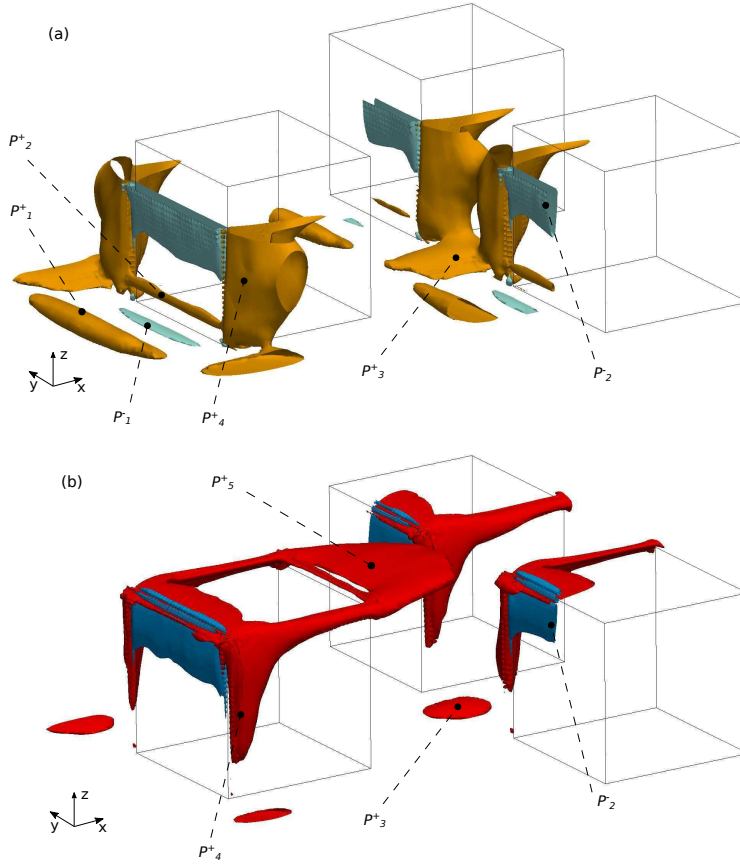


Fig. 9 Three-dimensional visualization of production, normalized by u_τ^3/h . For the sake of clarity, only three cubes are shown. (a) Close-up inside the urban canopy with iso-contours of $P = 10$ (orange) and $P = -10$ (light blue). Iso-contours are only shown below $z = 3h/4$. (b) View of production iso-contours $P = 25$ (red) and $P = -25$ (dark blue).

572 flow in this region, P_1^+ corresponds to the side of the strong clockwise up-
 573 stream recirculation region located in front of the cube, where a high upward
 574 flow (normal to the wall) can be observed. This region corresponds to **S1** in
 575 Fig. 10a. A secondary P peak (P_2^+) is visible on the lower part of the wind-
 576 ward face of the cube near **S4** (Figs. 9a and 11). It is an elongated spanwise
 577 structure located near the small secondary counterclockwise recirculation at
 578 the foot of the cube observed in Fig. 11. In this region, a wall-normal flow is
 579 also observed. Regions P_1^+ and P_2^+ are clearly linked to the near-wall mean
 580 flow upstream of a cube.

581 The third high production region close to the ground (P_3^+) is nearly circular
 582 in the horizontal plane and situated between the front faces of two cubes. Its
 583 center is located near **S2**, where the flow converges in the spanwise direction

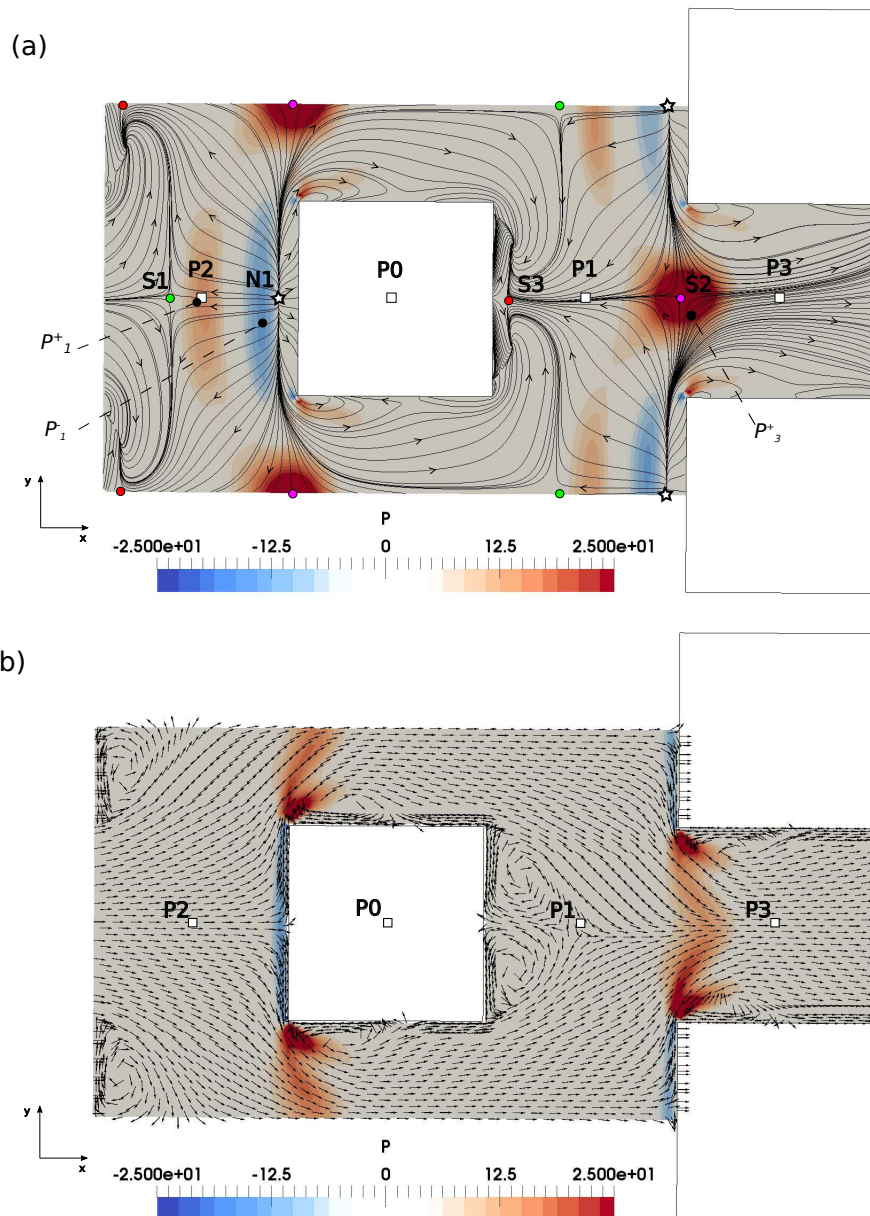


Fig. 10 Top view of the horizontal transect (X,Y) of production normalized by u_τ^3/h . Wind travels from left to right. (a) Near the ground ($z = h/40$) with planar velocity streamlines, where S and N locations stand for saddle point and node, respectively. (b) In the middle of the cube ($z = h/2$) with a mean velocity vector field. Vectors are of equal length in order to better visualize the flow structures.

584 due to the circumvention of the cubes (Fig. 10a, 9 and 11). Production here
 585 exceeds $P = 25$.

586

587 Extending up to $z = h/2$, P_3^+ merges with two high production regions
 588 (P_4^+) attached to the vertical edges of the windward face of the cube. These
 589 production regions at P_4^+ persist, strengthen with increasing height up to
 590 $z = h$. They also merge at $z = h/2$ in the spanwise space between two cubes
 591 (Figs. 10b and 9a). These regions correspond to the side of a lateral (xy)-plane
 592 recirculation zone along the vertical edge of the cube (visible in the vector field
 593 in Fig. 10b).

594 Other high production regions are observed (Fig. 9b) on the four top face
 595 edges. The strongest production area, P_5^+ , starts from the trailing edge of a
 596 cube (downwind edge of the top face) and expands downwind to reach the sec-
 597 ond row of cubes with nearly $P > 25$ (as mentioned in Meinders and Hanjalić
 598 (1999)). Production intensity in this area which corresponds to the shear layer
 599 decreases with downwind distance from the cube and spreads in all directions
 600 but mainly upwards (see Fig. 11). Above $z = h/2$, all high production regions
 601 around the cube are clearly linked to flow separation on the sharp corners.

602 From the above description, we can state that high P regions are clearly corre-
 603 lated with separation regions. Close to solid surfaces, these separation regions
 604 are visualized by saddle points **S1**, **S2** and **S4**. These points are associated
 605 with tremendous outwards wall-normal motion. On cubes, they are located at
 606 the edges where flow separates. These flow regions may be linked to vortex
 607 shedding sources. Let us note that **S3** is also a saddle point, but not visible in
 608 Fig. 9 because the flow velocity is very low in this region.

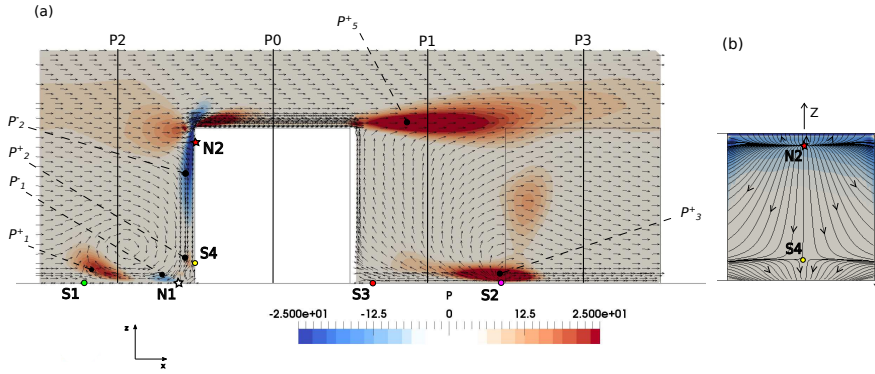


Fig. 11 (a) Vertical transects of production normalized by u_τ^3/h in the middle of the cube, with a projection of the mean velocity vector field. Vectors are of equal length in order to better visualize the flow structures. (b) Production on the wind face of a cube with wall streamlines.

609

610 The canopy flow also exhibits areas where P is negative, meaning that energy is extracted from turbulence and returned to the mean flow (Pope, 2001).
 611 For $z < h/2$, a spanwise elongated zone P_1^- with weak negative production
 612 ($P \approx -15$) is observed at the ground, near **N1** and parallel to P_1^+ (Figs. 10a
 613 and 11a). Point **N1** is a repelling line (Helman and Hesselink, 1989), representing a flow impinging on a surface. Here, it lies very close to the re-attachment
 614 zone situated between the large clockwise recirculation upwind of the cube
 615 and the secondary counterclockwise recirculation at the foot of the cube.
 616 The region with the most highly negative production ($P < -25$), called P_2^- ,
 617 starts at the cube's leading edge and extends downwards along the windward
 618 face of the cube with decreasing intensity to reach $P = -10$ at approximately
 619 $z = h/2$ (Figs. 11 and 9b). This region, near **N2** in Fig. 11 is also a repelling
 620 node (or line) where the mean turbulent flow is impacting the cube face and
 621 deflecting downwards. Instantaneously, it is likely that some of the vortices
 622 shed by leading edges of the previous cube (see instantaneous view in Coceal
 623 et al. (2006)) are being destroyed when impacting the subsequent cube, thus
 624 leading to a destruction of turbulence and an increase in the mean flow mag-
 625 nitude (down draft).
 626 Similar regions of negative production were observed by Yakhov et al. (2006)
 627 around an isolated wall-mounted cube. They particularly decomposed produc-
 628 tion terms to explain its negative sign on the front face of the cube and linked
 629 them to mean flow features. However, in the present case, the spatial extent of
 630 P_1^- and its relative importance compared to P_2^- differ (in our work $P_2^- > P_1^-$).
 631 This difference can be attributed to the very different 3D organization of the
 632 turbulent flow, the dense staggered arrangement preventing the free expansion
 633 of the horseshoe vortex observed around an isolated cube.
 634
 635

636 5 Conclusion

637 In order to determine the turbulent mechanisms at play inside the UCL of an
 638 urban-like boundary layer, a large-eddy simulation was performed over a stag-
 639 gered array of cubes at $Re = 50,000$ ($Re_\tau = 500$). The simulation performed
 640 used a dedicated dynamic Smagorinsky subgrid scale model allowing for en-
 641 ergy backscatter along with a $h/32$ mesh size and added refinements close to
 642 surfaces to resolve the viscous sublayers ($z^+ < 5$).

643 The high resolution of the LES presented in this work and the individ-
 644 ual computation of each TKE budget terms made it possible to discuss the
 645 highly heterogeneous distribution of TKE terms inside the UCL. The role of
 646 advection, turbulent transport and pressure transport that are of secondary
 647 importance in the case of a flat plate away from the surface, are here clearly
 648 shown. Additionally, significant positive and negative values of turbulence pro-
 649 duction were found close to the ground surface.

650 This work showed, for the first time, that substantial TKE production ar-
 651 eas in a staggered arrangement of cubes were located not just in the shear
 652 layer after a cube, as described in the literature, but also near surfaces. Sev-

653 eral locations on the ground and on some cube surfaces were identified where
654 P is far from being negligible. Highly positive and negative production regions
655 were observed, which allowed localizing where TKE is generated and where
656 it returns to the mean flow. This finding is important to understanding how
657 turbulence is generated and the boundary layer maintained in an urban-like
658 canopy. This information can be valuable to build simplified urban canopy
659 models. The TKE production process inside the urban canopy clearly differs
660 from that of a flat plate and of an isolated wall-mounted cube. Although the
661 turbulence production process is unsteady by its very nature, strong produc-
662 tion areas could be identified at fixed locations other than in the shear layer
663 or along the sharp edges of the obstacles.

664 In analyzing both high positive and negative production areas near sur-
665 faces, it is clear that each of them is related to distinctive features of the mean
666 flow. High production areas are associated to saddle points. By definition, at
667 a saddle point of a surface, there is a high convergence of the flow in the plane
668 tangent to the surface. In the present configuration, the wall streamlines con-
669 vergence is caused by the deflection of the flow around obstacles (as at S2)
670 or by the presence of the recirculating area upwind of a cube (as at S1). The
671 flow convergence results in both horizontal divergence and out-of-plane flow
672 by virtue of mass conservation for incompressible flows. In a turbulent flow,
673 this out-of-plane flow is very likely to produce TKE. Highly negative produc-
674 tion areas close to surfaces are clearly correlated with node points. Repelling
675 nodes (or repelling lines) are observed when the flow direction is normal to
676 the surface as at the upwind face of the obstacle (N2) or at the junction of
677 two recirculating flow regions (N1). Because of the divergence free condition
678 it leads to a high divergence of the flow in the plane parallel to the surface.
679 A node can be seen as a re-attachment zone. The TKE present in the flow
680 is destroyed when impacting a surface and energy is transferred back to the
681 mean flow resulting in a negative production of turbulence.

682 This finding is very likely to remain valid when changing the cube arrange-
683 ment, array density or wind direction, meaning that high and low production
684 areas near surfaces can simply be anticipated through analyzing the mean
685 flow. To some extent, this statement may also be valid for configurations fea-
686 turing square shapes such as buildings. Finally, the share of production at fixed
687 locations compared to instantaneous advected vortices in the domain would
688 provide an interesting subject to further analyze the turbulent production
689 process.

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References

- Adrian RJ (2007) Hairpin vortex organization in wall turbulence. *Physics of Fluids* 19(4):041,301
- Blackman K, Perret L (2016) Non-linear interactions in a boundary layer developing over an array of cubes using stochastic estimation. *Physics of Fluids* 28(9):095,108
- Blackman K, Perret L, Calmet I, Rivet C (2017) Turbulent kinetic energy budget in the boundary layer developing over an urban-like rough wall using PIV. *Physics of Fluids* 29(8):085,113
- Boppana VBL, Xie ZT, Castro IP (2010) Large-Eddy Simulation of Dispersion from Surface Sources in Arrays of Obstacles. *Boundary-Layer Meteorology* 135(3):433–454
- Bou-Zeid E, Overney J, Rogers BD, Parlange MB (2009) The Effects of Building Representation and Clustering in Large-Eddy Simulations of Flows in Urban Canopies. *Boundary-Layer Meteorology* 132(3):415–436
- Brooke JW, Hanratty T (1993) Origin of turbulence-producing eddies in a channel flow. *Physics of Fluids A: Fluid Dynamics* 5(4):1011–1022
- Calmet I, Magnaudet J (1997) Large-eddy simulation of high-Schmidt number mass transfer in a turbulent channel flow. *Physics of Fluids* 9(2):438–455
- Castro IP, Cheng H, Reynolds R (2006) Turbulence Over Urban-type Roughness: Deductions from Wind-tunnel Measurements. *Boundary-Layer Meteorology* 118(1):109–131
- Castro IP, Xie ZT, Fuka V, Robins AG, Carpentieri M, Hayden P, Hertwig D, Coceal O (2017) Measurements and Computations of Flow in an Urban Street System. *Boundary-Layer Meteorology* 162(2):207–230
- Cheng H, Castro IP (2002) Near wall flow over urban-like roughness. *Boundary-Layer Meteorology* 104(2):229–259
- Cheng H, Hayden P, Robins A, Castro I (2007) Flow over cube arrays of different packing densities. *Journal of Wind Engineering and Industrial Aerodynamics* 95(8):715–740
- Christen A, Rotach MW, Vogt R (2009) The Budget of Turbulent Kinetic Energy in the Urban Roughness Sublayer. *Boundary-Layer Meteorology* 131(2):193–222
- Coceal O, Thomas TG, Castro IP, Belcher SE (2006) Mean flow and turbulence statistics over groups of urban-like cubical obstacles. *Boundary-Layer Meteorology* 121(3):491–519
- Coceal O, Thomas TG, Belcher SE (2007a) Spatial Variability of Flow Statistics within Regular Building Arrays. *Boundary-Layer Meteorology* 125(3):537–552
- Coceal O, Dobre A, Thomas TG, Belcher SE (2007b) Structure of turbulent flow over regular arrays of cubical roughness. *Journal of Fluid Mechanics* 589:375–519
- Dwyer MJ, Patton EG, Shaw RH (1997) Turbulent kinetic energy budgets from a large-eddy simulation of airflow above and within a forest canopy. *Boundary-Layer Meteorology* 84(1):23–43

- 742 Eisma H, Tomas J, Pourquie M, Elsinga G, Jonker H, Westerweel J (2018)
743 Effects of a fence on pollutant dispersion in a boundary layer exposed to a
744 rural-to-urban transition. *Boundary-layer meteorology* 169(2):185–208
- 745 Ferziger JH, Perić M, Street RL (2002) *Computational methods for fluid dy-*
746 *namics*, vol 3. Springer
- 747 Finnigan J (2000) Turbulence in plant canopies. *Annual review of fluid me-*
748 *chanics* 32(1):519–571
- 749 Germano M, Piomelli U, Moin P, Cabot WH (1991) A dynamic subgridscale
750 eddy viscosity model. *Physics of Fluids A: Fluid Dynamics* 3(7):1760–1765
- 751 Giometto MG, Christen A, Meneveau C, Fang J, Krafczyk M, Parlange
752 MB (2016) Spatial Characteristics of Roughness Sublayer Mean Flow and
753 Turbulence Over a Realistic Urban Surface. *Boundary-Layer Meteorology*
754 160(3):425–452
- 755 Helman J, Hesselink L (1989) Representation and display of vector field topol-
756 ogy in fluid flow data sets. *Computer* (8):27–36
- 757 Herpin S, Perret L, Mathis R, Tanguy C, Lasserre JJ (2018) Investigation of
758 the flow inside an urban canopy immersed into an atmospheric boundary
759 layer using laser Doppler anemometry. *Experiments in Fluids* 59(5)
- 760 Hudson JD, Dykhno L, Hanratty T (1996) Turbulence production in flow over
761 a wavy wall. *Experiments in Fluids* 20(4):257–265
- 762 Inagaki A, Kanda M (2010) Organized structure of active turbulence over an
763 array of cubes within the logarithmic layer of atmospheric flow. *Boundary-*
764 *layer meteorology* 135(2):209–228
- 765 Jackson PS (1981) On the displacement height in the logarithmic velocity
766 profile. *Journal of Fluid Mechanics* 111:15
- 767 Kanda M, Moriwaki R, Kasamatsu F (2004) Large-eddy simulation of turbu-
768 lent organized structures within and above explicitly resolved cube arrays.
769 *Boundary-Layer Meteorology* 112(2):343–368
- 770 Kastner-Klein P, Rotach MW (2004) Mean Flow and Turbulence Charac-
771 teristics in an Urban Roughness Sublayer. *Boundary-Layer Meteorology*
772 111(1):55–84
- 773 Kim J, Moin P, Moser R (1987) Turbulence statistics in fully developed channel
774 flow at low reynolds number. *Journal of fluid mechanics* 177:133–166
- 775 Kono T, Tamura T, Ashie Y (2010) Numerical Investigations of Mean Winds
776 Within Canopies of Regularly Arrayed Cubical Buildings Under Neutral
777 Stability Conditions. *Boundary-Layer Meteorology* 134(1):131–155
- 778 Leonardi S, Castro IP (2010) Channel flow over large cube roughness: a direct
779 numerical simulation study. *Journal of Fluid Mechanics* 651:519
- 780 Lilly DK (1992) A proposed modification of the Germano subgridscale closure
781 method. *Physics of Fluids A: Fluid Dynamics* 4(3):633–635
- 782 Lyons S, Hanratty T, McLaughlin J (1989) Turbulence-producing eddies in
783 the viscous wall region. *AIChE journal* 35(12):1962–1974
- 784 Macdonald RW (2000) Modelling the mean velocity profile in the urban canopy
785 layer. *Boundary-Layer Meteorology* 97(1):25–45
- 786 Meinders E, Hanjalić K (1999) Vortex structure and heat transfer in turbulent
787 flow over a wall-mounted matrix of cubes. *International Journal of Heat and*

- fluid flow 20(3):255–267
- 788 Monnier B, Goudarzi SA, Vinuesa R, Wark C (2018) Turbulent Structure of a
789 Simplified Urban Fluid Flow Studied Through Stereoscopic Particle Image
790 Velocimetry. *Boundary-Layer Meteorology* 166(2):239–268
- 791 Oke TR (1997) Urban environments. *The surface climates of Canada* pp 303–
792 327
- 793 Perret L, Blackman K, Savory E (2016) Combining Wind-Tunnel and Field
794 Measurements of Street-Canyon Flow via Stochastic Estimation. *Boundary-*
795 *Layer Meteorology* 161(3):491–517
- 796 Perry A, Henbest S, Chong M (1986) A theoretical and experimental study of
797 wall turbulence. *Journal of Fluid Mechanics* 165:163–199
- 798 Pope SB (2001) *Turbulent flows*. IOP Publishing
- 799 Raupach MR, Antonia RA, Rajagopalan S (1991) Rough-wall turbulent
800 boundary layers. *Applied mechanics reviews* 44(1):1–25
- 801 Reynolds RT, Castro IP (2008) Measurements in an urban-type boundary
802 layer. *Experiments in Fluids* 45(1):141–156
- 803 Rotach MW (1999) On the influence of the urban roughness sublayer on tur-
804 bulence and dispersion. *Atmospheric Environment* 33(24):4001–4008
- 805 Roth M, Inagaki A, Sugawara H, Kanda M (2015) Small-scale spatial variabil-
806 ity of turbulence statistics, (co)spectra and turbulent kinetic energy mea-
807 sured over a regular array of cube roughness. *Environmental Fluid Mechan-*
808 *ics* 15(2):329–348
- 809 Scarano F, Riethmuller ML (2000) Advances in iterative multigrid piv image
810 processing. *Experiments in Fluids* 29(1):S051–S060
- 811 Smagorinsky J (1963) General circulation experiments with the primitive equa-
812 tions: I. the basic experiment. *Monthly weather review* 91(3):99–164
- 813 Tomas J, Eisma H, Pourquie M, Elsinga G, Jonker H, Westerweel J (2017)
814 Pollutant dispersion in boundary layers exposed to rural-to-urban transi-
815 tions: varying the spanwise length scale of the roughness. *Boundary-Layer*
816 *Meteorology* 163(2):225–251
- 817 Tomas JM, Pourquie M, Jonker HJJ (2016) Stable stratification effects
818 on flow and pollutant dispersion in boundary layers entering a generic urban
819 environment. *Boundary-Layer Meteorology* 159(2):221–239
- 820 Xie Z, Castro IP (2006) LES and RANS for turbulent flow over arrays of
821 wall-mounted obstacles. *Flow, Turbulence and Combustion* 76(3):291–312
- 822 Xie ZT, Coceal O, Castro IP (2008) Large-Eddy Simulation of Flows over
823 Random Urban-like Obstacles. *Boundary-Layer Meteorology* 129(1):1–23
- 824 Yakhot A, Liu H, Nikitin N (2006) Turbulent flow around a wall-mounted cube:
825 A direct numerical simulation. *International Journal of Heat and Fluid Flow*
826 27(6):994–1009
- 827 Yue W, Meneveau C, Parlange MB, Zhu W, Kang HS, Katz J (2008) Turbulent
828 kinetic energy budgets in a model canopy: comparisons between LES and
829 wind-tunnel experiments. *Environmental Fluid Mechanics* 8(1):73–95
- 830 Zang Y, Street RL, Koseff JR (1993) A dynamic mixed subgridscale model and
831 its application to turbulent recirculating flows. *Physics of Fluids A: Fluid*
832 *Dynamics* 5(12):3186–3196
- 833