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https://doi.org/10.1007/s12273-020-0689-z

Position Paper

CFD modelling: The most useful tool for developing mesoscale urban canopy parameterizations

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Article History
Received: 11 December 2019 / Revised: 03 July 2020 / Accepted: 16 July 2020

1 Introduction

The fact that most of the world's population lives in cities (UN-Habitat 2016) has increased interest in urban meteorology. Mesoscale models, such as the Weather Research and Forecasting (WRF) model (www.mmm.ucar.edu/weather-research-and-forecasting-model), are used to reproduce the meteorology and climatology over cities and around them, where the complex interactions between the atmosphere and urban surfaces (buildings, vegetation, urban obstacles, etc.) induce strong heterogeneity in the flow properties within the urban canopy layer (UCL) (Di Sabatino et al. 2013; Lateb et al. 2016; Tominaga and Stathopoulos 2016). The other option is to employ CFD (Computational Fluid Dynamics) models. However, due to the available numerical resources, the numerical domain of CFD cannot usually cover a whole city and its surroundings. Usually, the sizes of real urban districts simulated with CFD are around 1–2 km^2 (e.g., Buccolieri et al. 2011; Sanchez et al. 2017; Santiago et al. 2017a, b; Borge et al. 2018). More recent works have simulated wider urban areas. For example, the areas modelled by Jeanjean et al. (2015) and Toparlar et al. (2018) were approximately 4 km^2. Moreover, an entire mid-size city (42 km^2 approximately) was simulated by Rivas et al. (2019), but this required a large computational load. Mesoscale models with urban canopy parameterizations (UCPs), then, are still needed in the coming years to simulate whole cities and their surroundings.

Mesoscale models are designed to represent features with spatial dimensions in the order of tens to hundreds of kilometres. Consequently, their horizontal resolution is in the order of 1 km^2 (or hundreds of meters times hundreds of meters) to keep the number of grid points manageable for current computational resources. Therefore, the related variables are representatives of spatial averages over the volume of the grid cell. Typical time steps of mesoscale models at km resolutions are around 10 s. Smaller motion occurring at a time-scale is mainly turbulent, and thus fully parameterized. For this reason, when dealing with urban environments, mesoscale models employ UCPs to represent the effects of urban obstacles, typically obstacles of a building size or smaller, which cannot be explicitly resolved. Single-layer UCPs consider the lowest atmospheric model level as the roof top (or more correctly, the displacement height) and combine the effects of all the buildings in the surface fluxes (Masson 2000; Kusaka et al. 2001). The atmospheric behaviour in the UCL is diagnosed starting from analytic functions like the log-law used to link the urban canopy's air temperature with the air temperature of the lowest model level (assumed to be in the inertial sublayer, ISL) and to derive the momentum sink (e.g., the friction velocity u_*), which affects the wind speed at the lowest model level (again assumed in the ISL) or the exponential law used to extrapolate the wind speed from the lowest model level (above the canopy) to the canopy. This variable is important to compute the heat exchanges at walls and road. On the other hand, multilayer UCPs place the lowest model level at the road's surface and are, therefore, coupled with the meteorological model at several levels within the UCL. Here, the effect of buildings is modelled by drag forces. The

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energy exchange between urban surfaces and the atmosphere is considered by assuming simple street canyons; see, for example, the Building Energy Parameterization Scheme (BEP) proposed by Martilli et al. (2002) and the BEP combined with the Building Energy Model (BEM) proposed by Salamanca et al. (2010), which are both included in WRF. This configuration is usually employed to simulate urban environments (e.g., Salamanca et al. 2011, 2012; Gutiérrez et al. 2015) and has been coupled, in some cases, to CFD simulations (Sanchez et al. 2017; Borge et al. 2018; Santiago et al. 2020). There is a fundamental difference between these two approaches:

- Single layer UCPs need to represent the integral effect of all the buildings and translate it into a surface flux applied at the displacement height (the lowest level of the mesoscale model). With this approach, for example, the momentum sink due to the presence of buildings must be represented as a flux through a horizontal surface and parametrized as a function of the wind speed at the lowest model level, e.g., at a certain height above the buildings, outside of the UCL.
- Multilayer UCPs, on the other hand, account for the presence of buildings using a drag force that must be parametrized as a function of the wind speed and direction within the UCL at the same height where the force is applied to the fluid. Similarly, the heat fluxes are a function of the gradient between the temperature of the urban surfaces and the temperature of the air within the UCL.

Such differences in the ways that building effects are represented in the model have significant consequences on the type of parameterization used and the values of the different parameters. Mesoscale models using multilayer UCPs resolve the flow features with a vertical resolution around 5 m and need to parameterize, for example, the effect of buildings on the flow properties at this scale because the wind speed profile is very distant from a logarithmic vertical profile. This factor is crucial in several mesoscale-model applications like pollutant dispersion in urban environments, where traffic emissions are located close to the ground. The spatial variability of the flow properties within the UCL is strong in areas around the size of mesoscale cells. Due to these flow heterogeneities, then, very high-resolution information is necessary to compute the horizontally-averaged variables representative of the whole cell. Such spatially-averaged variables include not only the mean wind speed, turbulence kinetic energy, or momentum fluxes but also the length scales and coefficients required to estimate the drag forces or surface heat fluxes, which are input parameters of UCPs. Therefore, to develop (and eventually improve) new UCPs, information about variables with sufficient spatial resolution is needed to capture these heterogeneities and compute spatial averages that are representative of the area of the cell. In this context, the following research question emerges: How can this information be obtained?

Our answer to this research question is that CFD models are the most useful tool to provide the very high-resolution information needed for developing mesoscale UCPs. CFD models can, in fact, explicitly resolve the wind flow around buildings and provide detailed information in urban environments. Other approaches currently used to develop UCPs are mainly based on field or wind-tunnel/water channel measurements. As detailed in the following sections, we propose that field measurements are not completely adequate for this task because, even though sensors are now an affordable way to collect high-spatial-resolution field data, this process requires large resource expenditures to estimate the spatial averages in the UCL and can never realize the spatial resolution achievable with a CFD model (millions of points in the UCL). Thus, it would be difficult to use lab and field measurements to estimate spatial averages in the UCL—something needed for both multilayer and single layer UCPs (for the latter, to deduce the analytical formulas to extrapolate the above canopy values to the canopy—i.e., the region where people live). Wind-tunnel or water channel measurements, on the other hand, may have higher spatial resolutions in the UCL, but in the literature, there is a lack of experimental data under non-neutral conditions. However, recent works carried out at the University of Surrey have shown how non-neutral flows can be simulated in wind-tunnels (Marucci et al. 2018; Marucci and Carpentieri 2019, 2020). In these cases, performing sensitivity studies by varying many physical parameters would require a large number of experiments and different scale geometries that may be difficult and expensive to prepare. Needless to say, these experimental data are fundamental for the evaluation and validation of CFD models and the performance of simulations.

A framework proposed to develop or improve UCPs is shown in Figure 1. This methodology can be used to develop new UCPs by including other physical processes not previously considered or improving current UCPs by obtaining a better parameterization of UCPs parameters. Mesoscale models are not usually applied to calculate flows over idealized building geometries, and CFD models do not simulate the whole mesoscale domain. Thus, the application of UCP to real urban environments involves two main steps.

- CFD simulations are performed over idealized building geometries. From these results, some of the physical parameters required as UCP inputs are parameterized as a function of the urban morphology and meteorological conditions. For example, for arrays of cubes, the drag coefficient is parameterized as a function of the building

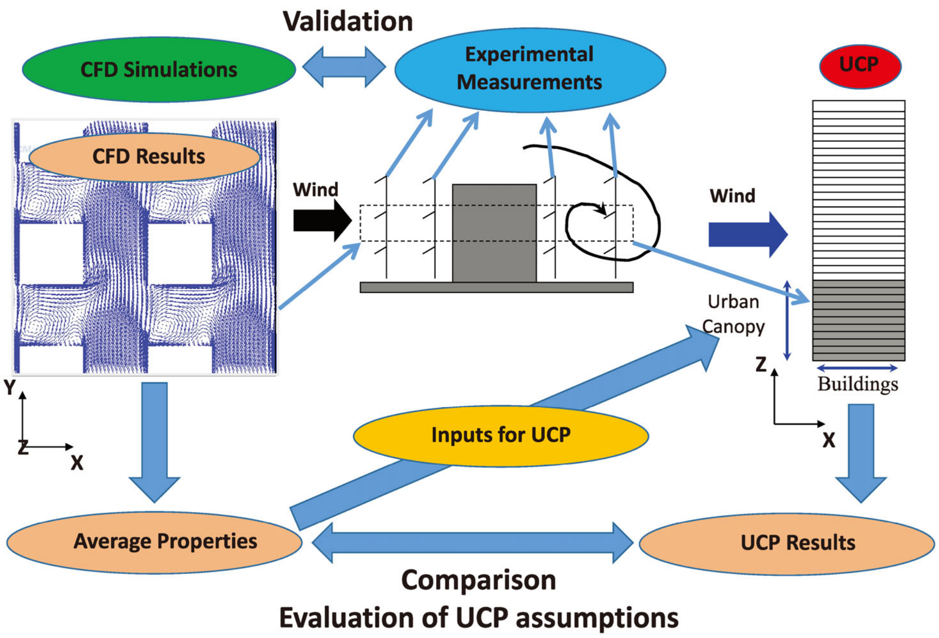

Fig. 1 A general framework summarizing the use of the computational fluid dynamics (CFD) tool to develop (and eventually improve) urban canopy parameterizations (UCPs)

packing density. Note that within the canopy, only spatially-averaged properties can be used for these parameterizations because the flow properties obtained with UCPs represent the spatially-averaged values in the mesoscale cells;

- Mesoscale models with UCPs are applied to real cities, and, at each mesoscale cell within the city (in addition to the land use information), information about urban morphology (building height, aspect ratio of the street(s), etc.) is needed. Then, using these data, the corresponding values of these parameters, previously parameterized with the CFD results, can be selected in each urban cell. For example, data on the packing density in each cell is necessary to select each cell's appropriate drag coefficient to run the UCP. Examples include studies by Santiago and Martilli (2010) and Gutiérrez et al. (2015). As we discuss below, the first study observed the dependency of the drag coefficient on the building packing density, while the second used this parameterization to compute the UCP inputs (in this case, BEP/BEM coupled with the WRF model) in each mesoscale urban cell for New York city. The authors simulated this area and obtained a better agreement between the wind and temperature data computed throughout the city by employing the new parameterization compared to the older model that did not consider the dependence of the drag coefficient with packing density. However, the increasing use of CFD models in real urban environments makes it possible to change the first step of the previous scheme to reduce the uncertainties because the physical input parameters for UCP are parameterized by using CFD simulations in simplified configurations. Therefore, as future research, we propose developing new parameterizations of UCP inputs by using CFD results over real urban environments and investigating how these parameterizations can be generalized compared to currently available parameterizations that were developed through simulations over simplified domains.

2 Counter arguments

The approaches commonly employed to study flow in an urban environment include full-scale field measurements, physical modelling (or reduced-scale experiments, mainly using wind tunnel and water channel experiments), and CFD simulations (see, for example, Vardoulakis et al. (2003) and Lateb et al. (2016) for a brief summary of various existing methods for flow and pollutant dispersion investigations, including their advantages and limitations). In this context, the main arguments against our thesis can be summarized as follows:

1) <u>Counter argument 1</u>: CFD does not reflect reality like field data, and some physical processes (such as buoyancy) are not commonly included or well established in CFD simulations.
2) <u>Counter argument 2</u>: Physical modelling is also performed under a controllable environment.
3) <u>Counter argument 3</u>: CFD simulations require a high-resolution representation of urban geometry and knowledge of the boundary conditions for all relevant flow variables.
4) <u>Counter argument 4</u>: A challenge in CFD modelling is

simulating the broad spectra of scales in turbulent flows.

The above counter arguments are clearly supported by the following statements:

1) Full-scale field measurements are performed under real atmospheric conditions. They have the advantages of being able to study a real situation and consider the full complexity of a problem. Most CFD studies have been performed under isothermal conditions and/or have not considered all processes—for example, buoyancy is usually neglected. There are several possible reasons for this issue. First, most studies simplify the problem by focusing on the mechanical effects of the urban geometry on flow structure and pollutant dispersion to find useful correlations between the geometry and the resulting flow. Second, wall models with thermal BCs remain a challenge. The computational grid must be sufficiently fine to allow thermal boundary layers to be resolved over the tops of buildings and within canyons; this process has become more affordable only recently with increasing computational power and resources. Finally, wind tunnel experiments are performed in non-isothermal conditions. Thus, the data for validation are recent.
2) Compared to field measurements, physical modelling, which is usually performed in wind-tunnels or water-channels, has the advantages that the boundary conditions can be chosen based on the problem and that the stationary flow conditions can be maintained throughout the test. It thus allows one to study different configurations under controllable conditions (Meroney et al. 1999; Cheng et al. 2007; Gromke and Ruck 2007; Hagishima et al. 2009).
3) Urban geometry should be discretized. Further, the numerical methods employed to resolve model equations introduce inaccuracy into simulations. Detailed information on the building geometry is required, which is not always easily available, and simplifications should be undertaken, depending on the available data. On the other hand, some urban obstacles like vegetation cannot be resolved in detail for two main reasons: a) the small size of the flow features that must be modelled (and thus the large number of cells needed); b) the small amount of available information. For example, the trunks, branches, and leaves of urban trees are not modelled and should instead be parameterized (Buccolieri et al. 2018). Another issue is the uncertainty in the set-up information (e.g., the urban morphology and inlet conditions) and their influence on the CFD results (García-Sanchez et al. 2014; Santiago et al. 2020).
4) The governing equations of mesoscale and fluid dynamics models, including large-eddy simulations (LES), are similar but with very different types of assumption and thus different model coefficients. In addition, the turbulence flow properties are difficult to reproduce for numerical models.

Despite the strengths of the counterarguments discussed above, in the context of our thesis and our position on the employment of CFD as the most useful tool to develop mesoscale urban parameterizations, these assertions can be refuted for the following reasons.

1) Although field measurements provide the true values (not accounting for measurement errors) of the different variables at one location and time, their representativeness is very limited in space due to the strong spatial gradients of flow variables in the urban environment within the UCL. Field measurements can include all the scale motions, and properly located tower measurements can capture more homogeneous signals in the ISL. However, focusing on the physical processes within the UCL, the extrapolation from ISL using log-law is not able to accurately compute the flow properties. Multilayer UCPs compute flow properties within the UCL, and it is crucial to obtain good estimates for different applications (e.g., in urban air quality problems where the most important pollutant emissions are located on the ground). In addition, inputs for multilayer UCPs, such as drag coefficients, wall surface heat coefficient transfers, etc., require the flow properties within the UCP for their computation. In this context, such measurements give only an incomplete, albeit very faithful, representation of the thermo-dynamic behaviour of the atmosphere in the UCL. However, to determine the spatial averages, we need complete (e.g., every point) information. Even single layer UCPs require information on the UCL and assumptions about the flow properties. Notably, these assumptions cannot be checked/derived from tower measurements above the roughness sublayer. More details about this aspect are provided in Section 3. In addition, other properties, such as the drag forces over buildings, cannot be computed from such measurements because the pressure at the building surfaces is needed, which is not likely to be measured in field campaigns. Wind-tunnel experiments are very helpful for this purpose. Another important issue is the reduced number of scenarios that field campaigns can cover and the difficulties in extrapolating the results to improve parameterizations. To investigate a larger number of scenarios, field campaigns need to be conducted for a long enough period of time and over a large number of different locations, something that may be difficult and expensive to do. Furthermore, field experiments are necessarily performed under uncontrollable atmospheric conditions, making it difficult to isolate the importance of different factors on the flow behaviour. Moreover, CFD models are increasingly implementing more relevant processes, such as the thermal

effect, in order to simulate the best non-neutral conditions (Blocken 2014, 2015; Toparlar et al. 2017). For this purpose, wall models for CFD simulations with thermal boundary conditions remain a challenge. However, a review by Toparlar et al. (2017) described several studies considering thermal effects, including CFD model evaluations against measurements with suitably accurate mean flow properties, that were performed in recent years.

2) Physical modelling also suffers from a limited set of spatial points but addresses the issue of controlling the atmospheric conditions of the scenarios studied. In addition, a denser grid of flow measurements and measurements of other useful properties like drag forces can be easily performed using a wind-tunnel, rather than field experiments (Cheng et al. 2007; Hagishima et al. 2009). Further studies by Buccolieri et al. (2017, 2019) measured the drag force with varying packing density by direct methods (using a load cell or by estimating it through pressure measurements at the building surfaces). However, developing a study spanning a large parameter space requires performing a large number of experiments. Moreover, different scale geometries need to be prepared. Consequently, compared to CFD modelling, a much lower number of scenarios can be studied. Moreover, the cost (i.e., personnel, instrumentation and others) and set-up are much more expensive and require adherence to similarity criteria, which can be problematic for many applications, such as buoyant flows (Blocken 2015). Wind-tunnels or water-channels are usually focused on neutral conditions, although non-neutral flows have been recently investigated using wind-tunnel experiments (Marucci et al. 2018; Marucci and Carpentieri 2019, 2020). Non-neutral cases are more commonly studied by CFD modelling (Milliez and Carissimo 2007; Santiago et al. 2014; Antoniou et al. 2019). However, the experimental data are crucial for validation purposes, and numerous CFD studies use wind-tunnel experiments or water-channels to evaluate their results (e.g., Santiago et al. 2007, 2010; Blocken et al. 2008; Gromke et al. 2008; Tominaga and Stathopoulos 2009; Gromke and Blocken 2015).

3) The inaccuracy of the model results due to the inaccuracy of the set-up information is becoming less significant, as increasingly more information about urban morphology is being made available, and more complex CFD simulations are being performed (with real geometries, wider domains, coupling with mesoscale models, the inclusion of vegetation parameterization, etc.) with the aid of the increasing computational resources (Toparlar et al. 2015; 2018; Sanchez et al. 2017; Santiago et al. 2017a, b; Borge et al. 2018; Blocken 2018; Rivas et al. 2019; Antoniou et al. 2019). The commonly employed Reynolds-Averaged Navier–Stokes (RANS) turbulence models have problems with reproducing specific details of the flow (e.g., close to edges). RANS models do not require large computational resources because an integral approach for the whole turbulence spectrum is considered; thus, assumptions of turbulence modelling are necessary for the statistical closures. Nevertheless, Blocken (2018), in his review, concluded that RANS models remain very popular for applications such as wind comfort and near-field pollutant dispersion in urban areas with a high plan area density, urban thermal environments, the natural ventilation of buildings, and indoor airflow. Studies following best practice guidelines have obtained acceptable average flow results in most cases. However, the evaluation of CFD simulations against experimental measurements always remains necessary. Notably, studies considering more processes or more complex treatments of turbulence can be carried out with LES (albeit at a great CPU cost) or direct numerical simulations (DNS). The LES methodology applies a spatial filtering operation to the Navier–Stokes equations, explicitly solving the unsteady larger turbulence scales, while the effects of small-scale motions are modelled based on the resolved ones. LES provides more accurate and reliable results than RANS, but the computational cost and the complexity of the simulations are much higher. The most accurate results are obtained by DNS, where all scales of turbulence motion are solved. However, DNS are restricted to simulating the flow around a limited number of obstacles due to the computational costs. There are numerous best practice guidelines for using CFD simulations, particularly RANS models, in urban environments (Franke et al. 2007, 2011; Tominaga et al. 2008; Di Sabatino et al. 2011; Blocken 2015). These guides provide information about the features of the domain size, mesh, etc. in order to appropriately apply numerical methods to solve fluid equations. As previously explained, evaluating the model before using the results for UCP is crucial. In the first step for developing or improving UCP, simple configurations simulated by CFD could be used to elucidate new relevant processes for UCP (Santiago and Martilli 2010; Santiago et al. 2013; Simón-Moral et al. 2014).

4) Modelling the turbulence properties of a flow is challenging. However, for the purposes of these kinds of studies, CFD simulations—following best practice guidelines and evaluated against experimental measurements—can provide useful knowledge. Notably, the methodology presented and discussed here is not limited to RANS-type CFD models. Results from other types of CFD models, such as LES or DNS, could be used. LES and DNS reproduce the turbulence fields more accurately than RANS, albeit at a higher CPU cost, so they can be used

to compute turbulence statistics. In addition, the objective of using CFD in the context of our thesis is to improve UCPs that provide the average flow properties over cells of the horizontal dimensions in the order of 1 km^2. In this regard, if UCPs were able to achieve the performance of even a RANS model, this experiment would be a full success. Thus, we need to balance the accuracy of the simulations and the number of cases studied to provide the variation in UCP inputs as a parameter. However, it is also crucial, as mentioned before, that RANS simulations must be evaluated against experimental measurements.

3 Arguments

The main arguments supporting our thesis are summarized as follows:

1) Argument 1: Information at a very high spatial resolution within the UCL, only attainable with CFD, is needed to estimate the relevant average parameters for UCPs. The few point measurements within the UCL are not enough.
2) Argument 2: CFD provides a controllable environment, which is very desirable when seeking to understand a process and develop parametrizations. CFD allows one to easily span the parameter space, studying different configurations and atmospheric stabilities and identifying the relevance of various morphological features.
3) Argument 3: CFD provides the possibility to model, in detail, every building in the study area and explore all flow properties at the same time. The effects of urban obstacles, both porous (i.e., vegetation) and solid (i.e., walls and cars), as well as traffic-produced turbulence, can be simulated.
4) Argument 4: A methodology using CFD allows one to compare the vertical profiles of variables from newly developed UCPs featuring a horizontal spatial average over mesoscale cells from detailed CFD simulations. In this process, UCPs can be improved by changing the parameterization of their inputs using the CFD results.

The above arguments are clearly supported by the following statements:

1) To illustrate argument 1, the spatially-averaged flow properties deduced from high resolution CFD results are compared against the averages obtained using only few points, mimicking those that can be obtained from a set of measurements. An aligned array of cubes was selected as an idealized urban environment. Periodic CFD simulations were performed and evaluated with wind-tunnel measurements and DNS (further details can be found in Santiago et al. (2014) and Martilli et al. (2015)). Figure 2(a) shows the numerical domain and the locations of the three points where the flow properties were extracted, representing the possible positions of the measurement towers. Measurements at P1 from a wind tunnel experiment with a similar configuration (Brown et al. 1999, 2001) are also shown. This experiment was also used to evaluate RANS-CFD simulations over this geometry (Lien and Yee 2004; Santiago et al. 2007). Note that, in this case, the simulations are performed over a periodic domain, and the experimental data were taken from the third street canyon of an array. The results obtained show that the stream-wise velocity U is accurately captured, while the TKE and the velocity vertical component W are slightly underestimated, showing general agreement with other studies. Notably, deploying three measurement towers in an urban environment would be extremely expensive and has not been done so far, even in the most complete field campaigns. In the BUBBLE experiments (Rotach et al. 2005), for example, only one tower was used. Data from three towers, therefore, represented an exceptionally complete dataset. In Figures 2(b)–(d), it can be observed that at each height within the canopy, the horizontally-averaged values are notably different. This is due to the strong spatial variability of the flow in the urban canopy, as indicated by the vertical profiles at three points. Using only a few points for the average may induce important errors which, depending on the height, can be greater than 100% or even have suggest an opposite result (Figures 2(b)–(d)). In addition, this example was carried out using simple geometry. This effect can be even worse with more realistic geometry. Thus, despite its accuracy limitations, CFD modelling can provide more comprehensive information for developing UCPs. It is important to keep in mind that CFD simulations should be performed following best practices and evaluated with experimental measurements to correctly estimate their accuracy for the cases studied.
2) CFD models provide a controllable environment, making it possible to simulate different scenarios by changing one parameter at a time in each simulation. This makes it easier to understand the dependence of each parameter (e.g., geometry and inlet flow properties) on the average properties. For example, CFD allows simulations with and without a certain factor (buildings, vegetation, physical processes, etc.). Parametric studies with CFD can be more easily performed on geometries that are too complex to be realized in a wind-tunnel or used to reproduce conditions that cannot be consistently measured or cannot be realized in experimental tests. Example of such applications include measuring the aerodynamic forces of moving vehicles (rolling contact forces influence the measurement of aerodynamic forces) or modelling buoyant forces in complex urban environments (for pollutant dispersion studies), which might not be properly investigable through wind tunnel tests using only data

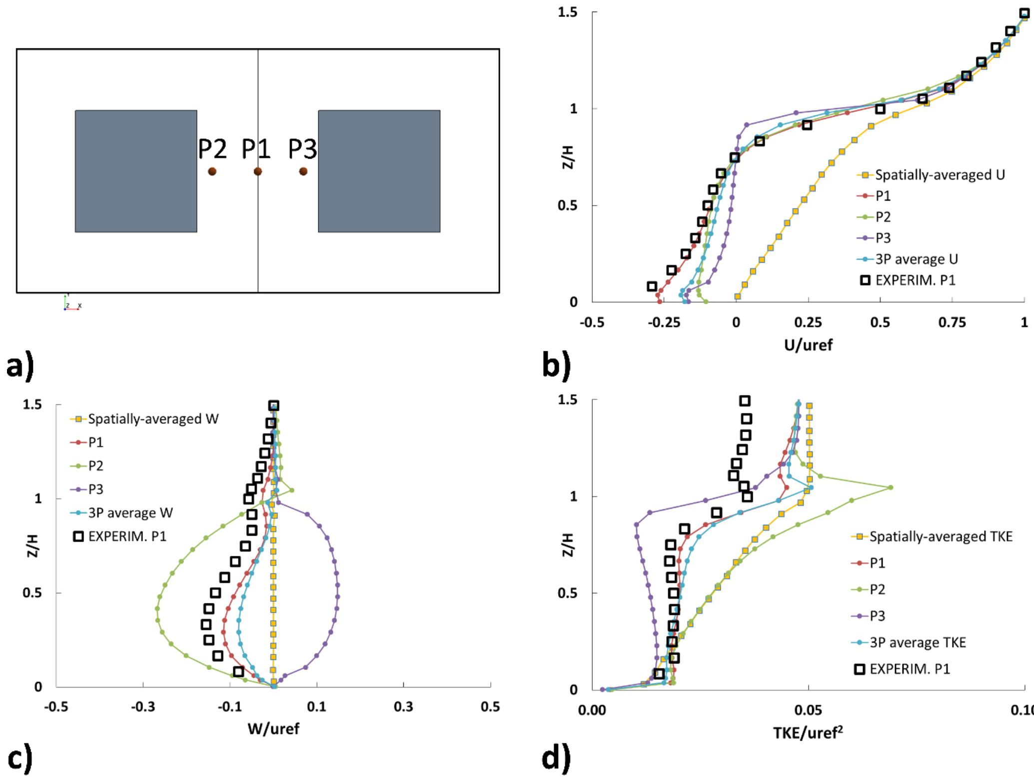

Fig. 2 (a) A scheme of the numerical domain with the location of the vertical profiles. (b) Vertical profiles of the spatially-averaged mean stream-wise velocity (*U*) over horizontal slices, normalized by a reference velocity u_{ref}, obtained at three different locations, with the profile computed as the average of the three former profiles; (c) same as (b) but for mean vertical velocity (*W*); (d) same as (b) but for turbulence kinetic energy (TKE). Experimental data from wind-tunnel experiments with similar configurations (Brown et al. 1999, 2001) are included

from recent wind-tunnel experiments on non-neutral flows (Marucci et al. 2018; Marucci and Carpentieri 2019, 2020). Wind tunnel tests on still vehicles or under neutrally buoyant conditions should be used to evaluate numerical models that can be subsequently used to reproduce more complex conditions. Consequently, CFD allows one to easily span the parameter space, studying different configurations and atmospheric stabilities and identifying the relevance of morphological features. In this way, the UCP inputs can be parametrized from CFD results. Some examples can be found in Santiago and Martilli (2010), Santiago et al. (2013), and Simón-Moral et al. (2014). Santiago and Martilli (2010) simulated staggered arrays of cubes for the same inlet flow properties (i.e., the incidence of the wind perpendicular to the array) while changing the packing density (in terms of the planar area index λ_p) but keeping the layout. From these CFD simulations, the drag coefficient, length scale, and displacement height (inputs of UCPs) as a function of packing density were computed. Figure 3 illustrates the configuration studied and the parameters included in the BEP/BEM, UCP coupled with the WRF model. Santiago et al. (2013) determined the form that a UCP must take to reproduce wind-turning effects within the canopy. In that work, the same building configuration (an aligned array of cubes) was simulated for different inlet wind directions. Simón-Moral et al. (2014) studied the variation in the drag coefficient and turbulent length scale (UCP inputs) of an aligned array of cubes as a function of its geometrical layout. For the same packing densities, different layouts were simulated.

3) CFD models allow one to study all flow properties at the same time without additional effort (this is different for measurements where different devices are needed). In a recent review, Blocken (2014) presented a perspective on the past, present, and future, summarizing the past 50 years of Computational Wind Engineering (CWE), which has successfully transitioned from an emerging field into an increasingly established field in wind engineering research, practice, and education. More recently, Toparlar et al. (2017) provided a review of research reported in journal publications on the use of CFD for microclimate research. The authors documented the increasing popularity of the research area over the years. Early CFD microclimate studies were conducted for model development, and later studies applied CFD to real case studies. Later, after

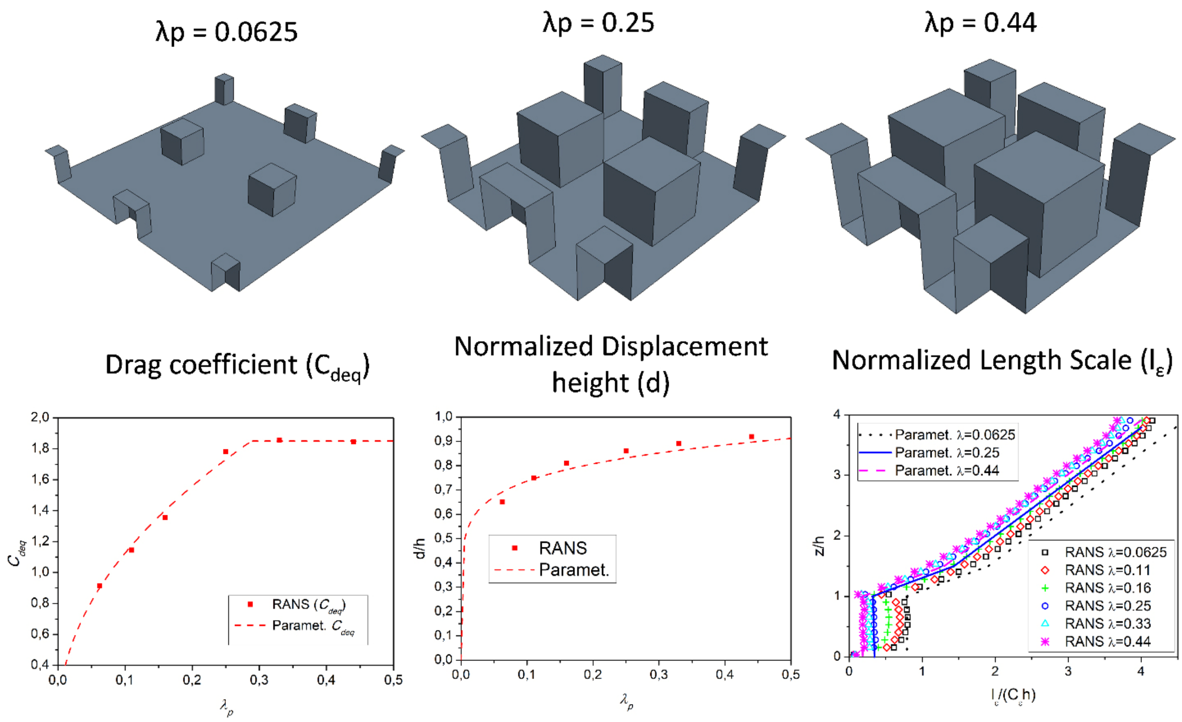

Fig. 3 The top panels show the three configurations studied by Santiago and Martilli (2010) with different packing densities. The bottom panels show the dependency of the drag coefficient, the displacement height, and the length scale (l_ε) obtained with the RANS simulations and the parameterization proposed by Santiago and Martilli (2010) (some parts of the figure are adapted from Santiago and Martilli (2010), reproduced with the permission © 2010 Springer)

establishing simulation set-ups, research efforts shifted to case studies. Such widespread CFD modelling exercises and expert applications have been essential to extract information on the physical processes within the canopy in a parameterized form (depending on urban morphology and meteorological conditions). These results inspired the development of subgrid parameterizations suitable for mesoscale weather models (Di Sabatino 2017). In this way, the impact of building morphology, vegetation, thermal stability, and even the turbulence induced by traffic on the average flow properties can be simply computed and parameterized for inclusion in UCP. Studies by Santiago and Martilli (2010) and Gutiérrez et al. (2015) showed the use of CFD to quantify the variation of drag coefficients with lambda-parameters (building packing densities), as well as the parameterization of turbulent length scales and its usefulness in mesoscale models. Notably, the introduction of a drag coefficient that varies with the building plan-area fraction increases the accuracy of a mesoscale model in predicting the surface wind speed in complex urban environments, particularly in areas with tall buildings. This was corroborated via simulations over New York city, with BEP/BEM UCP coupled with the WRF model. Santiago et al. (2014) parameterized the influence of buoyancy forces on the drag coefficient in terms of the solar position and h/L_{urb}. Here, L_{urb} is an urban length scale analogous to the Obukhov length, defined as $L_{\mathrm{urb}} = u_\tau^3 T_{\mathrm{ref}} \rho C_{\mathrm{p}} / (g Q_{\mathrm{h}})$, where u_τ is a scale velocity, Q_{h} is the total heat flux defined by the heat from all surfaces divided by the plan area, C_{p} is the specific heat of the air, T_{ref} is the reference temperature, g is the acceleration due to gravity, and ρ is the air density (Figure 4). The effect of tree foliage on the flow in urban areas was parameterized by Krayenhoff et al. (2015). Obstacle-resolving CFD simulations were used to determine the source and sink terms required for the momentum and TKE equations to represent the impact of trees on the horizontally-averaged mean flow within the urban canopy. Work remains ongoing to further test improved drag coefficients for tall buildings to capture not only wind speed but also wind direction at high resolution for the high-rise and compact city of Hong Kong. Results are encouraging and show that the urban microclimate of coastal high-rise cities can be realistically predicted, provided that the complexity of the urban morphology is appropriately captured and described (Wang et al. 2017). The required simple-yet-robust parameterization of urban morphology within weather prediction models would not have been possible without the large research efforts devoted to CFD modelling and companion experimental work undertaken in recent decades (Blocken 2014).

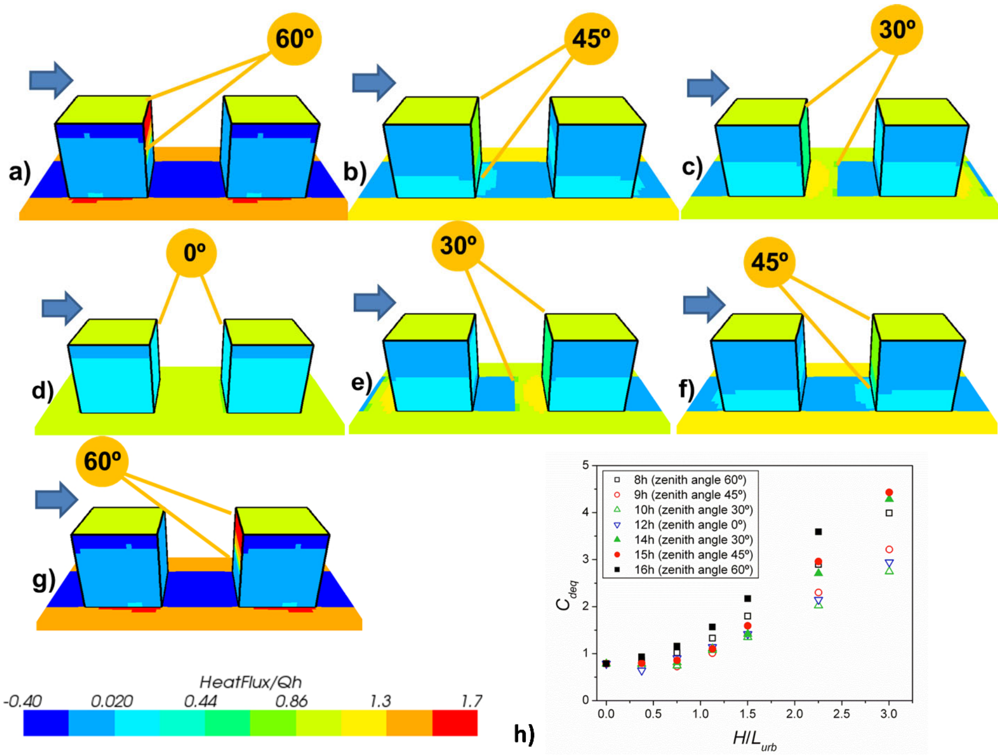

Fig. 4 Sensible heat flux distribution imposed on the building surfaces corresponding to (a) 8 local solar time (LST) to (g) 16 LST. (h) Drag coefficient for different heat fluxes and sun positions (adapted from Santiago et al. (2014), reproduced with the permission © 2014 Elsevier)

4) In the process to develop or improve UCP, CFD results are used to compute the spatially-averaged flow properties (including turbulent kinetic energy) and parameterize the input of the UCP depending on different parameters (building morphology, vegetation scenarios, inlet wind conditions, etc.). In addition to this advantage, the performance of the improved UCP can be evaluated by comparing the vertical profiles of the different flow properties averaged from the CFD results with the results obtained with the new UCP. The CFD model and new UCP can be run with the same conditions (using UCP with the inputs computed from CFD). Thus, the differences between the vertical profiles of the spatially-averaged properties computed from CFD and the UCP results are only due to the simplifications made by UCP. This evaluation allows one to assess the inaccuracy of the new UCP due to the inaccuracy of its simplifications caused by its coarse spatial resolution. Therefore, by developing UCP simulations with different assumptions, it is possible to evaluate the importance of these approaches on each flow property in the urban environment being simulated. Following this methodology and comparing the horizontally-averaged flow properties from CFD simulations with the UCP results, Santiago et al. (2013) showed that, for incoming flow not normal to the building faces, a UCP is able to reproduce the wind direction change due to the height within the canopy if a height-dependent drag coefficient is used. Figure 5 illustrates this point, where the results for different drag parameterization approaches in UCP are provided. Simón-Moral et al. (2014) found that, taking into account the dependency of the drag coefficient with the geometrical layout (not only packing density), UCP is able to provide suitable wind speed and turbulence kinetic energy values, which are different for different layouts with the same packing density. Martilli et al. (2015) showed that UCP is able to reproduce the pollutant dispersion within aligned and staggered arrays of cubes when the dispersive fluxes computed by CFD simulations are considered. Simón-Moral et al. (2017) improved their UCP results by considering the dependency of the length scales and drag coefficient with thermal stability and accounting for dispersive stress; all of these variables were computed with the CFD results (Santiago et al. 2014).

4 Summary and conclusions

Mesoscale meteorological models need to represent cities in their simulations and use UCPs for this purpose. Urban obstacles cannot be resolved by UCPs, and their results

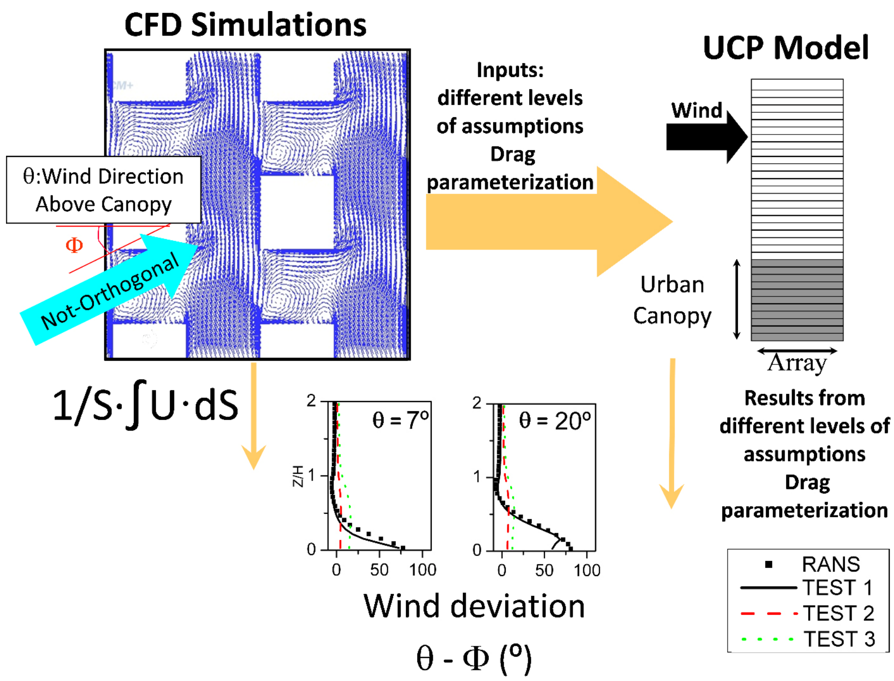

Fig. 5 Scheme of the approach followed by Santiago et al. (2013) to improve the parameterization of drag in the UCP considering inlet wind directions. Test 1 considers the drag coefficient values directly computed from the CFD, including the height dependence; two components of the drag coefficient are considered. Test 2 considers two components of the drag coefficient constant with height, and Test 3 considers one drag coefficient value constant with height (some parts of the figure are adapted from Santiago et al. (2013), reproduced with the permission © 2013 Springer)

correspond to the horizontally-averaged properties of the flow over mesoscale cells, typically 1 km^2 or hundreds of meters by hundreds of meters in size. Therefore, to develop a UCP, accurate information on the spatially-averaged flow properties is necessary. Since the interaction between the atmosphere and urban obstacles induces strong heterogeneities in the flow properties within the UCL, high spatial resolution information is needed to compute the horizontal averages. Obtaining the necessary spatial averages within the canopy for the UCPs, for many configurations and atmospheric conditions, is extremely difficult (albeit not impossible) with just laboratory and field measurements. On the other hand, this is much easier to achieve with CFD models. In this sense CFDs are the most useful tools to design UCPs. With the word "most", we do not mean that CFDs are perfect—the reader should be fully aware of the many limitations (numeric, uncertainty, etc.) of CFDs. Rather, we are making a relative judgement compared to other approaches. With the word "useful", we mean that this is the technique that can most easily provide the information needed for UCPs. However, CFD models also need to be validated and calibrated using lab and field measurements. In addition, different urban configurations and atmospheric conditions can be simulated by CFD under a controllable environment, allowing one to perform a parametric study useful for the development of UCP. These simulations can include detailed models of urban obstacles (buildings, trees, etc.) and provide information about all flow properties at the same time without any additional effort. The methodology using CFD allows one to compare the UCP's vertical profiles with the horizontal spatial averages from the detailed CFD simulations in some cases; thus, the assumptions made during the UCP's development can be tested. In this way, an improved (or new) UCP could be ready for use in real cities using the parameterization developed with CFD simulations along with the detailed input data of urban morphology corresponding to each mesoscale cell.

The use of CFD to develop (and eventually improve) UCPs will provide a better representation of cities in mesoscale meteorological models. The increase in computational resources and available urban morphology data is leading to increasingly more realistic CFD simulations with more detailed urban geometry, wider numerical domains, and more physical processes. In addition, the model results will be able to be evaluated with experimental measurements that are more common in urban environments. In this way, CFD simulations will become more realistic and accurate and thus provide a better representation of the city effects in mesoscale meteorological models. This will improve the meteorological and pollutant dispersion models within the cities where people live. It is worth mentioning that all currently existing UCPs are based on simplified geometry. Thus, it is not unreasonable to validate/test UCPs against idealized CFD simulations. The question is to what extent these idealized configurations represent real urban morphology. Here, again, CFD models can be extremely useful because they allow one to compare idealized and real morphologies. Thus, by using these models we can determine the simplest urban morphology that most accurately represents a real case and use it to build UCPs. This is something unattainable with field or laboratory measurements.

Acknowledgements

This study has been supported by EXCLUR (CGL2016-80154-R) project funded by Spanish Ministry of Science and Innovation.

Funding note: Open access funding provided by Università del Salento.

References

Antoniou N, Montazeri H, Neophytou M, Blocken B (2019). CFD simulation of urban microclimate: Validation using high-resolution field measurements. *Science of the Total Environment*, 695: 133743.

Blocken B, Stathopoulos T, Carmeliet J (2008). Wind environmental conditions in passages between two long narrow perpendicular buildings. *Journal of Aerospace Engineering*, 21: 280–287.

Blocken B (2014). 50 years of Computational Wind Engineering: Past, present and future. *Journal of Wind Engineering and Industrial Aerodynamics*, 129: 69–102.

Blocken B (2015). Computational Fluid Dynamics for urban physics: Importance, scales, possibilities, limitations and ten tips and tricks towards accurate and reliable simulations. *Building and Environment*, 91: 219–245.

Blocken B (2018). LES over RANS in building simulation for outdoor and indoor applications: A foregone conclusion? *Building Simulation*, 11: 821–870.

Borge R, Santiago JL, de la Paz D, Martín F, Domingo J, et al. (2018). Application of a short term air quality action plan in Madrid (Spain) under a high-pollution episode - Part II: Assessment from multi-scale modelling. *Science of the Total Environment*, 635: 1574–1584.

Brown MJ, Lawson RE, Decroix DS, Lee RL (1999). Mean flow and turbulence measurements around a 2-D array of buildings in a wind tunnel, Report LA-UR-99-5395, Los Alamos National Laboratory, Los Alamos, NM, USA.

Brown MJ, Lawson RE, DeCroix DS, Lee RL (2001). Comparison of centerline velocity measurements obtained around 2D and 3D buildings arrays in a wind tunnel, Report LA-UR-01-4138, Los Alamos National Laboratory, Los Alamos, USA.

Buccolieri R, Salim SM, Leo LS, Di Sabatino S, Chan A, et al. (2011). Analysis of local scale tree–atmosphere interaction on pollutant concentration in idealized street canyons and application to a real urban junction. *Atmospheric Environment*, 45: 1702–1713.

Buccolieri R, Wigö H, Sandberg M, Di Sabatino S (2017). Direct measurements of the drag force over aligned arrays of cubes exposed to boundary-layer flows. *Environmental Fluid Mechanics*, 17: 373–394.

Buccolieri R, Santiago JL, Rivas E, Sanchez B (2018). Review on urban tree modelling in CFD simulations: Aerodynamic, deposition and thermal effects. *Urban Forestry & Urban Greening*, 31: 212–220.

Buccolieri R, Sandberg M, Wigö H, Di Sabatino S (2019). The drag force distribution within regular arrays of cubes and its relation to cross ventilation – Theoretical and experimental analyses. *Journal of Wind Engineering and Industrial Aerodynamics*, 189: 91–103.

Cheng H, Hayden P, Robins AG, Castro IP (2007). Flow over cube arrays of different packing densities. *Journal of Wind Engineering and Industrial Aerodynamics*, 95: 715–740.

Di Sabatino S, Buccolieri R, Olesen HR, Ketzel M, Berkowicz R, et al. (2011). COST 732 in practice: The MUST model evaluation exercise. *International Journal of Environment and Pollution*, 44: 403–418.

Di Sabatino S, Buccolieri R, Salizzoni P (2013). Recent advancements in numerical modelling of flow and dispersion in urban areas: a short review. *International Journal of Environment and Pollution*, 52: 172.

Di Sabatino S (2017). Progress in local scale flow and dispersion modelling. In: Proceedings of Air Pollution Modeling and its Application XXV.

Franke J, Hellsten A, Schlünzen H, Carissimo B (2007). Best practice guideline for the CFD simulation of flows in the urban environment. COST Office Brussels.

Franke J, Hellsten A, Schlünzen KH, Carissimo B (2011). The COST 732 Best Practice Guideline for CFD simulation of flows in the urban environment: A summary. *International Journal of Environment and Pollution*, 44: 419–427.

García-Sánchez C, Philips DA, Gorlé C (2014). Quantifying inflow uncertainties for CFD simulations of the flow in downtown Oklahoma City. *Building and Environment*, 78: 118–129.

Gromke C, Ruck B (2007). Influence of trees on the dispersion of pollutants in an urban street canyon—Experimental investigation of the flow and concentration field. *Atmospheric Environment*, 41: 3287–3302.

Gromke C, Buccolieri R, Di Sabatino S, Ruck B (2008). Dispersion study in a street canyon with tree planting by means of wind tunnel and numerical investigations—Evaluation of CFD data with experimental data. *Atmospheric Environment*, 42: 8640–8650.

Gromke C, Blocken B (2015). Influence of avenue-trees on air quality at the urban neighborhood scale. Part I: Quality assurance studies and turbulent Schmidt number analysis for RANS CFD simulations. *Environmental Pollution*, 196: 214–223.

Gutiérrez E, Martilli A, Santiago JL, González JE (2015). A mechanical drag coefficient formulation and urban canopy parameter assimilation technique for complex urban environments. *Boundary-Layer Meteorology*, 157: 333–341.

Hagishima A, Tanimoto J, Nagayama K, Meno S (2009). Aerodynamic parameters of regular arrays of rectangular blocks with various geometries. *Boundary-Layer Meteorology*, 132: 315–337.

Jeanjean APR, Hinchliffe G, McMullan WA, Monks PS, Leigh RJ (2015). A CFD study on the effectiveness of trees to disperse road traffic emissions at a city scale. *Atmospheric Environment*, 120: 1–14.

Krayenhoff ES, Santiago JL, Martilli A, Christen A, Oke TR (2015). Parametrization of drag and turbulence for urban neighbourhoods with trees. *Boundary-Layer Meteorology*, 156: 157–189.

Kusaka H, Kondo H, Kikegawa Y, Kimura F (2001). A simple single-layer urban canopy model for atmospheric models: comparison with multi-layer and slab models. *Boundary-Layer Meteorology*, 101: 329–358.

Lateb M, Meroney RN, Yataghene M, Fellouah H, Saleh F, Boufadel MC (2016). On the use of numerical modelling for near-field pollutant dispersion in urban environments—A review. *Environmental Pollution*, 208: 271–283.

Lien F-S, Yee E (2004). Numerical modelling of the turbulent flow developing within and over a 3-D building array, part I: A high-resolution Reynolds-averaged Navier–Stokes approach. *Boundary-Layer Meteorology*, 112: 427–466.

Martilli A, Clappier A, Rotach MW (2002). An urban surface exchange parameterisation for mesoscale models. *Boundary-Layer Meteorology*, 104: 261–304.

Martilli A, Santiago JL, Salamanca F (2015). On the representation of urban heterogeneities in mesoscale models. *Environmental Fluid Mechanics*, 15: 305–328.

Marucci D, Carpentieri M, Hayden P (2018). On the simulation of thick non-neutral boundary layers for urban studies in a wind tunnel. *International Journal of Heat and Fluid Flow*, 72: 37–51.

Marucci D, Carpentieri M (2019). Effect of local and upwind stratification on flow and dispersion inside and above a bi-dimensional street canyon. *Building and Environment*, 156: 74–88.

Marucci D, Carpentieri M (2020). Dispersion in an array of buildings in stable and convective atmospheric conditions. *Atmospheric Environment*, 222: 117100.

Masson V (2000). A physically-based scheme for the urban energy budget in atmospheric models. *Boundary-Layer Meteorology*, 94: 357–397.

Meroney RN, Leitl BM, Rafailidis S, Schatzmann M (1999). Wind-tunnel and numerical modeling of flow and dispersion about several building shapes. *Journal of Wind Engineering and Industrial Aerodynamics*, 81: 333–345.

Milliez M, Carissimo B (2007). Numerical simulations of pollutant dispersion in an idealized urban area, for different meteorological conditions. *Boundary-Layer Meteorology*, 122: 321–342.

Rivas E, Santiago JL, Lechón Y, Martín F, Ariño A, Pons JJ, Santamaría JM (2019). CFD modelling of air quality in Pamplona City (Spain): Assessment, stations spatial representativeness and health impacts valuation. *Science of the Total Environment*, 649: 1362–1380.

Rotach MW, Vogt R, Bernhofer C, Batchvarova E, Christen A, et al. (2005). BUBBLE – an urban boundary layer meteorology project. *Theoretical and Applied Climatology*, 81: 231–261.

Salamanca F, Krpo A, Martilli A, Clappier A (2010). A new building energy model coupled with an urban canopy parameterization for urban climate simulations—part I. formulation, verification, and sensitivity analysis of the model. *Theoretical and Applied Climatology*, 99: 331–344.

Salamanca F, Martilli A, Tewari M, Chen F (2011). A study of the urban boundary layer using different urban parameterizations and high-resolution urban canopy parameters with WRF. *Journal of Applied Meteorology and Climatology*, 50: 1107–1128.

Salamanca F, Martilli A, Yagüe C (2012). A numerical study of the Urban Heat Island over Madrid during the DESIREX (2008) campaign with WRF and an evaluation of simple mitigation strategies. *International Journal of Climatology*, 32: 2372–2386.

Sanchez B, Santiago JL, Martilli A, Martin F, Borge R, et al. (2017). Modelling NOX concentrations through CFD-RANS in an urban hot-spot using high resolution traffic emissions and meteorology from a mesoscale model. *Atmospheric Environment*, 163: 155–165.

Santiago JL, Martilli A, Martín F (2007). CFD simulation of airflow over a regular array of cubes. Part I: Three-dimensional simulation of the flow and validation with wind-tunnel measurements. *Boundary-Layer Meteorology*, 122: 609–634.

Santiago JL, Dejoan A, Martilli A, Martin F, Pinelli A (2010). Comparison between large-eddy simulation and Reynolds-averaged navier–stokes computations for the MUST field experiment. Part I: study of the flow for an incident wind directed perpendicularly to the front array of containers. *Boundary-Layer Meteorology*, 135: 109–132.

Santiago JL, Martilli A (2010). A dynamic urban canopy parameterization for mesoscale models based on computational fluid dynamics Reynolds-averaged Navier–Stokes microscale simulations. *Boundary-Layer Meteorology*, 137: 417–439.

Santiago JL, Coceal O, Martilli A (2013). How to parametrize urban-canopy drag to reproduce wind-direction effects within the canopy. *Boundary-Layer Meteorology*, 149: 43–63.

Santiago JL, Krayenhoff ES, Martilli A (2014). Flow simulations for simplified urban configurations with microscale distributions of surface thermal forcing. *Urban Climate*, 9: 115–133.

Santiago JL, Borge R, Martin F, de la Paz D, Martilli A, et al. (2017a). Evaluation of a CFD-based approach to estimate pollutant distribution within a real urban canopy by means of passive samplers. *Science of The Total Environment*, 576: 46–58.

Santiago JL, Rivas E, Sanchez B, Buccolieri R, Martin F (2017b). The impact of planting trees on NO_x concentrations: The case of the Plaza de la Cruz neighborhood in Pamplona (Spain). *Atmosphere*, 8: 131.

Santiago JL, Sánchez B, Quaassdorff C, de la Paz D, Martilli A, et al. (2020). Performance evaluation of a multiscale modelling system applied to particulate matter dispersion in a real traffic hot spot in Madrid (Spain). *Atmospheric Pollution Research*, 11: 141–155.

Simón-Moral A, Santiago JL, Krayenhoff ES, Martilli A (2014). Streamwise versus spanwise spacing of obstacle arrays: parametrization of the effects on drag and turbulence. *Boundary-Layer Meteorology*, 151: 579–596.

Simón-Moral A, Santiago JL, Martilli A (2017). Effects of unstable thermal stratification on vertical fluxes of heat and momentum in urban areas. *Boundary-Layer Meteorology*, 163: 103–121.

Tominaga Y, Mochida A, Yoshie R, Kataoka H, Nozu T, Yoshikawa M, Shirasawa T (2008). AIJ guidelines for practical applications of CFD to pedestrian wind environment around buildings. *Journal of Wind Engineering and Industrial Aerodynamics*, 96: 1749–1761.

Tominaga Y, Stathopoulos T (2009). Numerical simulation of dispersion around an isolated cubic building: Comparison of various types of k-ε models. *Atmospheric Environment*, 43: 3200–3210.

Tominaga Y, Stathopoulos T (2016). Ten questions concerning modeling of near-field pollutant dispersion in the built environment. *Building and Environment*, 105: 390–402.

Toparlar Y, Blocken B, Vos P, van Heijst GJF, Janssen WD, et al. (2015). CFD simulation and validation of urban microclimate: A case study for Bergpolder Zuid, Rotterdam. *Building and Environment*, 83: 79–90.

Toparlar Y, Blocken B, Maiheu B, van Heijst GJF (2017). A review on the CFD analysis of urban microclimate. *Renewable and Sustainable Energy Reviews*, 80: 1613–1640.

Toparlar Y, Blocken B, Maiheu B, van Heijst GJF (2018). Impact of urban microclimate on summertime building cooling demand: A parametric analysis for Antwerp, Belgium. *Applied Energy*, 228: 852–872.

UN-Habitat (2016). Urbanization and Development: Emerging Futures. World Cities Report 2016. United Nations Human Settlements Programme (UN-Habitat), Nairobi, Kenya. Available at http://wcr.unhabitat.org/main-report. Accessed 30 Sept 2019.

Vardoulakis S, Fisher BEA, Pericleous K, Gonzalez-Flesca N (2003). Modelling air quality in street canyons: a review. *Atmospheric Environment*, 37: 155–182.

Wang Y, Di Sabatino S, Martilli A, Li Y, Wong MS, Gutiérrez E, Chan PW (2017). Impact of land surface heterogeneity on urban heat island circulation and sea-land breeze circulation in Hong Kong. *Journal of Geophysical Research: Atmospheres*, 122: 4332–4352.

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