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High-resolution air quality modeling: Sensitivity tests to horizontal resolution and urban canopy with WRF-CHIMERE

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ABSTRACT

The European Directive (2008/50/EC) encourages the use of models in the assessment and forecasting of air quality, and assigns them a supporting or replacing role with respect to fixed ground-based measurements. A thorough knowledge of performance of the modeling tools over urban areas is therefore required. In this study, we analyze sensitivity tests with the WRF-CHIMERE modeling system in order to investigate the effect of (1) the horizontal model grid size, (2) the resolution of the anthropogenic emission inventory, and (3) the introduction of urban canopy models. The work focuses on L'Aquila and Milan, two Italian cities widely differing for the number of inhabitants, the extension and the geographical location. We found a clear advantage in increasing the model resolution up to ∼4 km, but a further increase at ∼1 km resolution does not seem to be justified. Moreover, we found that the ozone simulation is generally degraded at higher resolution. The introduction of a more detailed treatment of the urban canopy and of the anthropogenic emissions suggests the potential for further improvement, but this requires a fine tuning on the area of application. For example, the Building Environment Parameterization corrects the surface wind speed daily cycle, but it also increases the planetary boundary layer height, resulting in excessive dilution of primary pollutants. The anthropogenic emissions should be refined proportionally to the increase in dynamic model resolution, possibly through new bottom-up inventories, rather than through a downscaling of a coarser inventory. We suggest that future work should primarily focus on intensive campaign periods, where a comprehensive observational characterization of the three dimensional structure and evolution of the planetary boundary layer is available.

1. Introduction

World and European agencies for human health and environmental protection treat air pollution as an urgent topic. World Health Organization (WHO) provides significant data about pollution-related premature deaths, with an amount of more than 2 million each year (WHO Guidelines, 2006). According to the European Environmental Agency (EEA), in European countries the most harmful pollutants are particulate matter (PM), nitrogen dioxide (NO_2), and ozone (O_3). In Europe, the rate of life loss is estimated in the range of 400,000–500,000 premature deaths (EEA Report, 2016). In Italy, the entity of premature deaths attributable to PM2.5, NO2 and O3 in 2013 is estimated in 66630, 21040 and 3380, respectively (EEA Report, 2016). The expected increase of urban population during 21st century makes urban air quality a crucial issue. According to data by European Commission, almost 75% of the European population lived in an urban area in 2015. It is estimated that just over 80% of the European population and almost two thirds of the world's population will be living in urban areas by 2050 (Eurostat, 2016). Initiatives aimed at controlling air quality, including regulatory requirements, are yielding reductions of key pollutants (Bloomer et al., 2009; Falasca et al., 2016). However, in the future, European ecosystems and citizens are likely to be increasingly affected by the transboundary transport of air pollutants from developing countries such as those in South-East Asia (EEA Report, 2016).

In this work, we analyze the air quality in two Italian urban areas (Milan and L'Aquila) characterized by different number of inhabitants, extension and geographical location using the modeling tool composed by the Weather Research and Forecasting model (WRF, Skamarock et al., 2008) and the chemistry and transport model CHIMERE (Menut et al., 2013). Milan is located in the Po Valley, one of the pollution “hot spots” in Europe, and the phenomenology of air pollution there is well characterized (e.g. Putaud et al., 2010; Bigi and Ghermandi, 2014; Curci et al., 2015 and references therein). L'Aquila is located in Central Italy, in a mountain valley, and it is generally much less polluted than Milan. The number of exceedances of PM10 and ozone limit values is

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Abbreviations

BEP	Building Environment Parameterization
CTM	chemistry-transport models
EEA	European Environmental Agency
PBL	Planetary Boundary Layer
PM	particulate matter
T2m	temperature at 2 m height
U10m	wind speed at 10 m height
UCM	Urban Canopy Models
WHO	World Health Organization
WRF	Weather Research and Forecasting model

generally below the threshold of EU and national legislation (Di Carlo et al., 2007; Curci et al., 2012), and the site receives a significant contribution from long-range transport and natural sources (Pitari et al., 2014, 2015). However, the development of state-of-art air quality modeling tools is justified also in less polluted places, such as L'Aquila, because models may complement or substitute the standard observational monitoring network, according to the current legislation (EU 50/2008, D. Lgs. 155/2010).

In this context, Eulerian chemistry-transport models (CTM) are widely used tools and there is a clear trend in specializing the applications at high horizontal resolution for their application at the urban scale (Terrenoire et al., 2015). The need for high-resolution simulations (up to 1 km) stems from the fact that a better representation of small scale processes is crucial for a more accurate simulation of

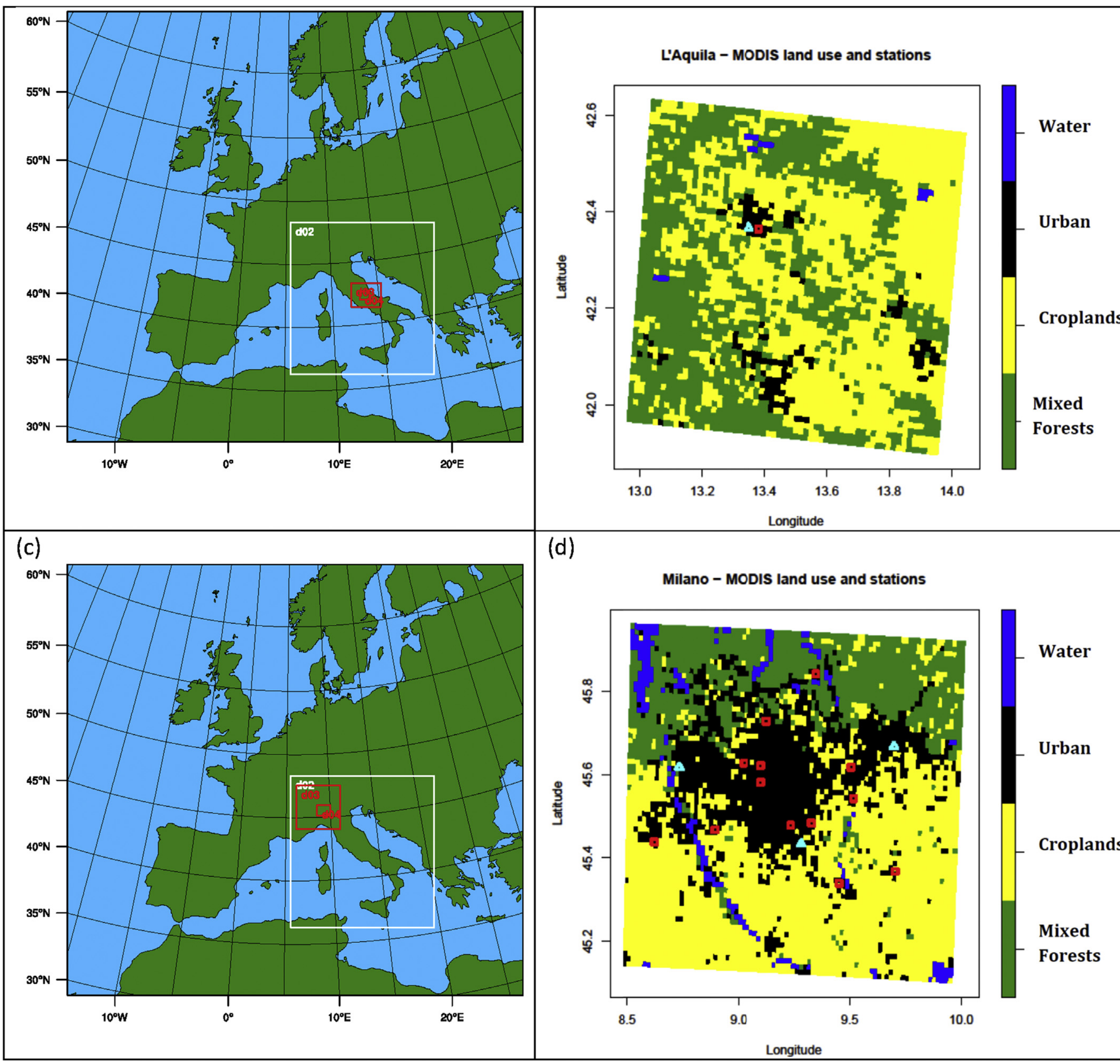

Fig. 1. Simulation domains over (a) L'Aquila and (c) Milan. Panels (b) and (d) show land use classification (from MODIS) used in the highest resolution domains. Cyan triangles denote NOAA meteorological stations, while red squares denote air quality Airbase stations. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

Table 1
Definition of simulation domains.

Area	WRF meteorological model			CHIMERE chemistry-transport model		
	Label	Resolution (km)	n. cells (lon x lat)	Label	Resolution (degrees)	n. cells (lon x lat)
Europe	EUR36	36	108 × 102	EUR05	0.5	82 × 55
Italy	ITA12	12	102 × 108	ITA015	0.15	87 × 72
Central Italy	ABR04	4	63 × 51	ABR004	0.04	51 × 35
North-Western Italy	NW04	4	93 × 93	NW004	0.04	113 × 70
L'Aquila	AQU01	1.33	60 × 54	AQ0015	0.015	53 × 34
Milan	MI01	1.33	84 × 66	MI0015	0.015	92 × 48

Table 2
Physics options used for WRF simulations.

Category (namelist variable)	namelist.input option	
Microphysics (mp_physics)	WSM6	
Longwave radiation (ra_lw_physics)	rrtmg scheme	
Shortwave radiation (ra_sw_physics)	rrtmg scheme	
Surface layer (sf_sfclay_physics)	Revised MM5 Monin-Obukhov	
Land Surface (sf_surface_physics)	unified Noah land-surface model	
Planetary Boundary Layer (bl_pbl_physics)	Bougeault and Lacarrere (BouLac)	
Urban Physics (sf_urban_physics)	Bulk	BULK
	UCM	Urban Canopy Model
	BEP	Building Environment Parameterization

Table 3
Labels and description of numerical experiments.

Label	WRF Urban model	WRF Urban parameters	Emissions reallocation
REF	Bulk	–	No
UCM	UCM	Default	No
UCMt	UCM	Tuned	No
BEP	BEP	Default	No
BEPt	BEP	Tuned	No
GLOB	Bulk	–	Yes

meteorological and chemical-dispersion processes (Schaap et al., 2015; Terrenoire et al., 2015; Mircea et al., 2016). Increased resolution, however, is not the solution to all simulation biases, which are still found especially under stable night-time conditions (e.g. Mircea et al., 2016). Moreover, there is a limit to the use of current turbulence parameterizations in meteorological and chemistry-transport model, that prevents a meaningful application on grids finer than ~1 km (Wyngaard, 2004). Indeed, the improvement in simulating meteorological and composition quantities tends to saturate as model grids approach spacing of a few km (Kuik et al., 2013).

The increase of model resolution should be generally accompanied by a proportional increase in the underlying emission inventories (Schaap et al., 2015). The ideal case is the development of new, highly resolved, bottom-up inventories that result in the most accurate representation of emissions (Timmermans et al., 2013; Zhou et al., 2017). When a high-resolution bottom-up inventory is unavailable, a coarse-resolution inventory may be downscaled by use of high-resolution proxy variables. For example, Kuik et al. (2013) obtained satisfactory results downscaling the 7 km × 7 km TNO-MACC III inventory to 1 km × 1 km, through traffic and population density as proxy variables. In this work, we develop a downscaled version of the 5 km × 5 km national CTN-ACE emissions inventory (Deserti et al., 2008), using GlobCover land use as proxy variable to reallocate anthropogenic emissions on 1 km × 1 km model grids.

When the focus of the study is specifically an urban area, the use of Urban Canopy Models (UCM), for a better representation of the effect on turbulent dispersion of the complex urban texture, is becoming another common practice. The simulation of daytime temperature near the surface is usually satisfactory also without the use of an UCM module (Salamanca et al., 2011), but this is needed for a more accurate simulation of night-time stable conditions (Martilli et al., 2003). The wind speed and pollutant concentrations near the surface are generally reported to be better reproduced when an increased complexity is introduced in the treatment of the urban canopy (Martilli et al., 2003; Salamanca et al., 2011; Liao et al., 2014; De la Paz et al., 2016). Specialization of UCM internal parameters with characteristics specific of the city (e.g. average building height, artificial surfaces albedo and thermal inertia, etc.) was also found to improve simulations (Kuik et al., 2013). Here we compare results applying a bulk urban parameterization (Chen et al., 2011) and two UCM available in WRF (Kusaka et al., 2001; Martilli et al., 2002).

The work presented here is aimed at testing the three main aspects summarized from the recent literature in the two urban areas of Milan and L'Aquila: the effect of increasing model horizontal resolution, the effect of the spatial reallocation of anthropogenic emissions, and the effect of the introduction of urban canopy models. In section 2, we describe the setup of WRF and CHIMERE models, the spatial reallocation procedure of anthropogenic emissions, and the observations used for comparison with simulations. The results of sensitivity tests are illustrated in section 3, organized into three subsections dedicated to the spatial resolution, urban schemes and the emissions reallocation, and are discussed and summarized in final section 4.

Table 4
Thermal parameters used in urban canopy models (UCM and BEP). We list default values (first column), a range from the literature (second and third columns), and those used here for adjusting values to Italian cities (fourth column).

Parameter for UCM and BEP Urban Canopy Models	Default	Kusaka et al. (2001)	Kim et al. (2013)	This work
Heat capacity of roof, building walls, road (J m^{-3} K^{-1})	1.0×10^6	2.1×10^6	2.1 × 106	2.1 × 106
Thermal conductivity of roof, building walls (W m^{-1} K^{-1})	0.67	2.28	2.28	2.28
Thermal conductivity of road (W m^{-1} K^{-1})	0.4004	2.28	2.28	0.7
Surface albedo of roof, building walls, road	0.2	0.2	0.2	0.2
Surface emissivity of roof and building wall	0.90	0.97	0.97	0.97
Surface emissivity of road	0.95	0.97	0.97	0.97
Lower boundary temperature for roof, walls and road	293.00	n.a.	n.a.	293.00

Table 5
List of NOAA weather and AirBase air quality stations. Location of stations is displayed in Fig. 1.

Urban area	Network	International code	Name	Latitude	Longitude	Type
Milan	NOAA-NCDC	160660	Malpensa	45.617	8.733	–
Milan	NOAA-NCDC	160760	Orio al Serio	45.667	9.700	–
Milan	NOAA-NCDC	160800	Linate	45.433	9.283	–
L'Aquila	CETEMPS	–	–	42.367	13.984	–
Milan	AirBase	IT0524A	Cassano d'Adda	45.542	9.516	Background
Milan	AirBase	IT0706A	Limito	45.483	9.328	Background
Milan	AirBase	IT0839A	Crema – Via XI febbraio	45.367	9.705	Background
Milan	AirBase	IT1010A	Magenta	45.467	8.893	Background
Milan	AirBase	IT1418A	Montanaso	45.335	9.453	Background
Milan	AirBase	IT1463A	Osio sotto	45.621	9.102	Background
Milan	AirBase	IT1466A	Trezzo d'Adda	45.617	9.506	Background
Milan	AirBase	IT1518A	NO - Verdi	45.438	8.621	Background
Milan	AirBase	IT1648A	Cantù	45.727	9.126	Background
Milan	AirBase	IT1650A	Saronno	45.627	9.024	Background
Milan	AirBase	IT1692A	MI - Pascal	45.478	9.236	Background
Milan	AirBase	IT1734A	Valmadrera	45.841	9.349	Background
Milan	AirBase	IT1743A	Monza - Machiavelli	45.581	9.102	Background
L'Aquila	AirBase	IT1856A	Amiternum	42.364	13.382	Traffic

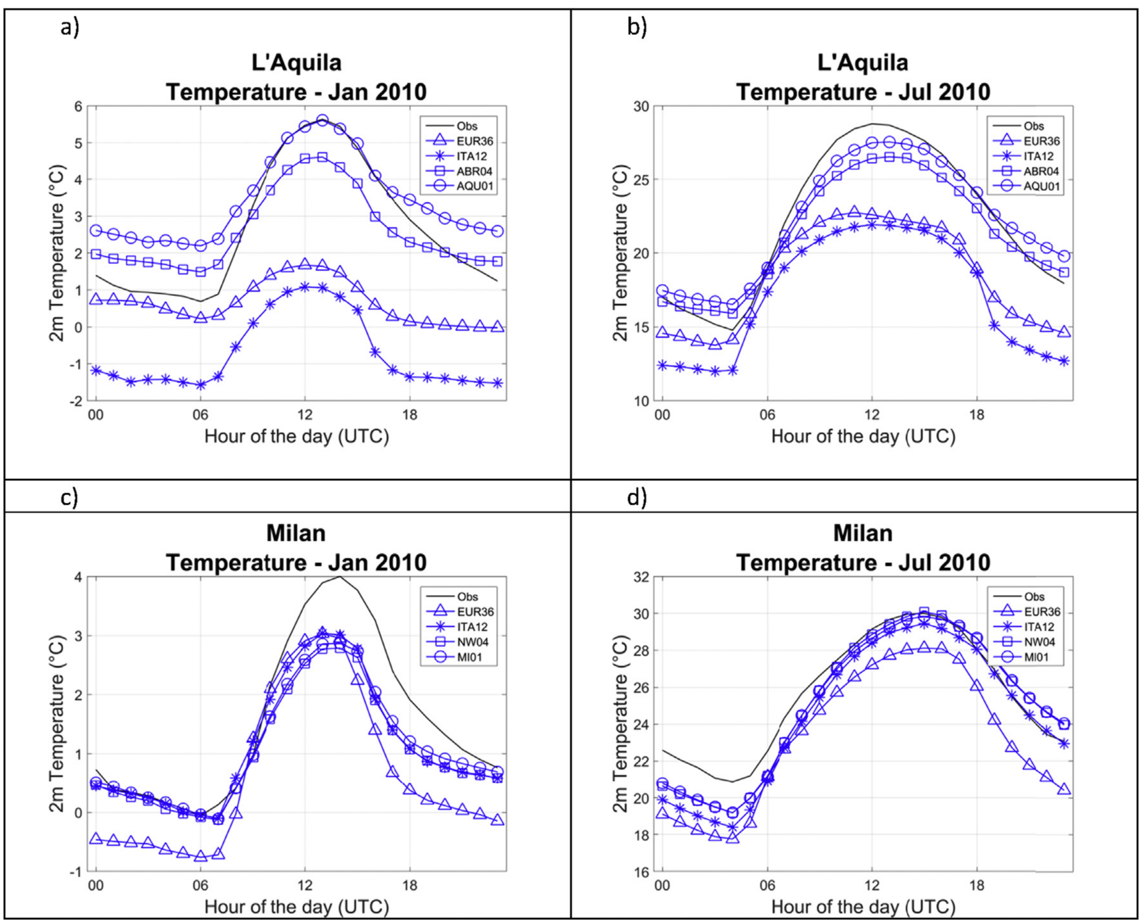

Fig. 2. Daily cycles of temperature at 2 m height (°C) average over available stations, at varying model horizontal resolution (see for the definition of domains). The BULK urban scheme is used. (a) L'Aquila in January 2010, (b) L'Aquila in July 2010, (c) Milan in January 2010, and (d) Milan in July 2010.

2. Methodology

The modeling chain used in this work is based on the Weather Research and Forecasting (WRF) model (Skamarock et al., 2008) and the Chemistry and Transport Model CHIMERE (Menut et al., 2013), with WRF outputs provided as input to CHIMERE. We evaluate the modeling system in the urban context studying its sensitivity to the horizontal spatial resolution, the resolution of anthropogenic emission inventory, and to the urban canopy modeling through six targeted numerical experiments. We consider two urban areas that share the two larger domains covering Europe and Italy, and differ for two inner domains, as illustrated in Fig. 1. For all numerical experiments the simulated period includes a winter month and a summer month of 2010, namely January and July.

Milan is the second most populated city in Italy with about 1,300,000 inhabitants and it is located south of the Alps in the Po

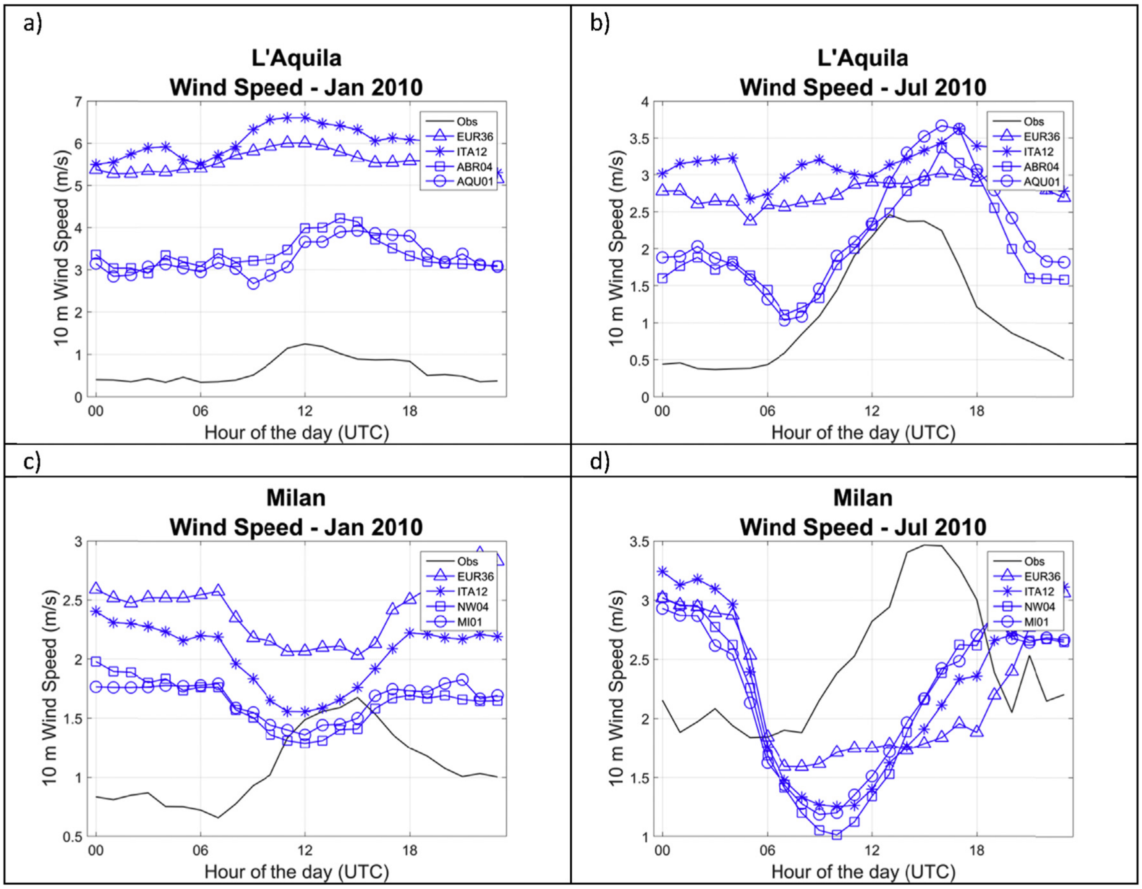

Fig. 3. Same as Fig. 2, but for wind speed at 10 m height (m/s).

Valley. L'Aquila is located in a valley at 721 m above sea level, surrounded by the highest mountains of the Appennines, in the Central Italy and it has about 70,000 inhabitants.

2.1. WRF setup

The mesoscale Weather Research and Forecasting (WRF) model is a fully compressible and non-hydrostatic model whose technical description can be found in Skamarock et al. (2008). We use WRF version 3.7.1 to perform simulations over four one-way nested domains having increasing horizontal resolution with grid ratio of 4, from 36 to 1.3 km. Geographical areas covered by domains are shown in Fig. 1, and the number of cells for each domain is listed in Table 1. All domains have 33 eta vertical levels with 11 levels below 1000 m, the lowest one at about 23 m and the top at 50 hPa. Initial and global boundary conditions are taken from the Global Forecasting System (GFS) operational analyses, provided by the National Center for Environmental Prediction (NCEP), at a spatial resolution of $1^\circ \times 1^\circ$ and a temporal resolution of 6 h. We perform simulations in 30-h blocks, starting at 18 UTC of each day, and discarding the first 6 h as model spin-up.

We use the physics options reported in Table 2: they are common to all the simulations listed in Table 3, except for the urban surface option. As for the latter, we alternatively use the zero-order urban BULK parameterization (Chen et al., 2011), the Single-layer Urban Canopy Model (UCM, Kusaka et al., 2001) and the Multi-layer Building Environment Parameterization (BEP, Martilli et al., 2002), in order of complexity. For each of UCM and BEP schemes, we carried out two experiments: one using default input values for thermal and geometric parameters, related to building materials and city morphology typical of large American cities, and the other using default values for geometric parameters and adjusting thermal input to values considered more proper for Italian cities (Pichelli et al., 2014). The value of the thermal conductivity was extracted from the table available online at the link of the architecture department of an Italian university: http://www.architettura.unina2.it/docenti/areaprivata/90/documenti/Conducibilit%C3%A0.pdf. Table 4 shows the default values and those used in the adjusted test, taken from Kusaka et al., (2001) and Kim et al., 2013. For completeness, the BULK parameterization uses the following parameters values for urban surface: roughness length of 0.8 m, surface albedo of 0.15, volumetric heat capacity of $3.0\ \mathrm{J\,m^{-3}\,K^{-1}}$, and soil thermal conductivity of $3.24\ \mathrm{W\,m^{-1}\,K^{-1}}$. Since the MODIS dataset used in this study includes 20 land use categories and does not distinguish the three types of urban texture (commercial, high residential, low residential) as expected by the UCM and BEP schemes, we employ the same value for the three types. The extension of urban areas and prevailing land use classes are shown in Fig. 1.

2.2. CHIMERE setup

CHIMERE is an Eulerian off-line chemistry and transport model whose detailed description is given in Menut et al. (2013). The model version used in this study is 2014b. Geographic areas covered by domains are similar to those of WRF, but CHIMERE is defined on lat-lon horizontal grids, thus interpolation of meteorological fields from the Lambertian WRF projection is needed. As detailed in Table 1, the horizontal grid size decreases from 0.5° of the domain covering Europe

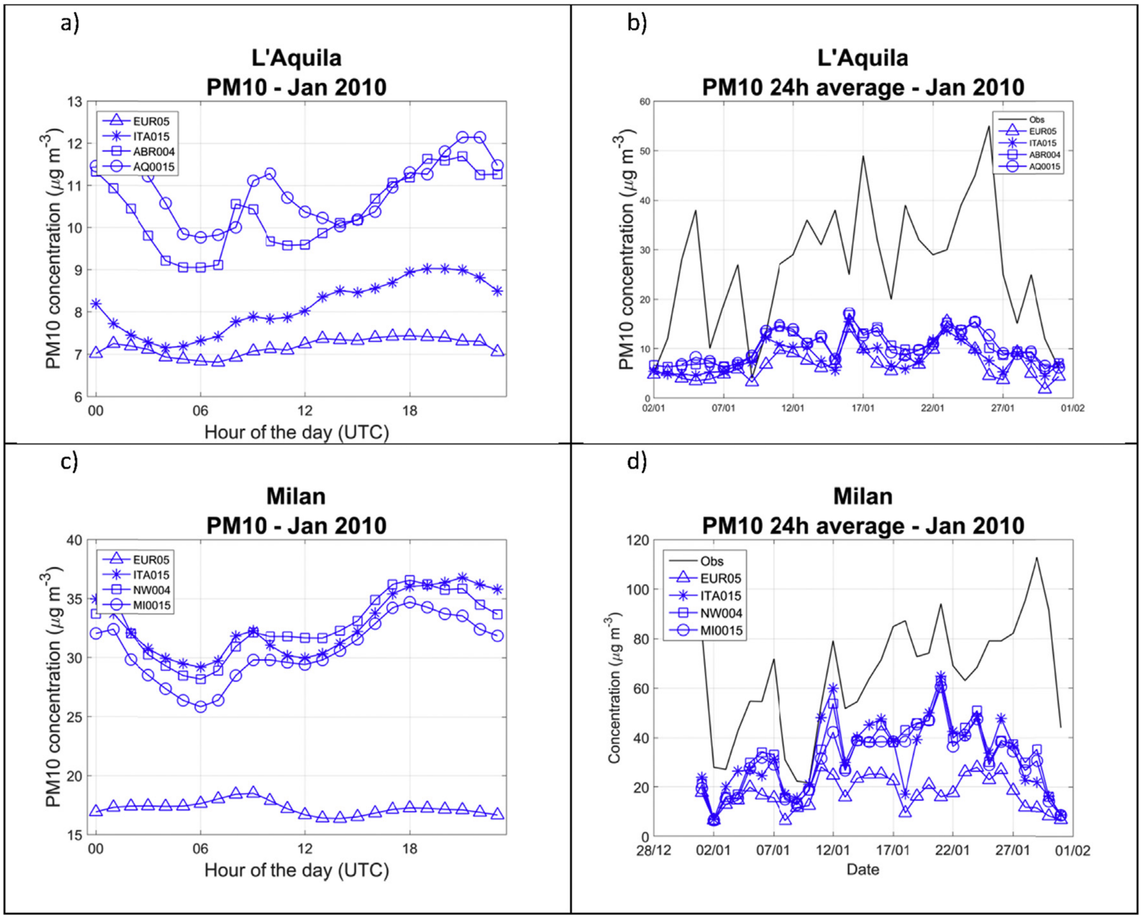

Fig. 4. Average daily cycles and monthly time series of PM10 in January 2010, at varying model horizontal resolution (see Table 4 for the definition of domains). (a) L'Aquila, daily cycle, (b) L'Aquila, monthly time series, (c) Milan, daily cycle, and (d) Milan monthly time series.

to 0.015° of the urban domains. The number of vertical sigma levels is 12 with the top pressure at 500 hPa, 7 levels below 1000 m, and the first level of about 21 m height. Vertical diffusion coefficients are re-calculated in CHIMERE based on the boundary layer height using the parameterization by Troen and Mahrt (1986) without counter-gradient term (Menut et al., 2013). Anthropogenic emissions are taken from the European Monitoring and Evaluation Programme (EMEP, http://www.emep.int), at a resolution of 0.5° × 0.5° and used on the European domain, and from the National Thematic Center for Atmosphere, Climate, Emissions (CTN-ACE, Deserti et al., 2008), at by a resolution of 5 km × 5 km and used for the inner domains.

2.3. The reallocation of anthropogenic emissions

Since the horizontal resolution of the available anthropogenic emission inventory over Italy is 5 km, we applied a downscaling technique in order to reallocate emissions for the high-resolution urban domains. The procedure consists in the subdivision of original emissions onto the fine grid of a land use database, and reallocating them prevalently in pixels classified as urban areas. Here we use the GlobCover land use database (Bicheron et al., 2008) at a resolution of about 300 m, and perform numerical tests with and without the reallocation of anthropogenic emissions using the BULK urban scheme (see Table 3).

2.4. Observations

For meteorological variables (temperature and wind speed), we use data from the National Climatic Data Center of the National Oceanic and Atmospheric Administration (NOAA-NCDC, ftp://ftp.ncdc.noaa.gov/pub/data/noaa) stations for the Milan area, and from the CETEMPS' weather station for L'Aquila (http://meteorema.aquila.infn.it/tempaq/main.html). Observed values of pollutant concentrations (ozone and PM10) are from the European AirBase network (https://www.eea.europa.eu/data-and-maps/data/airbase-the-european-air-quality-database-7). Features of weather and monitoring stations are listed in Table 5.

3. Results and discussion

We present here results of the numerical experiments described in section 2 and summarized in Table 3. This section is arranged into three subsections, focusing on the effect of (1) the horizontal resolution of model grid, (2) the spatial reallocation of anthropogenic emissions, and (3) the urban canopy modeling. We present the analysis in terms of daily cycles averaged over the stations listed in Table 5 and displayed in Fig. 1. We assume that point measurements can be compared with numerical data, appropriately interpolated at the geographic coordinates of the stations (Salamanca et al., 2011). For air quality quantities, we show results also in terms of time series of daily values, specifically the daily maximum of 8-h average for ozone and the 24-h

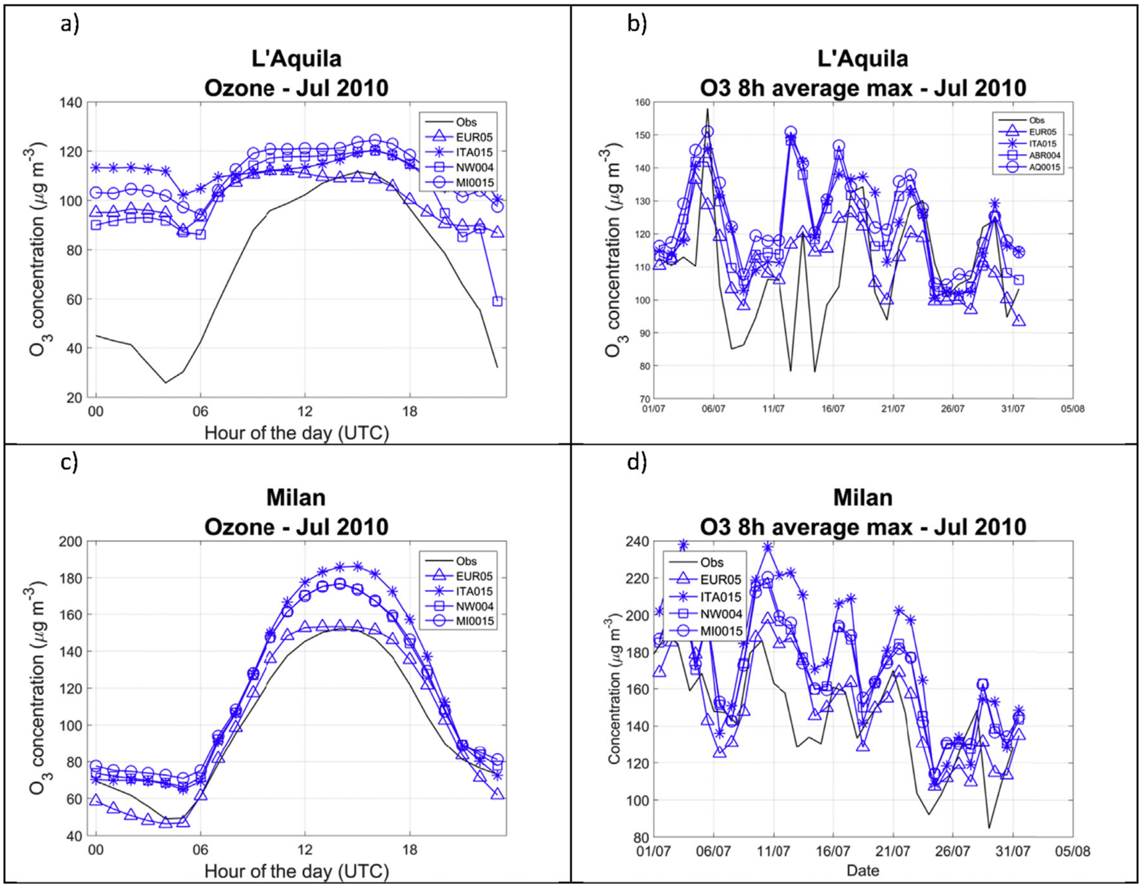

Fig. 5. Same as Fig. 4, but for daily maximum of 8-h ozone in July 2010.

average for PM10, consistently with the European Directive 2008/50/EC. Furthermore, since the exceedances of regulated limits typically take place in winter for PM10 and in summer for ozone, we show PM10 data for January and ozone data for July. Additional figures and tables with statistical indices are available for further details in the online supplement to this article.

3.1. Horizontal resolution of model grid

In this section, we give evidence of the effect of increasing horizontal grid resolution on the BULK numerical experiment.

3.1.1. Meteorology

Fig. 2 shows the average daily cycle of temperature at 2 m height (T2m) at L'Aquila and Milan for January and July 2010. For L'Aquila, we found a sharp improvement for runs at the regional and local scales (ABR04, AQU01) with respect to those at larger scales (EUR36, ITA12). The worst performance is on ITA12 for both January (underestimation by ~3 °C at 00:00 UTC and ~5 °C at 12:00 UTC) and July (underestimation by ~4 °C at 00:00 UTC and ~7 °C at 12:00 UTC). The best performance is on the highest resolution domain AQU01, with the exception of nighttime temperature, which is better reproduced on ABR04. In Milan, we found a marginal improvement among higher resolution simulations, which display a noticeable negative bias of ~1 °C during the day in winter and of ~2 °C during the night in summer. The low resolution simulation (EUR36) has an almost constant underestimation throughout the day, of ~1 °C and ~3 °C in winter and summer, respectively.

In Fig. 3 we show results for wind speed at 10 m height (U10m). In L'Aquila, all test cases overestimate the velocity throughout the day, but the bias is reduced from ~5 m/s at moderate resolution to ~2 m/s at high resolution in winter. In summer, higher resolution simulations reproduce much better the daily cycle, specifically the transition from low wind speed at night to higher wind speed during the days, typical of a mountain-breeze dynamic (Curci et al., 2012). In Milan, higher resolution contributes to alleviate the model high bias in winter, but in summer has only a small effect. The daily cycle appears to be inverted with respect to the observations, with higher wind speeds at night with respect to the day. The shape of the modeled daily cycle resembles that expected at levels of 100–200 m above the ground (Wallace and Hobbs, 2006), thus calling into question a possible excessive vertical transport of momentum from upper levels toward the surface.

3.1.2. Air quality

The model tends to underestimate hourly and daily concentrations of PM10 with a clear benefit associated to the increase in resolution at both L'Aquila and Milan (Fig. 4). While for L'Aquila there is a progressive improvement from the large scale to the local scale, in the case of Milan performances at scales other than the coarse one are equivalent. There, PM10 hourly concentrations simulated at the continental scale are lower and nearly constant throughout the day. We note that the day-to-day variability of PM10 daily concentrations is better reproduced in Milan ($r \sim 0.5$) than in L'Aquila ($r \sim 0.4$).

For ozone both hourly and daily observed data are compared with numerical results (Fig. 5). In contrast to PM10, the model overestimates concentrations and there is no benefit from the increase in spatial

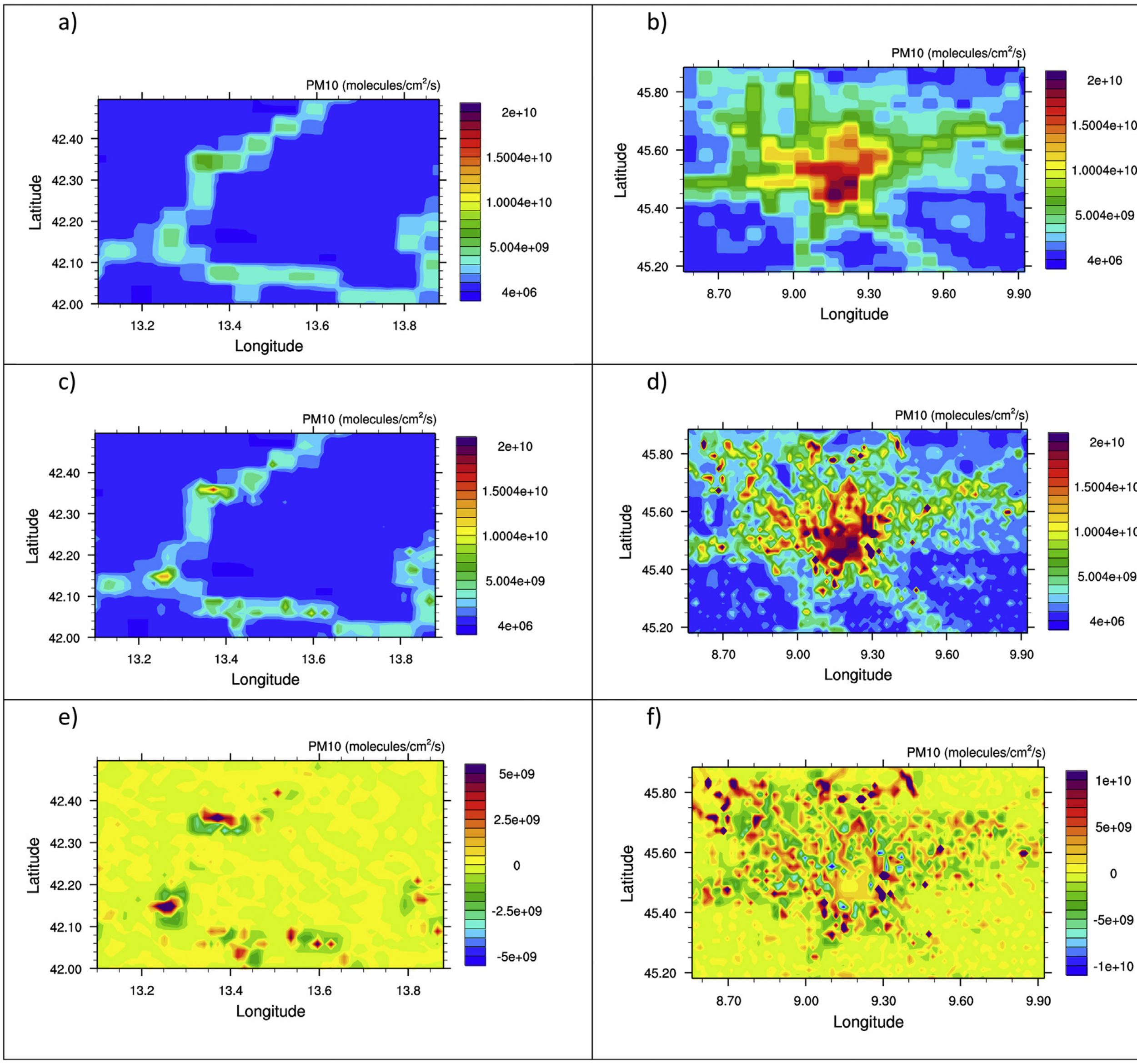

Fig. 6. PM10 surface emission flux at 12:00 UTC on a midweek day of January 2010 over the urban area of L'Aquila (left) and Milan (right). From top to bottom: (a–b) original emissions from the national inventory CTN-ACE at 5 km resolution; (c–d) emissions after spatial reallocation using the GlobCover land use dataset; (e–f) difference between the two cases.

resolution at both locations. The case with the coarser resolution has a nearly unbiased performance, especially in the central hours of the day. In L'Aquila, the model does not reproduce the observed excursion of ozone between night and day (the difference of observed hourly ozone is equal to about ~80 μg/m^3, while the simulated is ~30 μg/m^3).

Also the day-to-day variability is generally better reproduced at coarser scale, particularly in L'Aquila (r ~ 0.47 on EUR05 vs. r ~0.34 on ITA015). In Milan results at regional and local scales (NW004, MI0015) are virtually superimposed and results at national scale (ITA015) has the worst performance. This may point out a degradation of the quality of the anthropogenic emission inventory in that area, when passing from EMEP to CTN-ACE.

3.2. Horizontal resolution of anthropogenic emissions

The procedure of spatial reallocation of anthropogenic emissions is described in Section 2: in Fig. 6 we illustrate the product of this technique, comparing maps of PM10 emission fluxes without and with spatial reallocation, in L'Aquila and Milan. The spatial reallocation, driven by the underlying GlobCover land use database, adds much finer details to the maps. In L'Aquila, there is a clear shift of emission patterns from the suburban and rural areas toward the respective city centers. In Milan, the emissions are the same in the urban core, but becomes more patchy as one moves to the surroundings, reflecting the inhomogeneity of the alternating artificial and natural/agricultural surfaces.

Fig. 7 shows monthly trends of daily values simulated using the original and the spatially reallocated anthropogenic emissions inventory.

The reallocation of emissions causes a small improvement of simulated values, but this is largely insufficient to compensate the bias with respect to observations for both PM10 and ozone at both sites. The

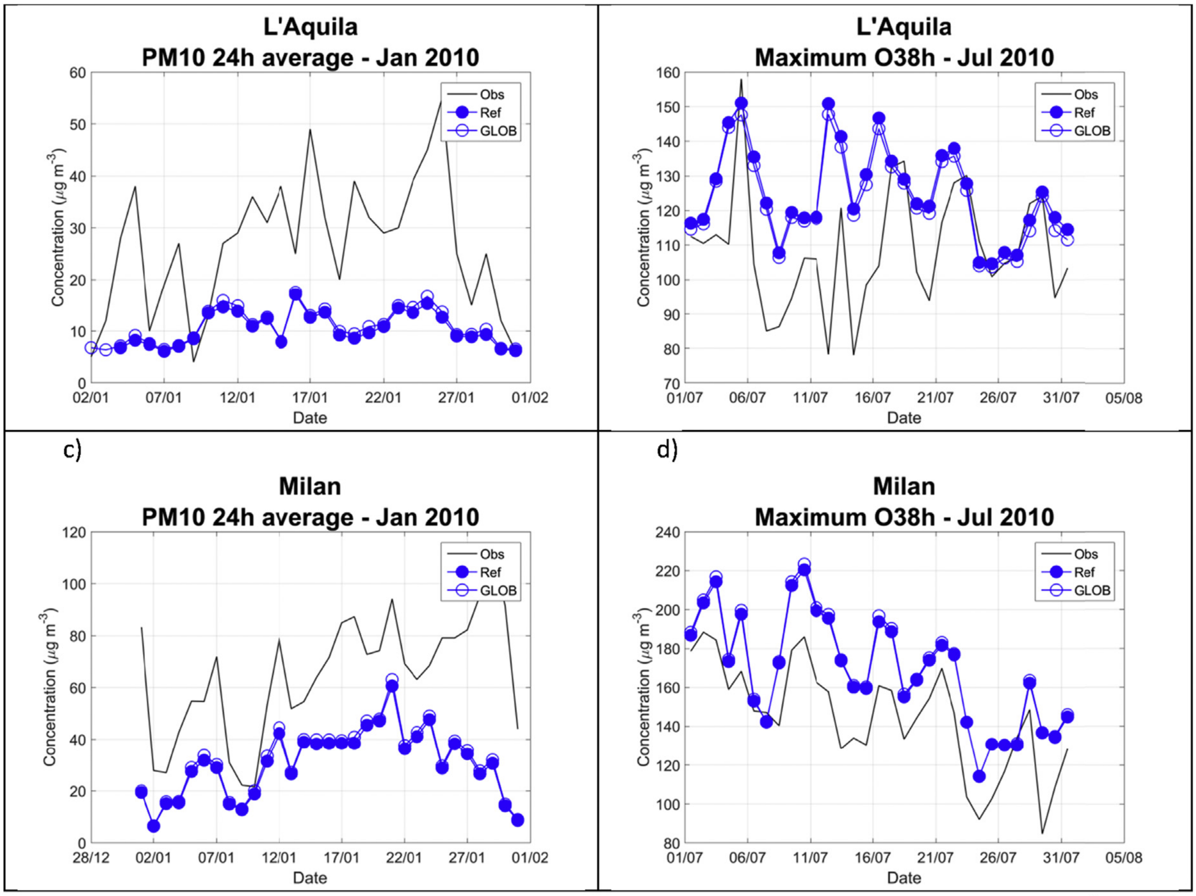

Fig. 7. Monthly time series of daily mean PM10 (January 2010) and daily maximum 8-h ozone (July 2010), without and with reallocation of anthropogenic emissions. Results are averaged over the available monitoring stations in L'Aquila (top) and Milan (bottom).

reallocation has negligible influence on day-to-day and hour-to-hour (not shown) variability.

3.3. Urban canopy models

In this section, we illustrate the effect of different urban canopy models, while maintaining the same Planetary Boundary Layer (PBL) scheme and other physical parameterizations. Here, we employ the Boulac-Lacarrere PBL scheme, even if the BULK and UCM schemes are not expected to work in optimal conditions (Salamanca et al., 2011). Previous studies generally changed simultaneously both the PBL and the urban scheme (Salamanca et al., 2011; Pichelli et al., 2014; De la Paz et al., 2016), making difficult the isolation of the effect of changing UCM only.

In addition to the figures of time series of T2m and U10m shown in this section, daily cycles of PBL height (PBLH) and maps of differences between the reference case and the test cases are included in the supplementary material. Furthermore, the supplementary material includes average daily cycles of PM10 in January 2010 and ozone in July 2010 for the different types of monitoring stations (rural, suburban and urban, as classified by the managing Regional Agencies, see Table 1 in the supplementary material).

3.3.1. Meteorology

In Fig. 8, we show differences among simulations for T2m in January and July 2010, in L'Aquila and Milan. We note larger differences among schemes during the night than during the day, for all sites and periods. In July, the differences during daytime are negligible.

In January, the reference case, that uses the simple BULK UCM scheme, displays a positive bias ($\sim 1\ ^\circ C$) in L'Aquila during night, and a negative bias ($\sim 1\ ^\circ C$) in Milan during the day. The UCMt canopy model performs better than any other at both sites, alleviating the reference model bias. UCM has a large negative bias at night ($\sim 3\ ^\circ C$), while BEP and BEPt overestimate T2m throughout the day (by $\sim$ 1–1.5 °C at L'Aquila and by $\sim$ 1.5–2 °C at Milan). In July, the reference model underestimates day temperature by $\sim 2\ ^\circ C$ only in L'Aquila, and overestimates (underestimates) by $\sim 2\ ^\circ C$ nighttime temperature in L'Aquila (Milan). In L'Aquila, none of the alternative urban schemes improves over the reference, while in Milan BEP and BEPt schemes remarkably reduce the bias.

We conclude that there is no single combination of urban canopy model that may help reducing the reference model bias in all situations. According to Liao et al. (2014), more realistic urban morphology and parameters are needed to improve the model performance. With the combination of schemes used here, we found that the increase in the value of thermal parameters in UCMt and BEPt compared to UCM and BEP (Table 4) yields a general increase in temperature overnight, but this is not necessarily associated to an improvement in model performance with respect to observations.

In Fig. 9 we show the comparison for U10m. In L'Aquila, the model qualitatively reproduces the daily cycle, with lower speed at night than daytime, but has substantial positive bias, especially in winter (2–3 m/s). The BEP urban scheme is the one performing better, and it alleviates model bias, especially in summer. This is consistent with results by De la Paz et al. (2016). The UCM scheme degrades the simulation, because it predicts wind speeds always larger than the reference. We also found a small difference when introducing modified physical characteristics in the urban schemes (UCMt, BEPt). In Milan, the introduction of the BEP scheme, also in the modified BEPt version, corrects the inversion, with respect to the observations, of the daily cycle manifested by the

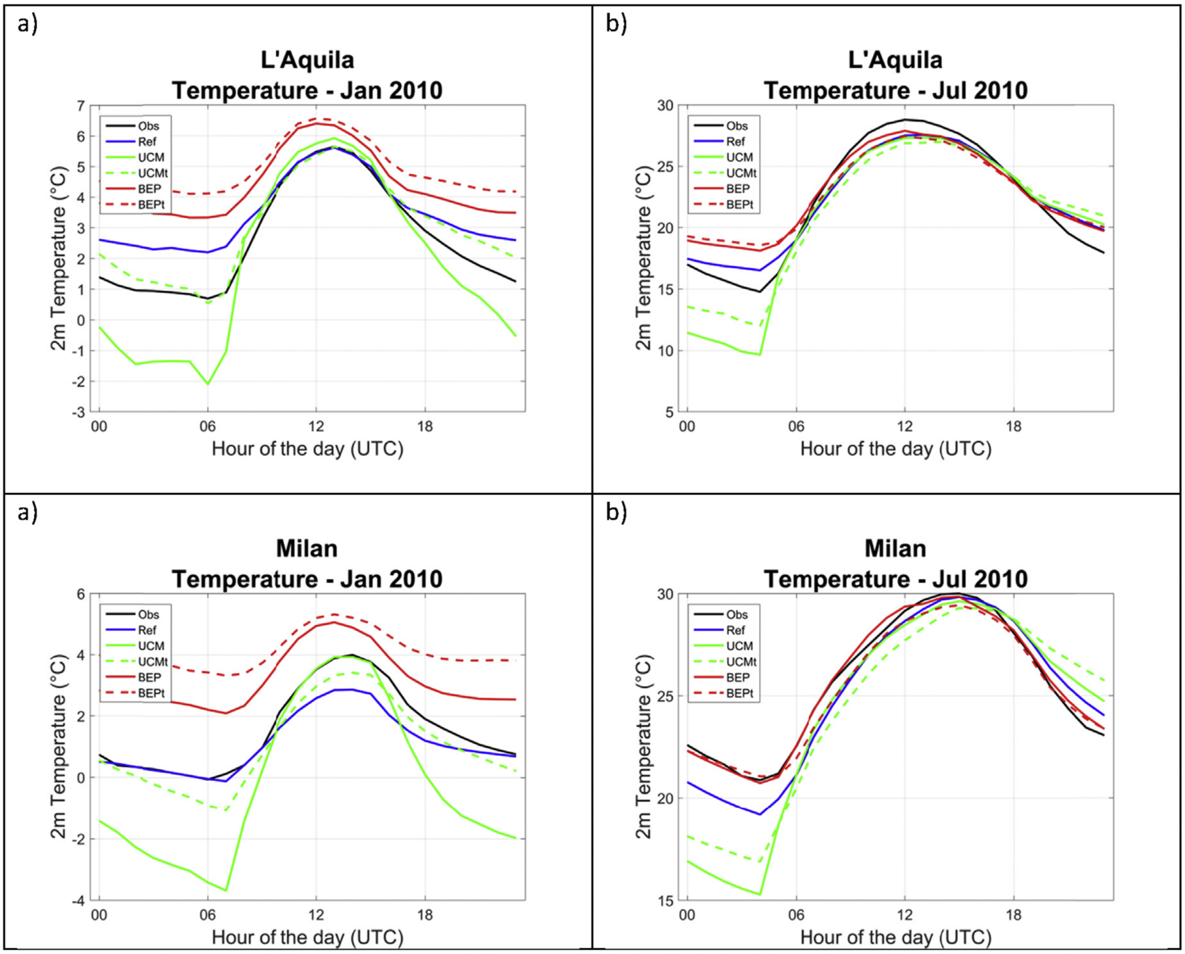

Fig. 8. Same as Fig. 2, but for test using different urban canopy models on the highest resolution domain (see Tables 3 and 4).

reference case. As for L'Aquila, UCM cases deteriorate model performances with respect to the reference case. A basic difference between UCM and BEP schemes is that the latter have an improved representation of surface drag by artificial surfaces, which may be the reason of the decreased momentum in the lower layers with respect to other configurations.

3.3.2. Air quality

In Fig. 10 we illustrate results from sensitivity tests on the urban canopy model for PM10. The daily cycle of PM10 has a similar behavior at both sites, characterized by a progressive build-up during daytime, with peaks in the morning and evening rush hours. The rise of the PBL justifies the reduction of PM10 concentrations in central hours. As observed by Shindler et al. (2013), during daytime, anabatic winds together with the urban heat island circulation enhance pollutants dispersion, while at night katabatic winds coming from the mountains clean the air.

We note that the effect of using different urban schemes is small compared to the large negative bias of the reference simulation with respect to observations. A marginal improvement (higher PM10 values with respect to the reference) is found adopting UCM schemes at both sites, and with the BEP scheme in L'Aquila. This happens despite the fact that UCM schemes predict larger wind speeds than other schemes, circumstance that should reduce PM10 levels through decreased removal. However, together with the wind speed, also the vertical extent of the mixing layer changes, and this may have a counteracting effect on pollutant concentrations. The crucial role of vertical mixing for PM10 is confirmed by the fact that in Milan the BEP cases have the slowest wind speeds, the highest PBL heights (shown in supplemental material), and the lowest levels of PM10. The potential benefit from improved simulation of the wind speed is thus offset by increased vertical dilution.

In Fig. 11 we show results for ozone concentrations. The urban canopy models have a generally smaller influence on the simulated concentrations during daytime than during nighttime. The scheme that tends to alleviate the positive model bias is BEP, which is the one having the best simulation of the wind speed, indicating that part of the model bias may be due to excessive removal of ozone and nitrogen oxides at night in the reference case.

In L'Aquila, we note that the daily cycle is characterized by a large difference between day and night that the model does not reproduce, in particular the nighttime decrease. This may be due to an insufficient titration of ozone during night by reaction with nitrogen oxide, as commonly found in urban areas.

In Milan, the differences among the schemes are larger than those found in L'Aquila, denoting a more important role played by the horizontal and vertical transport of locally produced pollutants. This is also confirmed by an analysis differentiated by station type (see supplementary material): at the rural station there is almost no difference among test cases, while at suburban and urban stations there is a slight improvement in the performance using the BEP scheme.

4. Conclusions

We performed numerical experiments using the modeling system WRF-CHIMERE over two Italian urban areas, the metropolitan area of

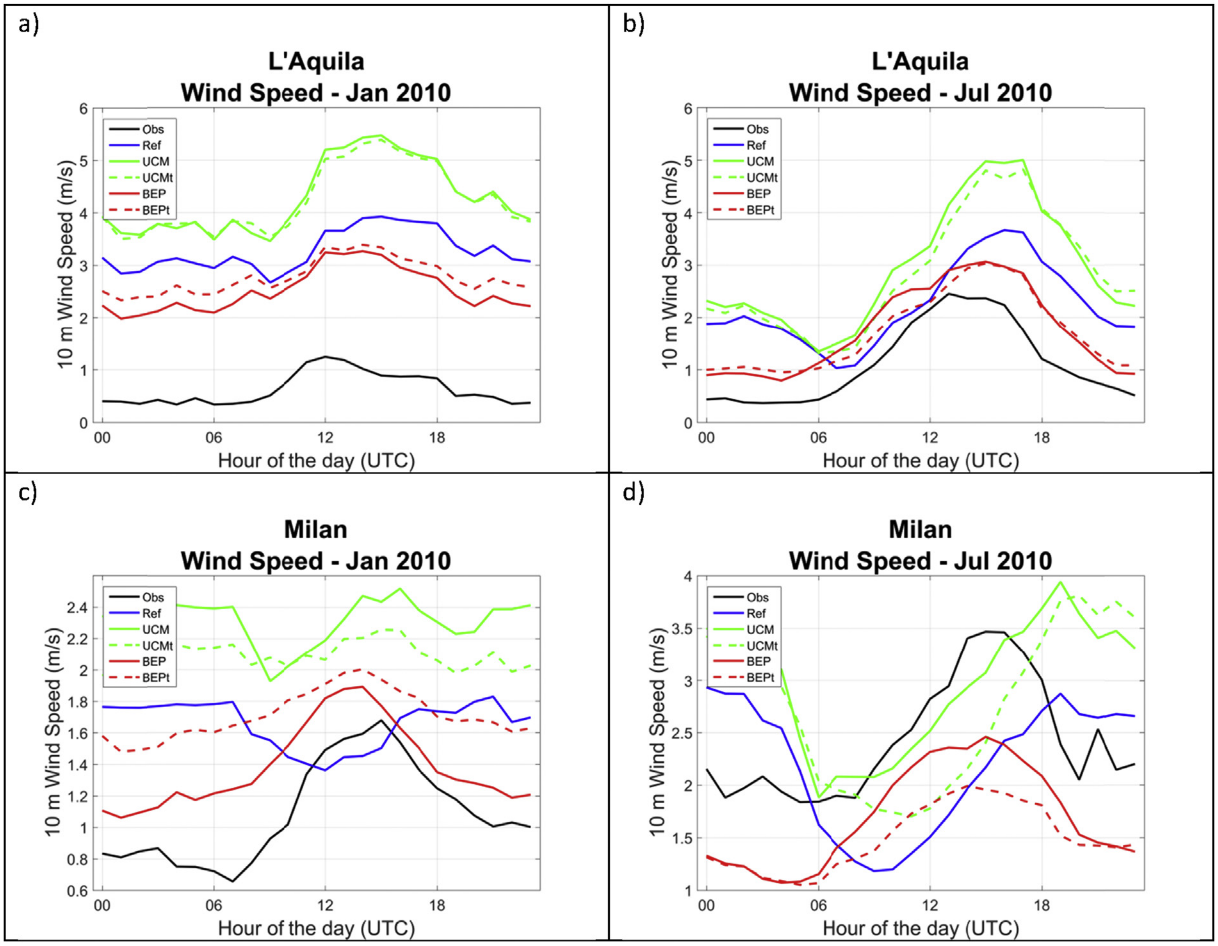

Fig. 9. Same as Fig. 8, but for wind speed at 10 m height.

Milan and the small city of L'Aquila. Sensitivity tests were designed to study the effect of (1) the horizontal model grid size, (2) the horizontal resolution of the anthropogenic emissions inventory, and (3) the urban canopy models. The horizontal grid dimension of the WRF model decreases from 36 km for domain over Europe to 1.333 km for domain over urban areas, while the horizontal grid size of CHIMERE decreases from 0.5° to 0.015°. Nesting is applied in one-way direction for both WRF and CHIMERE, thus the simulations on the inner domains are independent of the parent domain, but for the boundary conditions. The reference case uses an urban BULK parameterization and the national inventory CTN-ACE (5 km resolution). Test cases include simulations with two urban canopy models available in WRF, and we used alternatively default and "tuned" values of the thermal urban parameters. In a simulation, we downscaled the anthropogenic emission inventory through the spatial redistribution of emissions according to the land use.

We compared numerical results with available ground-based observations of the 2 m temperature (T2m), 10 m wind speed (U10m), ozone and PM10. Most of the comparison is illustrated in terms of daily cycles average over all stations and over the two months selected for the simulations, namely January and July 2010.

The coarse resolution simulation at the European scale present significant bias with respect to the observations both in L'Aquila e Milan urban areas. T2m is underestimated, in particular during the day in L'Aquila by ~5 °C and during night in Milan by ~3 °C. U10m is overestimated at both locations, in particular in winter by 3–4 m/s, and the observed diurnal cycle typical of the mountain-valley breeze system (higher wind speeds during the day with respect to the night) is reversed in the simulation. PM10 is underestimated by a factor of 2–3 at both locations, while ozone is generally well reproduced, with the exception of nighttime values in L'Aquila, where the simulated ozone is a factor of 3–4 higher than observations. In evaluating the sensitivity tests, we paid particular attention to the eventual correction of these model biases.

Increased horizontal resolution determines an improvement in model skill for all considered quantities, but for ozone. Much of the benefit in using a higher resolution is obtained already at a moderate resolution of 12 or 4 km (2nd and 3rd nested domains): we generally found little improvement, if any, with further increase of the resolution down to ~1 km (on the 4th nested domains). For example, in L'Aquila the wind diurnal cycle is corrected at 4 km resolution, while in Milan the cycle is not corrected even at 1 km resolution. PM10 simulation is improved at 4 km resolution, but there is no progress when going to 1 km. For ozone, the simulation generally deteriorates, becoming overestimated, when using resolutions higher than the coarse one.

The spatial reallocation of anthropogenic emissions, originally at available at 5 km resolution over Italy and using the urban land use class as proxy variable for downscaling, only yields a small improvement on the simulated levels of pollutants, but such improvement is negligible with respect to the model bias.

Concerning the use of different urban canopy models, we found that the BEP scheme introduces the clearest benefit on the simulation of the wind speed, because it corrects the diurnal cycle in Milan and further improves the simulation in L'Aquila. For the temperature, however, the UCM and BULK schemes perform better than BEP in L'Aquila. The improved simulation of the wind speed is not transferred directly to that of pollutants, especially PM10. The expectation from a more realistic (and lower) cycle of the wind speed was to have higher values of PM10, i.e. a

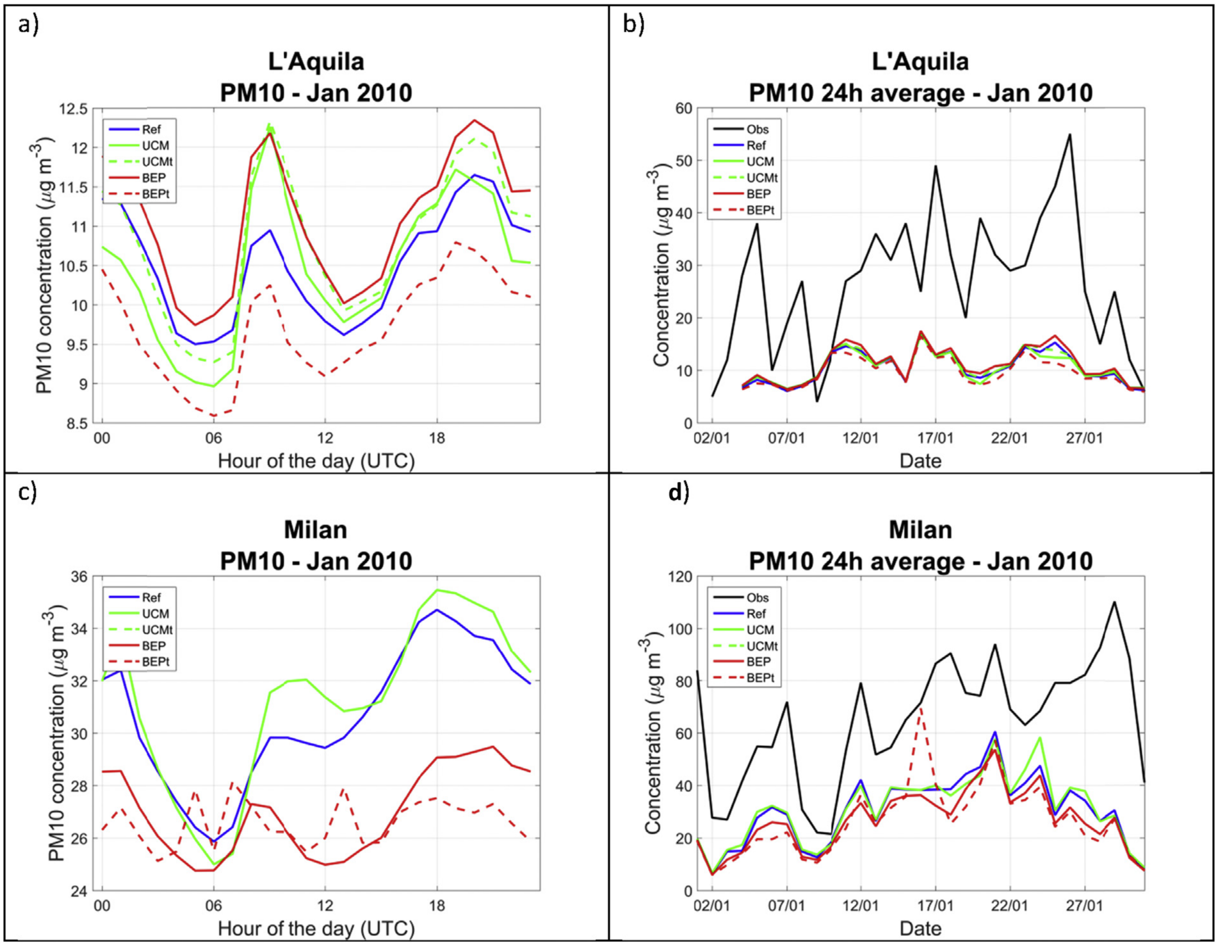

Fig. 10. Same as Fig. 4, but for test using different urban canopy models on the highest resolution domain.

change in the right sense for correcting model bias, due to decreased removal. However, we found that PM10 is actually lowered when using the BEP scheme, because it induces also a sharp increase in the mixing layer height, which favors an increased dilution of pollutants that more than offset the benefit from the better simulation of the wind. For ozone, urban canopy models influence nighttime concentration more than daytime concentrations. BEP scheme, which simulates lower wind speed values, has better skill in simulating ozone at night, and this suggests that the reference case has an excessive removal of ozone and nitrogen oxides. The introduction of "tuned" values for the thermal parameters in the canopy models makes generally a second-order change to the simulations.

In conclusion, the sensitivity tests on the WRF-CHIMERE air quality modeling system illustrated here indicate a clear advantage in increasing the resolution of the model up to ~4 km horizontal resolution, but a further computational effort to run the model at ~1 km resolution does not seem to be justified. This is consistent with conclusions by Kuik et al. (2013). The introduction of more detailed treatment of the urban canopy and anthropogenic emissions on the highest resolution domains at ~1 km suggests the potential for further improvement, but this will require a fine tuning on the area of application. There is no unique "best" choice, valid for all areas, of the urban canopy model, and the anthropogenic emissions should probably be refined through new bottom-up inventories at the same resolution of the model, rather than downscaling them from coarser resolution database (which was at 5 km in our case).

Future development of this work will be primarily focused on a better characterization of the modeled three dimensional structure of meteorological and micrometeorological dynamics in the planetary boundary layer, carried out in places and periods where comprehensive observational campaigns are available.

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Conflicts of interest

The authors declare no conflict of interest.

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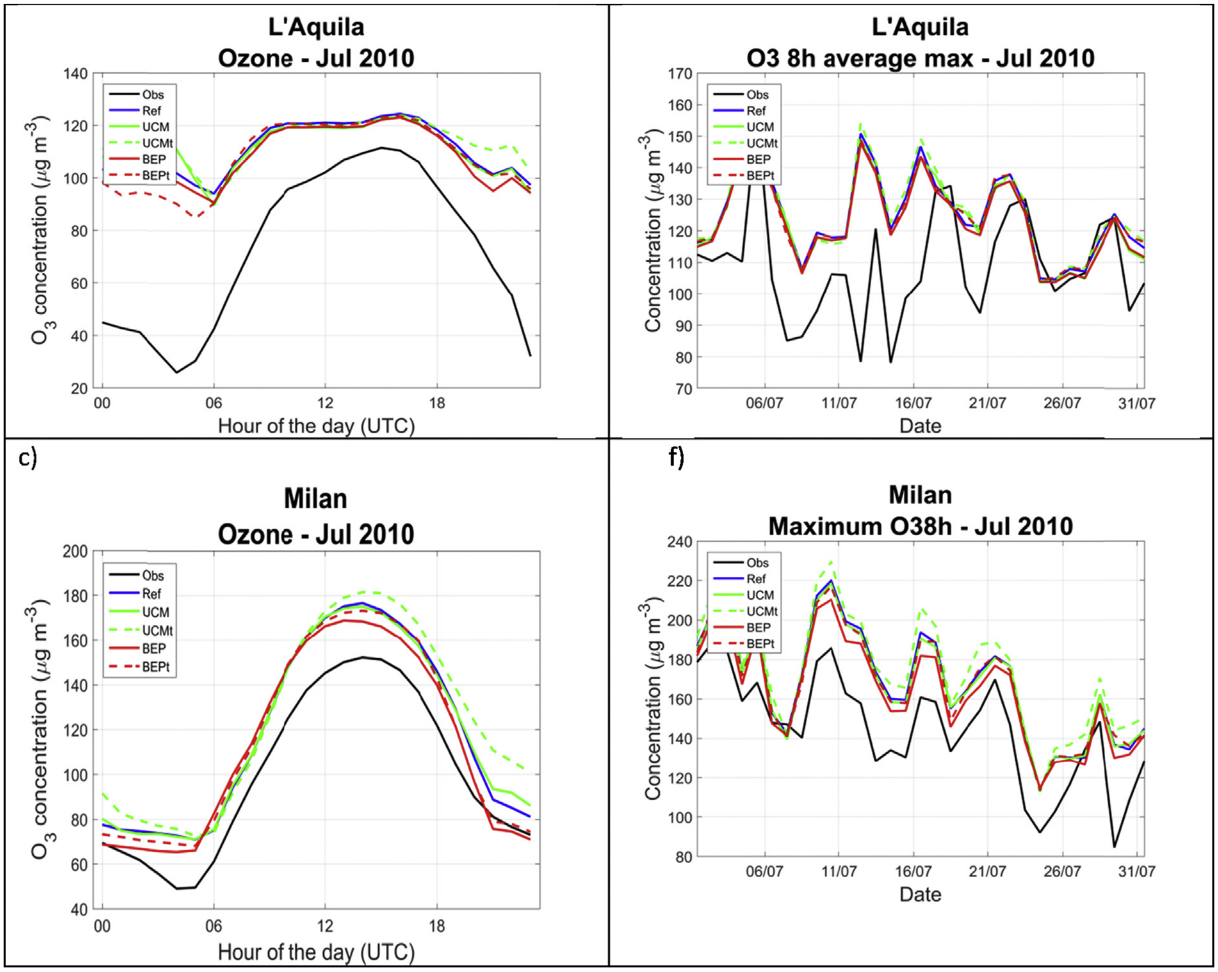

Fig. 11. Same as Fig. 5, but for test using different urban canopy models on the highest resolution domain.

Appendix A. Supplementary data

Supplementary data related to this article can be found at http://dx.doi.org/10.1016/j.atmosenv.2018.05.048.

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