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Bridging the scales in a eulerian air quality model to assess megacity export of pollution

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ABSTRACT

In Chemistry Transport Models (CTMs), spatial scale interactions are often represented through off-line coupling between large and small scale models. However, those nested configurations cannot give account of the impact of the local scale on its surroundings. This issue can be critical in areas exposed to air mass recirculation (sea breeze cells) or around regions with sharp pollutant emission gradients (large cities). Such phenomena can still be captured by the mean of adaptive gridding, two-way nesting or using model nudging, but these approaches remain relatively costly. We present here the development and the results of a simple alternative multi-scale approach making use of a horizontal stretched grid, in the Eulerian CTM CHIMERE. This method, called "stretching" or "zooming", consists in the introduction of local zooms in a single chemistry-transport simulation. It allows bridging online the spatial scales from the city (~1 km resolution) to the continental area (~50 km resolution).

The CHIMERE model was run over a continental European domain, zoomed over the BeNeLux (Belgium, Netherlands and Luxembourg) area. We demonstrate that, compared with one-way nesting, the zooming method allows the expression of a significant feedback of the refined domain towards the large scale: around the city cluster of BeNeLuX, NO_2 and O_3 scores are improved. NO_2 variability around BeNeLux is also better accounted for, and the net primary pollutant flux transported back towards BeNeLux is reduced. Although the results could not be validated for ozone over BeNeLux, we show that the zooming approach provides a simple and immediate way to better represent scale interactions within a CTM, and constitutes a useful tool for apprehending the hot topic of megacities within their continental environment.

1. Introduction

In 2010, there were 20 cities worldwide housing more than 10 million inhabitants, while 30 others had a population exceeding 7 million people (Molina and Molina, 2004; Lawrence et al., 2007). The chemical plumes produced by these megacities contain a large quantity of primary species (NO_x, volatile organic compounds – VOC, CO and particulate matter – PM) which, at the regional scale, lead to the formation of gaseous oxidants such as ozone as well as organic particulate matter. In addition to their adverse effects on human health (Bell et al., 2006; Gryparis et al., 2004) or ecosystems (Ashmore, 2005; Felzer et al. 2007) and to their contribution to the degradation of regional air quality, many of these compounds impact the radiative budget of the atmosphere at the global scale (Molina and Molina, 2004; Akimoto, 2003; Crutzen, 2004; Gurjar and Lelieveld, 2005). As a consequence, our ability to quantify the impact of megacities and other emissions hotspots on the composition and long-term evolution of the troposphere constitutes a scientific topic of sustained attention (Chow et al., 2004; Gurjar and Lelieveld, 2005). To address this question, one must be able to track the transport of pollutants originating from megacities, in order to characterize their impacts at multiple temporal and spatial scales.

Several studies have focused on the growing problem of megacities using global (Wild and Akimoto, 2001; Stohl et al., 2002; Lawrence et al., 2007, 2003) and regional (de Foy et al., 2006; Guttikunda et al., 2005) chemistry-transport models. All of them have highlighted the high potential of megacities for affecting the surrounding areas – the amplitude of their impact being strongly dependent on the regional-scale meteorological features prevailing over each individual city. The conclusions all support the

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importance of bridging local and regional scales when investigating the impact of megacities with Chemical Transport Models (CTM). The study of scale interactions is common to all scientific disciplines and several approaches are used (Voinov and Shugart, 2013; Pisoni et al., 2010; Boumans et al., 2002).

The most widespread approaches to represent the interactions between spatial scales in a CTM are the one-way and two-way nesting methods (Jakobs et al., 1995). One-way nesting consists in using a first broad simulation as initial and boundary conditions for a second simulation of different resolution. It is generally used to constrain, at its boundaries, a high-resolution simulation with the chemical or meteorological fields obtained from a simulation covering a larger domain at lower resolution. In this configuration, both simulations can be computed simultaneously or sequentially, but an important disadvantage of this technique is that there are no possible feedbacks between the small and the large domain. Despite this limitation, this method is widely used and remains appropriate when the impact of the small scale on the larger environment is not the focus of the study (Kaminski et al., 2002). Otherwise, the impact of the small scale the larger scale must be represented. In this case, implementing a two-way nesting approach is more appropriate: the fine and coarse domains are simultaneously simulated so as to allow the exchange of data at each time step of the calculations. This approach is not simple: it requires the elaboration of hypotheses about air mass distribution from large to small grid cells, and deep modifications in the computer code. Indeed, the communication from coarse to fine domains can lead to numerical problems (see Garcia-Menendez and Odman, 2011). Various mesh refinement techniques using structured grids (Srivastava et al., 2000) as well as mesh enrichment techniques on unstructured grids (Tomlin et al., 1997) were thus explored by Garcia-Menendez and Odman (2011). These techniques were developed from simple exercises and designed to prove the worthiness of adaptive gridding in air quality modelling tools, for pollution management purposes. This new type of gridding is promising. However, until now, it was principally used for plume simulation, and it requires further development to be integrated in a CTM.

Alternatively, the feedback of the regional to the larger scale can be represented using a nudging technique. Maurizi et al. (2011) have introduced such a parameterization in the Bolchem CTM (Mircea et al., 2008). This technique consists in nudging a high resolution sub-domain into a low-resolution larger domain. The main advantage of this method is that it allows coupling different models for each scale. However, feedbacks between the coarse and the fine domains cannot all be accounted for.

Stretched grids (also known as “zooming” approaches) are another alternative method. Stretching consists in gradually increasing the horizontal resolution of the model grid over given latitudinal and longitudinal bands. At the intersection of these bands, a grid which is finer than the rest of domain is obtained. Originally, this stretched-grid approach was principally used in weather numerical models, which were successfully used for operational short-term (24–48 h) forecasting (Schmidt, 1977; Staniforth and Mitchell, 1978). It was then introduced in a Global climate model (GCM) by Fox-Rabinovitz et al. (1997) to represent adequately the regional scale over an area of interest. The main interest of this approach resides in its capability to capture real-time feedbacks from the small to the large scale and reversely. The specificity of this technique is that it allows studying the scale interactions without changing the classical structure of CTM.

Our study presents the development and the results of implementing this alternative multiscale approach in the Eulerian CTM CHIMERE. We investigate here its capacity to better apprehend the chemical interactions between a high resolution area and its mesoscale environment. Through this analysis, we aim at evaluating the benefits of very simple refined gridding processes for the large and for the small domains, compared with classical one-way nesting approaches. In the first part of the paper, we introduce the models used for this study. The methodology that has been developed to bridge the scales in the model is then presented in the second part. Finally, the third part is devoted to a case study analysis.

2. Meteorological and chemical models

2.1. Description of the CHIMERE chemistry transport model

The CHIMERE model (see the model documentation at http://www.lmd.polytechnique.fr/chimere/download.php) uses the reduced MELCHIOR2 chemical mechanism, which is composed of 44 species, including 19 organic species, and 120 reactions. Photolysis rates are calculated under clear sky conditions as a function of height using the TUV model of Madronich et al. (1998). The aerosol module accounts for 14 species (primary particulate matter made of black carbon and organic carbon, but also several biogenic and anthropogenic secondary organic aerosol species – SOA –, sea salts, dust and water) and uses 8 sizes bins from 40 nm to 10 μm (Bessagnet et al., 2005). Dry deposition for gaseous species is parameterized from Wesely (1989) as a downward flux, and a resistance scheme is also included for the aerosols.

Boundary conditions for gaseous species are interpolated from LMDZ-INCA global model data. Anthropogenic emissions are those of the EMEP (http://www.emep.int/) inventory which considers NO_x, VOC, SO_x, CO, PM_{coarse} and PM_{fine} at a resolution of $0.5^\circ \times 0.5^\circ$. Biogenic emissions are calculated by the MEGAN model (Guenther et al., 2006).

The horizontal and vertical transport is prescribed by input meteorological fields, processed by the second order Van Leer scheme (Vanleer, 1979).

2.2. Description of the WRF mesoscale meteorological model

In this study, the meteorological fields used to drive the CHIMERE CTM are computed with the WRF ARW (Weather research and forecasting) model (Skamarock and Klemp, 2008). This model offers the possibility to perform one-way and two-way nested simulations. For the present study, we have used the two-way nested setup.

From these data, CHIMERE calculates a set of parameters and constrains some physical processes required for chemistry-transport simulations. The planetary boundary layer height is calculated with the Yonsei University scheme (Hu et al., 2010). The convection is parameterized with the Kain-Fritsch scheme (Kain and Fritsch, 1990), and cloud microphysics is described with the WRF Single-Moment 5-class scheme. Long wave and short wave radiations are calculated with the RRTMG scheme (Iacono et al., 2008). The land surface is represented with the RUC Land Surface Model with soil temperature and moisture being given inside six layers, multi-layer snow and frozen soil physics. The surface layer description is based on Monin-Obukhov with Carlson-Boland viscous sub-layer (Skamarock and Klemp, 2008). Finally, both components of the wind (u and v), as well as temperature and specific humidity are nudged towards the large scale NCEP/GFS meteorological reanalyzes with a relaxation time scale of 3, 3 and 14 h respectively. This nudging is applied to all vertical levels except in the boundary layer.

3. Development of a stretched grid

3.1. Technical description

The first step consists in creating an irregular grid from the default CHIMERE grid which uses a plate-carree projection (regular