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The challenges of air quality modelling when crossing multiple spatial scales

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Abstract
Multiscale air quality assessment implies understanding the interaction among atmospheric processes and scales. In this per-spective, the use of air quality models has a fundamental role and the way they address these interactions is very important for the quality of results. However, in multiscale air quality modelling, the relationship between models, simulation domains and resolutions remains a challenging research issue. This paper presents a state-of-the-art review on multiscale air quality modelling applications from the regional to the street level, identifying which models are used, the methodological principles and the required input datasets. Based on the findings, an analysis of the current limitations associated with the integration of different models and multiple spatial scales in a single modelling system is presented and discussed. Lastly, taking as support the reviewed contents, a set of guidelines for strengthening the synergy among scales and harmonizing different types of models within a system is proposed. Unsuitable or non-existent urban canopy parametrizations (UCP), limited grid resolutions, discarded micro-scale impacts on upper domains, inadequate input data and simplified chemistry are some important aspects contributing to large uncertainties when analyzing multiscale air quality results. To overcome these shortcomings in current multiscale modelling systems, more research aimed at improving the modelling performance is required, focusing on (i) UCP coupled to mesoscale models, (ii) developing modelling systems with two-way nesting capability to boost feedbacks among domains and (iii) pro-moting the use, improvement and development of multiscale online modelling systems, in order to have a comprehensive multiscale understanding of all atmospheric processes that govern the transport, dispersion, transformation and deposition of air pollutants.

Keywords Urban areas · Multiscale air quality modelling systems · Online models · Urban canopy parametrizations · Nesting approaches

Introduction

To date, ambient air pollution is responsible for huge damages, sometimes irreversible, on the environment and human health. According to the latest World Health Organization report, about three million deaths per year around the world are related to outdoor air pollution problems (WHO 2016). The exponential population growth throughout the last decades and consequent non-sustainable intensification of the human activity have been contributing to these records (Likhvar et al. 2015). From the point of view of the main pollution hotspots, particular attention should

be attributed to urban areas, because more than half of the world's population lives there, and normally a dense network of emission sources is present, namely transports, industry and households (Miranda et al. 2015). However, the causes of air pollution must be analyzed beyond the urban/local scales, since air pollutants are often transported across continents and ocean basins (Ramanathan and Feng 2009; APPRAISAL 2013; Thunis et al. 2016). Thereby, the use of modelling tools for assessing atmo-spheric concentrations in a wide spatio-temporal spectrum is a current practice to analyze the relative importance of the main emitting sources. These assessments involve the application of different air quality models depending on the research objectives, dimension of study domains and intended 3D resolutions (Srivastava and Rao 2011). For this purpose, mesoscale and mi-croscale models have been developed and applied, although in most cases following separated approaches.

Within the regional scale, Eulerian chemical transport models (CTM) are the most used by the scientific community

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for air quality assessment and management. Their use goes beyond the mesoscale, since these modelling tools are often applied for downscaling over lower spatial scales (urban or even local) (Kukkonen et al. 2012; Miranda et al. 2015; Thunis et al. 2016; Relvas and Miranda 2018). These advances are supported by the increasing computational processing power and the inclusion of different urban canopy parametrization (UCP) schemes. In this scope, Grimmond et al. (2010, 2011) provide an overview about urban surface energy balance models. UCP is included in some mesoscale atmospheric models (e.g. Weather Research and Forecasting model and Environment-High Resolution Limited Area Model), with the primary goal of representing the subgrid effects of urban surfaces by means of average input parameters (e.g. urban fraction, building height, albedo and roughness) on air flows and air pollution processes taking place in the urban canopy (i.e. atmospheric layer between the surface and the highest building height). In other words, it is aimed at incorporating average characteristics of the urban structure, like road network, building geometry and vegetation interfering with the energy balance components and accumulation/dissipation patterns of air flows (Tang and Wang 2007). However, the UCP's numerical and empirical methods triggered to model the urban/local air quality are simple approximations to describe fluid's turbulent flows, heat transfer mechanisms and associated phenomena occurring in urban environments, since these are mostly based on the assumptions of horizontal homogeneities (Baklanov and Nuterman 2009; Chen et al. 2011; Kim et al. 2015). These physical processes and the amount of air pollutants emitted from individual sources, as well as the involved chemical reactions, can be influenced by local weather patterns, including air temperature, precipitation, clouds, atmospheric water vapour and wind regimes (velocity and direction). In turn, the chemical composition of the atmosphere may have a feedback effect on the local weather, but such effect has usually been discarded in atmospheric modelling. To reverse this common practice of offline application of models (i.e. meteorology is only provided to the CTM as an input), the modelling community has been working on the development of online modelling tools that allow a full integration and parallel computing of both meteorology and chemistry components, sharing the same simulation grids (horizontal and vertical levels), physical parametrizations, transport schemes and vertical mixing (Grell et al. 2005). In addition to the Eulerian approaches, Lagrangian trajectory models are also quite used for simulating regional/urban air quality. These models are computationally simpler and allow an easy determination of transboundary flows. Moreover, they could be especially suitable for assessing the dispersion from individual emission sources, and their application over urban areas could be grounded in the longer reaction time scale of many chemical species than the travel time across the study area (Stein et al. 2007; Kukkonen et al. 2012).

From the local-scale point of view, if simplified chemical transformation processes are an option and decreasing the computational requirements, an objective, empirical or Gaussian models able to estimate the air pollutant dispersion around the local sources are normally used (APPRAISAL 2013). These approaches have progressively gained a prominent role in the local and street level modelling, or at least in connection with specific microscale tools, as the obstacle-resolved models and/or the computational fluid dynamics (CFD) models (Thunis et al. 2016). The use of CFD arises as a powerful modelling technique diffused in various research fields (e.g. industry and environment), which has the capability to deal with complex features and accurately evaluate their effects (Vardoulakis et al. 2003). CFD are numerical models extensively tested over simplified geometries (Borrego et al. 2003; Schlünzen et al. 2011; APPRAISAL 2013) that solve the Navier-Stokes equations over small domains (few hundreds of metres) at very high resolutions (metres or less), and can be divided into two main types: Reynolds Averaged Navier-Stokes (RANS) and large eddy simulations (LES). RANS approaches are less computationally time demanding and are only able to estimate steady-state flows (i.e. very simple flows), simulating the wind disturbances by means of averages in time. In turn, LES turbulence models are able to simulate unsteady flows and to accurately reproduce the flow recirculation inside the atmospheric boundary layer, parametrizing their effects at the subgrid level, such as changes on the thermodynamic and mechanical properties of the surfaces. Other LES advantages are related to the capabilities to simulate the transient turbulent structure and the intermittency through vortex shedding (McDonough 2007; Baklanov et al. 2009; Schlünzen et al. 2011; Srivastava and Rao 2011). Local-scale air quality (AQ) modelling using CFD requires urban features and atmospheric emissions defined at much higher resolutions (e.g. street-to-building scales) than those in mesoscale applications, allowing reproducing in a more realistic way the air flows, involved processes and resulting ambient concentrations (Kim et al. 2012). Furthermore, street canyon simulation experiments have also been used for computing UCP which take into account building effects on the local weather (e.g. wind speed, air temperature and turbulence), with the purpose of providing spatially averaged characteristics for the mesoscale models (Brown 2000; Masson 2006; Santiago and Martilli 2010). Besides the local features, it is also crucial to take into account the influence of larger scale processes, since the dispersion and atmospheric chemistry contribute to variations in polluted air arriving to a region from other regions and/or countries (APPRAISAL 2013). However, the background and time-dependent boundary chemical conditions provided from mesoscale modelling, in particular to study the behaviour of a CFD under complex terrain, are often greatly simplified mostly due to the nature of mesoscale-coupled UCP schemes

(Mensink et al. 2003; Baklanov and Nuterman 2009; Beevers et al. 2012; Kwak et al. 2015).

Despite the methodological advances in air quality modelling to promote the link between the scales, the subject is still a challenging research issue that needs more work and answers to decrease the uncertainties when analyzing urban-to-local modelling results.

Based on this general framework, the objective of this paper is twofold. Firstly, a state-of-the-art review on available modelling approaches for air quality assessment from regional to local scales is carried out, conceptually analyzing the basic principles and methodologies that are behind these multiscale approaches. The second part is aimed at identifying current limitations associated with the integration of different models and multiple spatial scales in a single air quality modelling system and discussing them in order to provide some recommendations for improving the modelling performance.

The paper is organized as follows. In "Overview of multiscale air quality modelling applications", several research works with multiscale air quality modelling applications are presented and analyzed. Current methodological limitations associated with these estimates are discussed in "Current limitations". "Guidelines for strengthening the synergy among scales" provides a set of guidelines for strengthening the synergy among scales. Lastly, some concluding remarks about this review study are presented.

Overview of multiscale air quality modelling applications

Multiscale modelling systems for air quality assessment have often been applied using nesting approaches aimed at simulating urban areas. Based on a literature review addressing multiscale features and assumptions, a summary of the reviewed applications is presented in Table 1 including information about the model type, scales of application, domains, resolutions and other configurations. This review focuses on manuscripts from 2000 to 2019 available from the Web of Science, JSTOR and Scopus databases, given preference to the most cited ones. The keywords/terms used for the search were "air quality", "multiscale modelling" and "nesting". The analysis of Table 1 is oriented towards urban/local areas, where the main air pollution problems are found.

The large majority of the reviewed multiscale modelling applications only consider atmospheric feedbacks from larger simulation domains to the inner ones (i.e. one-way nesting), mainly when different types of air quality models are used. It means, therefore, that the influence of microscale processes on the regional/urban air quality is usually neglected. Some coarser resolution models have been adapted to include UCP, like microscale-averaged characteristics, but these parametrizations do not realistically reproduce the direct effect

of the obstacles, only feasible using microscale models (Martilli 2007; Baklanov and Nuterman 2009; Schlünzen et al. 2011; Hood et al. 2018; Benavides et al. 2019). Moreover, once the air quality models that integrate the respective modelling systems were run independently, the input data and physical and chemical processes underlying each model are treated separately taking into account their application scales and study domains.

Looking at the regional and urban scales, Eulerian CTM with UCP have been the most used to provide background and boundary chemical conditions for higher resolution models. In some studies, Lagrangian and Gaussian models are used to make the connection with CTM (Mensink et al. 2003; Oxley et al. 2013; Hofman et al. 2014), and some Gaussian models were specifically configured for assessing the pollution dispersion in street canyons (Stein et al. 2007; Isakov et al. 2009; Beevers et al. 2012). Therefore, based on bottom-up emission inventories from mobile and stationary sources, it is possible to simulate the transport and plume dispersion from these local emission sources, even on complex surfaces, although these models do not properly resolve building effects and consider highly simplified atmospheric photochemical reactions of nitrogen oxides (NOx) and tropospheric ozone (Isakov et al. 2009; Beevers et al. 2012). To analyze the intraurban spatial variability, ensemble modelling techniques with dispersion models (e.g. ADMS, OSPM, AERMOD and HYSPLIT) focused on the main emitting sources have been applied; in the case of HYSPLIT, it is through a trajectory analysis allowing the determination of the origin of air masses and establishing source-receptor relationships (Stein et al. 2007).

The downscaling for the local/microscale is done through modelled meteorological and chemical data from the upper domain and requires a more detailed characterization of the study case, especially regarding the building volumetry and street configuration, so that street emissions and dispersion around these urban structures can be simulated (Brandt et al. 2012; Hofman et al. 2014). The different modelling-based experiments over densely built areas show that the urban geometry results in lower wind speeds leading to a less intense vertical mixing in contrast to suburban or rural areas (Vardoulakis et al. 2003; Borrego et al. 2003; Tang and Wang 2007; Baklanov et al. 2009; Beevers et al. 2012). Furthermore, in order to keep the numerical stability in the advection scheme, much smaller time steps linearly interpolated from mesoscale outputs and increasing horizontal and vertical resolutions (a few metres by a grid cell) are defined (Joe et al. 2014; Kwak et al. 2015). In terms of atmospheric chemistry, in Lagrangian and Gaussian models, local pollutant concentrations (e.g. NOx/NO_2 at traffic locations) are also derived from simplified chemical reactions (Brandt et al. 2012; Jensen et al. 2017), or through empirically tested quadratic relationships for rural, urban and roadside sites (Oxley et al. 2013).

Table 1 Brief characterization of the reviewed air quality modelling applications commonly used involving regional, urban and local scales

Modelling system/reference	Model	Type	Application scales	Domains/spatial resolution	Other configurations/comments
CALIOPE-Urban (Benavides et al. 2019)	The Community Multiscale Air Quality (CMAQ) model	Eulerian CTM	Regional to urban	3 nested domains over Europe, Iberian Peninsula and Catalonia (12, 4 and 1 km)	- WRF meteorology - CMAQ emission sources: EMEP for Europe and bottom-up/top-down approaches by SNAP for Spain
	Research LINE source dispersion model (R-LINE)	Gaussian model	Urban to local	Barcelona (roadside)	- Traffic counting data and fleet composition to estimate emissions for the R-LINE model were used - CMAQ provides background concentrations for the R-LINE - There is no double counting of traffic emissions between models - R-LINE was adapted to street canyons using urban geometry data, and it has a simplified NO-NO_2 chemistry
GEM-MACH (Russell et al. 2019)	Global Environmental Multiscale-Modelling Air-quality and Chemistry (GEM-MACH)	Online model (meteorology and chemistry are handled within a single model)	Regional to urban	4 nested domains from two-thirds of the operational GEM-MACH domain to the Canadian provinces of Alberta and Saskatchewan (10, 10, 2.5, 1 km)	- Meteorological boundary conditions from operational GEM forecasts (outermost domain) and data assimilation for the inner domains - Emission sources: stack monitoring and regional and national EI - Chemistry is embedded within the GEM physics module - It represents the particle distribution by sizes (12 and 2-bin) - Two-way nesting
Street-in-Grid model (Kim et al. 2018)	Polair3D	Eulerian CTM	Regional to urban	4 nested domains over western Europe, northern–central France, Île-de-France region, eastern Paris suburbs (0.5, 0.15, 0.04, 0.01°)	- WRF meteorology (1.5 km) - Polair3D emission sources: EMEP for domains 1 and 2 and Airparif EI for domains 3 and 4 - MOZART BC
	Model of Urban Network of Intersecting Canyons and Highways (MUNICH)	Street-network model	Local	577 street segments within domain 4	- At a street level, detailed traffic emissions, geographic data and meteorological and chemical background conditions provided from Polair3D were used - MUNICH is composed of two main components: street canyon and street intersection - CB05 chemical mechanism was implemented in both models - There is no double counting of emissions - Feedback between models

Table 1 (continued)

Modelling system/reference	Model	Type	Application scales	Domains/spatial resolution	Other configurations/comments
EMEP4UK–ADMS-Urban (Hood et al. 2018)	EMEP regional version focused on air quality in the UK (EMEP4UK)	Eulerian CTM	Regional to urban	2 nested domains over Europe and the UK (50 and 5 km)	- WRF meteorology (10 km) - EMEP4UK emission sources: UK National EI (5 km) and EMEP (50 km) outside the UK
	Atmospheric Dispersion Modelling System (ADMS-Urban)	Gaussian model	Urban to local	Greater London region	- ADMS-Urban used a detailed EI by a SNAP sector for London (1-km grid resolution) and measured background concentrations as BC - It has an "urban canopy" module calculating wind speed and turbulence as a function of the surface roughness (enters with a building volumetry and road network)
The THOR Integrated System (Jensen et al. 2017)	Danish Eulerian Hemispheric Model (DEHM)	Eulerian CTM	Regional	3 nested domains over Europe, Northern Europe and Denmark (50 × 16.7 and 5.6 km)	- MM5 meteorology - DEHM-UBM emission sources: EMEP for Europe and Danish EI from all sectors on a 1 × 1 km grid - DEHM was run in two-way nesting, using
	Urban Background Model (UBM)	Urban background pollution model	Urban	A few Danish cities (1 km)	Northern Hemisphere results (150-km resolution) from Brandt et al. (2012) as IC and BC
	Operational Street Pollution Model (OSPM)	Street canyon model	Local	98 selected streets in Copenhagen and 31 streets in Aalborg	- At a street level, geometry urban data, traffic volume and emissions, meteorological parameters and background concentrations provided from the UBM were used
Integrated Urban Air Quality Modelling System (Kwak et al. 2015)	CMAQ	Eulerian CTM	Regional to urban	3 nested domains over Seoul, Republic of Korea (9, 3 and 1 km)	- WRF meteorology - Mobile emissions are spatially allocated on roads of the CFD domain
	CFD	CFD model	Local/microscale	High-rise building area of Seoul (1600 × 1600 × 997 m)	- CMAQ and WRF provide initial and time-dependent boundary conditions for the CFD domain - The same chemical mechanism used in the CMAQ was implemented in the CFD model
Polair3D–SIREAM (Kim et al. 2015)	Polair3D SIze REsolved Aerosol Model (SIREAM)	Eulerian CTM Implemented aerosol model	Regional to urban	Part of Europe (0.5°), France (0.125°), Greater Paris (0.02°)	- WRF meteorology - EMEP emissions (0.5° × 0.5°) - INCA-LMDz IC and BC - Test different PBL schemes, with/without UCM
CMAQ–CALPUFF (Zhang et al. 2015)	CMAQ	Eulerian CTM	Regional to urban	Hong Kong Administrative Region (3 km)	- WRF meteorology for the CMAQ and CALMET. The latter produces finer scale meteorological fields for the CALPUFF
	California Puff (CALPUFF)	Multilayer non-steady-state puff dispersion model	Urban to local	Centred at Hong Kong (0.5 km)	- Emission sources: CMAQ used a bottom-up EI for some sources (3-km resolution), while CALPUFF used local emission data - CMAQ provide IC and BC for the CALPUFF - User-friendly system interface currently prepared for Hong Kong and Pearl River Delta region, but

Table 1 (continued)

Modelling system/reference	Model	Type	Application scales	Domains/spatial resolution	Other configurations/comments
					could be transferable to study other regions, providing a proper dataset
AURORA–IF-DM–OSPM (Hofman et al. 2014)	Air quality modelling in Urban Regions using an Optimal Resolution Approach (AURORA)	Eulerian CTM	Regional to urban	Antwerp city to street level	- Emission sources: industry, traffic, households - Local traffic emissions provided from the MIMOSA model - AURORA and IFDM were coupled using a method to avoid the double counting of the local emissions - IFDM and OSPM results were combined in order to get high-resolution concentrations
	Immission Frequency Distribution Model (IFDM)	Bi-Gaussian plume model	Urban to local		
	Operational Street Pollution Model (OSPM)	Street canyon model	Local		
Source-Oriented WRF/Chem with High Resolution (SOWC-HR) (Joe et al. 2014)	WRF/Chem	Online model (fully coupled meteorology and chemistry)	Regional to urban	3 nested domains over the Oakland region, California (12, 4 and 1 km)	- Higher resolution EI for domains 3 and 4 were developed - LES is coupled in WRF/Chem - Changes on the PBL schemes were made to allow the nesting of the LES within the multiscale parent domains - Requires very small time intervals to keep the numerical stability in the advection scheme - Street canyon and building effects are not resolved - Two-way nesting - Online coupling
	Large eddy simulation (LES)	Subgrid-scale turbulence model	Urban to local	Domain 4 focused on the Port of Oakland (250 m)	
The UK Integrated Assessment Model (UKIAM) (Oxley et al. 2013)	EMEP	Eulerian CTM	Regional	Europe (50 km)	- Emission sources: EMEP for non-UK areas; national and local EI for the UK - Gaussian PPM only includes small derivations for NO_2 concentrations - Source apportionment assessment from local and distant sources
	FRAME	Lagrangian CTM	Regional to urban	UK (5 km)	
	Primary Particulates Model (PPM)	Gaussian model	Urban	UK (1 km)	
	BRUTAL	Street canyon model	Local	Roadside	
CHIMERE–"Stretching" method (Siour et al. 2013)	CHIMERE	Eulerian CTM	Regional	Europe (0.5°) to Belgium-Netherlands-Luxembourg (0.1°)	- WRF meteorology - EMEP emissions (0.5° × 0.5°) - Zooming approach provides a simple and immediate way to better represent scale interactions within the CTM - One-way nesting
	"Stretching" method	Also called "zooming"	Regional to urban	Belgium-Netherlands-Luxembourg (300 m)	
The THOR Integrated System (Brandt et al. 2012)	DEHM	Eulerian CTM	Regional	Northern Hemisphere (NH—150 km); two nested domains: Europe	- MM5 meteorology - Emission sources: RCP for NH and NA, EMEP for Europe (both EI with 0.5° × 0.5°) - DEHM was run in two-way nesting

Table 1 (continued)

Modelling system/reference	Model	Type	Application scales	Domains/spatial resolution	Other configurations/comments
	UBM	Urban background pollution model	Urban	and North America (NA—50 km) A few cities (1 km)	- UBM includes a simple scheme for dispersion and transport, as well as a simple chemical model including NOx and O_3 reactions - OSPM used UBM outputs and emissions provided
	OSPM	Street canyon model	Local	Roadside	from a traffic model for simulating NO_2 dispersion and chemistry at the street scale
CMAQ–ADMS-Roads (Beevers et al. 2012)	CMAQ	Eulerian CTM	Regional to urban	London (3 km)	-WRF meteorology - Emission sources: EMEP (0.5° × 0.5°), E-PRTR and London EI (1-km resolution) - STOCHEM IC and BC - CMAQ predictions were downscaled for a 20-m grid using the bilinear interpolation method - ADMS represents the dispersion from road traffic ($NOx-NO_2-O_3$)
	Atmospheric Dispersion Modeling System (ADMS-Roads)	Gaussian model	Urban to local	Roadside (20 m)	
CCAM–TAPM (Thatcher and Hurley 2010)	Conformal Cubic Atmospheric Model (CCAM)	Semi-Lagrangian atmospheric model	Regional	Australia (60 km)	- CCAM requires only global IC (1° resolution GFS) - It provides BC for the TAPM - TAPM was selected due to its combined prognostic meteorological and air pollution modelling capability
	The Air Pollution Model (TAPM)	Eulerian CTM	Urban	Urban regions centred on Melbourne (dynamic downscaling of 30, 10 and 3 km)	
CMAQ–AER-MOD (Isakov et al. 2009)	CMAQ	Eulerian CTM	Regional to urban	US region (nesting from 36 to 12 km)	- MM5 meteorology - 1999 National EI - CMAQ was run for one year in nested mode - It provides regional background concentrations for the AERMOD - AERMOD is designed to capture local gradients from nearby sources, using highly simplified atmospheric chemical reactions. It uses "bottom-up" EI from mobile and stationary sources
	AERMOD	Gaussian model	Urban	New Haven (mobile and stationary source network)	
Enviro-HIRL-AM–M2UE (Baklanov and Nuterman 2009)	Environment-High Resolution Limited Area Model (Enviro-HIRLAM)	Online model (fully coupled meteorology and chemistry)	Regional to urban	Copenhagen (nesting from 3 to 0.5 km)	- Enviro-HIRLAM provides IC and BC for the M2UE - It was run in one-way nesting - It uses urban parameterizations: at a regional level, these are based on the roughness and flux
		CFD model	Local/microscale		

Table 1 (continued)

Modelling system/reference	Model	Type	Application scales	Domains/spatial resolution	Other configurations/comments
	Obstacle-resolved Microscale Model for Urban Environment (M2UE)			Selected area of Copenhagen (from 50 to 3 m)	correction approach (EMS-FUMAPEX), while BEP is considered at the urban scale - M2UE calculates obstacle-resolved flows and dispersion based on the RANS approach and two-equation turbulence closure
CMAQ–HYS-PLIT–AERM-OD (Stein et al. 2007)	CMAQ	Eulerian CTM	Regional to urban	Houston, Texas (1 km)	- CMAQ provides regional background concentrations and urban-scale photochemistry
	Hybrid Single-Particle Lagrangian Integrated Trajectory (HYSPLIT)	Lagrangian CTM	Urban to local	Stationary sources	- A simulated HYSPLIT concentration ensemble is used to assess the variability/dispersion from point sources, assuming non-reactive chemistry on subgrid scales (useful to model the uncertainty)
	AERMOD	Gaussian model	Urban to local	Selected road network	- AERMOD simulates the plume dispersion from mobile sources
ECHAM5/M-ESSy–CMAQ (Jiménez et al. 2006)	Fifth-generation atmospheric GCM/Modular Earth Submodel System (ECHAM5/MESSy)	Atmospheric chemistry GCM	Global	Global (1.8° × 1.8°)	- The ECHAM5/MESSy coupling allows simulating large-scale chemistry climate - Emission sources: EDGAR3.2 EI for ECHAM5/MESSy and EMEP (coarser domains) and high-resolution emissions (1 h and 1 km—inner domain) for CMAQ
	CMAQ	Eulerian CTM	Regional to urban	4 nested domains from Europe and Iberian Peninsula to a Catalonia area (72, 24, 6 and 2 km)	
MATCH (Gidhagen et al. 2005)	Multi-scale Atmospheric Transport and Chemistry (MATCH)	Eulerian CTM	Regional to urban	Stockholm—35 × 35 km (5 km down to 0.5 km)	- HIRLAM meteorology (22-km resolution) - The flat topography allows the downscaling to the urban grid (500 m) and also interpolation in time to yield hourly data, involving higher vertical resolutions (4 layers below 15 m) and a recalculation of the turbulence over the city - Street canopies and buildings are not resolved in the model

Table 1 (continued)

Modelling system/reference	Model	Type	Application scales	Domains/spatial resolution	Other configurations/comments
Integrated system AURORA (Mensink et al. 2003)	AURORA	Eulerian CTM	Regional to urban	Flemish region, Antwerp (1 km)	- ARPS meteorology (100-m resolution) - Detailed EI, described as a function of space, time and temperature - AURORA system integrates the OPS and SBM - OPS calculates concentrations and dry and wet depositions for primary and secondary components - SBM assumes a uniform concentration distribution over the street with the box dimensioned by the length and width of the street and the height of the surrounding built-up area
	Operational Priority Substances (OPS)	Lagrangian CTM	Regional to urban	Flemish region, Antwerp (1 km)	
	Street box module (SBM)	Street canyon model	Local	11 selected streets	

WRF the Weather Research and Forecasting model, *MM5* fifth-generation Penn State/NCAR Mesoscale Model, *GCM* general circulation model, *CALMET* California Meteorological Model, *EMEP* the European Monitoring and Evaluation Programme, *SNAP* Selected Nomenclature for Air Pollution, *MOZART* Model for Ozone and Related chemical Tracers, *INCA* Interaction with Chemistry and Aerosols model, *CB* carbon bond, *LMDz* Laboratoire de Meteorology Dynamique zoomed, *GFS* Global Forecast System, *ARPS* Advanced Regional Prediction System, *EI* emission inventory, *E-PRTR* the European Pollutant Release and Transfer Register, *RCP* Representative Concentration Pathways, *IC* initial conditions, *BC* boundary conditions, PBL planetary boundary layer, *UCM* urban canopy model, *BEP* Building Effects Parameterization

For each modelling system, when results from the model combination were compared with the high-resolution nested Eulerian CTM results and the available air quality measurements, a better statistical performance was achieved using the cascade of models. The coupling of models over different scales allows accounting for contributions from nearby and distant emission sources to the air quality at a specific location (e.g. in an industrial area, in rural areas or even in a street canyon) (Stein et al. 2007; Isakov et al. 2009; Brandt et al. 2012; Kim et al. 2018). However, the way the atmospheric emissions are included within the system requires particular attention, because the same emission sources may be considered by the different types of models and adding as a background the modelled concentrations from upper domains could result in double counting the impact of these sources.

Figure 1 shows the basic requirements involving a typical multiscale air quality modelling system, namely the information scheme needed to interactively combine models at different scales and applications.

The air quality modelling is divided into mesoscale and microscale taking into account the suitable spatial coverage and resolutions for application of the involved models, seeking, in a multiscale perspective, to ensure the harmonious link among them. To feed offline air quality models, three main input datasets are used: meteorology, initial and boundary conditions and atmospheric emissions. In the case of online models, the calculation of meteorology and chemistry is done in parallel, allowing the assessment of potential feedbacks including, for example, direct aerosol effects on the radiation scattering and the influence of local weather patterns on chemical reactions. Two main types of nesting techniques for the down- and/or upscaling can be chosen: (i) one-way nesting, when effects of the local/microscale on a larger scale are not considered, and (ii) two-way nesting, whose scale effects are felt in both directions (meso- to microscale and micro- to mesoscale). The two-way option is mainly used in mesoscale modelling, favouring the feedback between simulation domains.

Current limitations

As discussed in the previous section, combining air quality results within multiscale models is not straightforward. In general, the inconsistences found are related to the modelling assumptions and nature of the available input data.

Mesoscale CTM are particularly useful to simulate chemically reactive species and address their long-range transport (Stein et al. 2007; Srivastava and Rao 2011), but they fail in the realistic representation of atmospheric flows at lower spatial levels (e.g. city scale). This inaccuracy of the mesoscale modelling results over urban areas

Fig. 1 General structure of a multiscale air quality modelling system
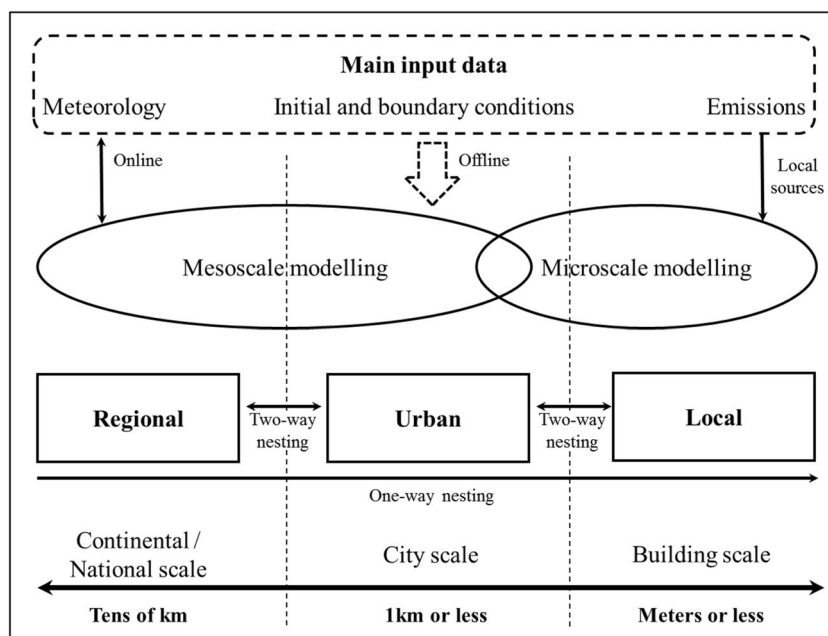
is associated with many factors, which should be highlighted:

(i) No urban parametrization or being unsuitable to characterize the 3D urban structure

The urban canopy (UC), a region where people live and human activities take place, has been a subject of much investigation (Baklanov et al. 2009; Schlünzen et al. 2011) given its highly complex atmospheric circulations, primarily due to the presence of multiple obstacles strongly modifying the air flows and the thermal land-atmosphere exchanges. In these circumstances, the use of CFD models to evaluate small-scale atmospheric dynamics is recommended; however, the common practice in multiscale modelling is to apply mesoscale models with increased resolution over urban areas without the adequate parametrizations or Gaussian models that despite the new developments to simulate urban areas are still limited (Baklanov and Nuterman 2009; Thunis et al. 2016). Taking as example the urban canopy model (UCM)-coupled WRF-Chem modelling system, high uncertainties are related to the required urban parameters and selection of the most representative values, especially due to the limited number of urban land use classes and value projection on a single layer (Kim et al. 2015). Notwithstanding all efforts to decrease the regional-to-urban modelling uncertainties, currently most of the operational mesoscale models do not consider the urban effects.

(ii) Limited grid resolution

Grid models are the best suited tools to deal with regional features. Nevertheless, when the goal is to estimate concentration fields very close to individual sources, the use of regional scale grid–based models is discouraged, since all emissions located within each cell are evenly distributed, not allowing the accurate simulation of the effects of these sources, either in the grid cell itself or in any of the nearby cells (Stein et al. 2007; APPRAISAL 2013). Furthermore, due to limitations in the mesoscale formulations, the highest typical grid resolution using these modelling tools (about 1 km) is inadequate to capture the urban morphology (obstacles) and thermal characteristics inducing dispersion of air flows and pollutants within the UC, primarily close to densely urbanized areas and with many pollution sources (Baklanov and Nuterman 2009; Talbot et al. 2012; Pay et al. 2014; Kwak et al. 2015; Thunis et al. 2016).

(iii) Local scale impacts on larger domains are often neglected

In air quality modelling, multiscale interactions can be represented through two-way nesting using a single CTM and/or large- and small-scale coupled models. This model coupling assumes that only the inner domain outputs resulting from large-scale simulations are passed to microscale models as initial and boundary conditions (i.e. in one-way mode). Not considering microscale effects over upper simulation domains can be critical in areas exposed to air mass recirculation (sea breeze cells) or around regions with high pollutant emission gradients (large cities) (Siour et al. 2013).

In turn, at microscale applications to resolve fine-scale pollutant variations, current limitations could be accounted as follows:

(i) Limited pollutant dispersion modelling in the presence of obstacles using Gaussian approaches

As mentioned in "Overview of multiscale air quality modelling applications", Gaussian models are often used to depict the pollutant dispersion around obstacles. However, the Gaussian formulations have been successfully employed in simplified flow configurations (under steady-state conditions) and for flat and unobstructed landscapes. In the presence of complex surfaces, the pattern observed in most cities, and the plume dispersion rate depending on the urban geometry, turbulence and distance from the pollution sources, is probably an over-simplification due to the use of empirical input parameters (i.e. all variables are ensemble averaged), and so, the validity of these models needs to be carefully evaluated (APPRAISAL 2013; Lateb et al. 2016).

(ii) Lack of proper input data

The use of local-scale atmospheric models is often hampered by a lack of adequate lateral boundary conditions to drive the flow in the finer domain, because, typically, these boundaries are extracted from regional/urban-scale results to produce time-varying local solutions, and they are often skewed due to the local meteorological dynamics, especially on complex terrain (Borrego et al. 2003; Talbot et al. 2012; APPRAISAL 2013). The desired resolution of the emission inventory is another concern in microscale air quality applications, since the spatial detail is frequently inadequate to fully characterize individual sources at the street-to-building scales (Likhvar et al. 2015; Thunis et al. 2016).

(iii) Simplified photochemistry

Local-scale dispersion models have been improved to provide a detailed description of the concentration patterns, but they are not properly treating the complex photochemical reactions and their effects, due to the longer reaction time of many chemical species than the travel time across an urban area (Stein et al. 2007). Thus, local-scale models are considering pollutants passive compounds or are using a simplified chemical kinetic mechanism. This could be considered an advantage because it simplifies the simulation and it is computationally cheap, but it has to be carefully assessed to be sure that important (fast) chemical reactions are represented. For instance, if VOC emissions are larger than NOx emissions, simplified photochemistry is not a valid approach. Moreover, the dimension of the domain has to be taken into account to understand how far the simplification of the chemistry can go.

The integration of complex chemistry mechanisms at the local scale is an important but also a challenging issue for the air quality modelling community, which must be duly weighed.

(iv) Temporal analysis of CFD results

Analyzing the evolution of modelled concentrations using CFD at the local/street level for long time periods is a challenge that still needs to be worked, due to the high complexity of the urban structure and computational requirements for processing information at very fine resolutions. When overcoming this issue, it will be possible to assess the influence of the main emission sources throughout a particular year and to evaluate the seasonality and dispersion and accumulation patterns in a wide range of weather conditions (Thunis et al. 2016).

Guidelines for strengthening the synergy among scales

In view of the current limitations and identified scientific developments in multiscale air quality modelling, additional efforts are needed to reduce uncertainties and differences among modelled atmospheric concentrations by comparing results from different scales and models. In this sense, the following set of guidelines to flexibly integrate regional-to-local–scale models and input data within a single system is proposed:

(i) Linking different types of air quality models

For a reliable representation of multiscale air quality, different types of air quality models need to be carefully coupled within the modelling system, and the relevant variables from the mesoscale (time-dependent boundary and background meteorological and chemical conditions) should be properly assimilated by a microscale model (Mensink et al. 2003; Brandt et al. 2012; Oxley et al. 2013; Hofman et al. 2014). Given the complexity of the involved atmospheric processes in the mixing layer, the option for online mesoscale models may allow a better characterization of the time-resolved dispersion of air pollutants and it has the advantage of integrating meteorology-chemistry feedbacks (Grell et al. 2004). Even the simplest urban canyon model requires a background concentration value as input, to account for the pollutant fraction that is not emitted within the simulated street (Vardoulakis et al. 2003). Obstacle-resolved simulations together with a canopy layer–based mesoscale approach are likely the simplest and the most promising way to include obstacle effects using structured grids in two-way nesting (Schlünzen et al. 2011). Another possibility to design a multiscale modelling system, though more complex to implement but with advantages, at least, in terms of computational efficiency, is the integration of a local/microscale model within the mesoscale CTM. Thus, as a starting point for successful multiscale simulations, the urban characteristics should be well indicated, namely the urban canopy structure, effects of the obstacles (e.g. building blocks and their distribution) and influence of the underlying surface (e.g.

orography, land use type, roughness, thermal properties and energy consumption sources) over the urban atmospheric dynamics (Baklanov et al. 2007). At the microscale, using combined plume and box models is feasible to numerically and accurately examine the intraurban spatial variability and dispersion of air flows associated with building geometry and street configuration (Mensink et al. 2003; Oxley et al. 2013; Kwak et al. 2015). When dispersion models are used in a knowledgeable way, they can be very useful to improve the understanding of the physical and chemical processes that govern the transport mediated by the advection scheme and chemical transformation of atmospheric pollutants (Vardoulakis et al. 2003). Hence, to suitably represent atmospheric phenomena at different spatial and temporal scales, the base equations have to be treated and integrated in joint meso-to-microscale modelling approaches, ensuring the consistency of processes, essentially due to the need of time-dependent boundary conditions for various pollutants (Baklanov and Nuterman 2009; Kwak et al. 2015).

(ii) Detailed emission inventories

Nowadays, emission inventories are recognized as one of the main uncertainty sources in air quality modelling applications. To improve the performance of the air quality models, a detailed knowledge of the pollutants emitted with high spatial and temporal resolutions is required. In the case of multiscale modelling systems, the emission inventory should be prepared to give response at multiple scales and disaggregated in time based on activity profiles by macrosetor (Russo et al. 2019). Nevertheless, the dynamical downscaling involving different models should be conducted carefully, because the background conditions used to drive the microscale simulations could result in double counting the impact of emission sources, mainly if local sources are included in mesoscale/urban modelling. In order to accurately assess the impact from local emission sources, two air quality simulations using a multiscale model system could be performed: one for the base case in which local emissions are included in both CTM and small-scale model (double counting) and another simulation in which local emissions are only included in the small-scale model. The absolute difference in the air concentrations between the two simulations provides an indication of the magnitude of these impacts (Isakov et al. 2009). This analysis is very useful for deciding whether local emission sources should be included or not in mesoscale simulations and thus avoiding the double counting issue to use the resulting modelled concentrations as a background of microscale tools.

(iii) Using techniques of data assimilation and inverse modelling

Data assimilation can be a way to improve results from multiscale modelling, and inverse modelling can help in identifying the most relevant emitting sources for the different scales. Data assimilation techniques within atmospheric models employ observations with the purpose of improving air quality estimates, whereas the inverse modelling uses these predictions and measured data to estimate pollutant emissions. Thus, the use of these two types of techniques under the multiscale modelling framework could be an added value. It is not a common practice yet to use these two types of techniques in multiscale modelling; they are used in single-model applications. A step forward would be to assess their application within the entire multiscale modelling system, as a whole. However, a balance between improved results and computational efforts, as well as the scales to be focused, has to be analyzed.

(iv) Increasing the spatial resolution of mesoscale models

This issue is designed as a priority research area, mainly for air quality assessment in urban environments, since results from high-resolution mesoscale models are needed to be compared with finer scale modelling outputs and measured data and also to allow an accurate forecasting of air pollution events. On the other hand, to provide the best air quality estimates, mesoscale models should jointly include local-scale features, long-range transport and photochemical transformations (Stein et al. 2007; Isakov et al. 2009; Siour et al. 2013). One way to increase the spatial resolution of mesoscale CTM (finer than 1 km) is to use fully embedded LES approaches, which allow the dynamic downscaling for grid resolutions around 200 m.

(v) Applying the modelling system with nesting capabilities

Nested atmospheric simulations arise as an appealing approach that can combine the strengths of the different modelling scales and enable high-resolution outputs (Talbot et al. 2012). Most studies involving multiscale modelling systems consider nesting using mesoscale models with a spatial ratio between simulation grids that should not exceed 3–5, since this ratio is primordial to keep the numerical stability, suitable approximation and accuracy of the models (Gidhagen et al. 2005; Stein et al. 2007; Baklanov and Nuterman 2009; Thunis et al. 2016). The link to the local scale or microscale should be ensured with specific microscale tools (e.g. CFD models), merging the different types of models, preferentially in two-way nesting mode.

(vi) Evaluating atmospheric feedbacks between simulation domains

Combining modelled results from the different simulation domains is the most computationally efficient way to

provide pollutant concentrations from nearby and distant sources (Isakov et al. 2009). The option of two-way nesting capability is a priori recommended, making it possible to incorporate the influence of small-scale features on broader domains, as well as assessing the opposite effect (i.e. larger scale to microscale), though it requires more computational power (Soriano et al. 2004; Brandt et al. 2012; Siour et al. 2013). For a comprehensive assessment of air quality problems in a specific area, it is advisable to analyze potential feedbacks from the microscale to larger scale processes and vice versa, as it happens when analyzing multiscale results provided from the Street-in-Grid and SOWC-HR modelling systems (Table 1). The comparison of overlapping areas will be another test to take into account, in order to avoid mass inconsistency and generation of numerical noise (Baklanov and Nuterman 2009).

Concluding remarks

Air pollution is closely associated with urban and local problems, which also depend and affect larger scale processes. Hence, its assessment in a multiscale perspective is recognized as an important research issue. Several modelling studies relating to the influence of the complex urban structure (e.g. road network, building volumetry and vegetation) on pollutant accumulation/dispersion patterns have been undertaken, with many of them assessing the resulting implications for the health and the environment. Most of the multiscale modelling systems are designed to capture regional to urban effects, using mesoscale nested approaches with generic urban parametrizations, but they do not reproduce local/street-scale phenomena given the high level of the UC heterogeneity. To that end, suitable microscale tools able to capture dynamic effects induced by the urban structure on the turbulent transport within the UC could be used.

When local models are integrated in modelling systems, the proper link from the mesoscale to the street level is a key determinant to obtain reliable multiscale air quality outcomes and to decrease the uncertainties when combining different domains and resolutions. To achieve this target, three relevant aspects in multiscale air quality modelling should be highlighted and require further investigation:

(i) Improving the UCP within mesoscale models

An enhanced representation of the urban structure and associated processes will allow, on the one hand, obtaining higher resolutions over limited areas and, on the other hand, reducing the discrepancies between meso-to-microscale modelling results.

(ii) Developing modelling systems with two-way nesting capability

Two-way grid nesting is currently available in many mesoscale atmospheric models, but if the objective is to cover multiple spatial scales using specific modelling tools, the models to integrate into the system should be adapted and carefully coupled to boost feedbacks among the different simulation domains.

(iii) Promoting the use, improvement and development of multiscale online modelling systems

The use of online models instead of the classic offline modelling systems represents an added value in atmospheric modelling, because the meteorological and chemical evolution of the atmosphere is modelled within the same system sharing the same simulation grids, with the potential to include chemistry-meteorology feedbacks. Nevertheless, additional efforts to improve and test the existing physical and chemical parametrizations, as well as to develop new transport and vertical mixing schemes and new online hybrid approaches combining different types of models and scales, are needed to have a comprehensive multiscale understanding of all atmospheric processes that govern the transport, dispersion, transformation and deposition of air pollutants.

In summary, for a multiscale air quality assessment, adequate modelling tools should be used and flexibly integrated into a system to accurately describe atmospheric phenomena and resulting pollutant concentrations at different scales, so that the decision-makers can use this information for effective policy development of air quality management at different administrative levels.

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