

## An integrated numerical methodology for describing multiscale interactions on atmospheric flow and pollutant dispersion in the urban atmospheric boundary layer



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### ABSTRACT

Interactions between different spatial and temporal scales play a major role in determining the flow structure over the urban canopy in densely built agglomerations. Aiming to address the limitations which arise as a result of the physical disparities between the different modelling scales, a two-way scheme has been introduced for coupling the mesoscale model MEMO and the microscale model MIMO, utilising a collection of interpolating metamodels. The coupled system was used to simulate meteorological fields over the Greater Paris area during a multi-day wintertime case study. Its performance as a meteorological driver model was further evaluated by introducing the calculated meteorological fields as driving input in air quality calculations performed using the Eulerian chemical dispersion model MARS-aero.

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### 1. Introduction

Simulating the flow field in and above the urban canopy involves an account of the interplay between obstacle effects, surface forcings and scale interactions that in most cases are impossible to resolve by a single physical model. The intense surface in-homogeneities of urban areas result in the generation of extra terms of turbulence which directly affect atmospheric transport within the urban canopy. Nevertheless, a detailed description of the effect of urban structures on the Urban Atmospheric Boundary Layer (UABL) has the potential to significantly improve the accuracy of the predicted flow and dispersion fields on both the local scale and the mesoscale. The main reason for that is that by including the microscale effects of the urban structures at the lower levels of the UABL in terms of local forcing, better predictions can be made for the evolution of atmospheric turbulence distribution over the urban canopy. Moreover, obstacle-induced flow features in small spatial and temporal scales can affect loads on tall structures, including wind turbines (Emeis, 2012). Validation studies of a number of model mesoscale simulations have shown that the presence of urban conglomerations in

the study domain compromises the accuracy of the air quality simulations, thus suggesting that new approaches for the description of urban effects should be adopted. During the last years the scientific community succeeded in the development of scale exchange procedures in several models. Efforts to introduce urban effects on mesoscale models have in general followed two different approaches. In the first one, corrections are applied in the mesoscale parameterisations within the lower computational layers, in an attempt to account for the specific characteristics of the urban canopy. Such approaches have the advantage of low computational requirements and offer a significant degree of flexibility by allowing a fine-tuning of the various parameterisations to the qualitative characteristics of different urban morphologies. On the other hand, they suffer from the introduction of a large number of parameters that need to be calibrated for a wide range of urban canopy characteristics such as building height and geometry, density of street canyons and thermal properties of the urban elements.

In regard to the second approach, research has focused on refining and further developing methods for coupling individual models, considering interactions between the various scales, aiming to assess the effect of such interactions on urban air quality. In this way a refined description of interactions between larger scale phenomena and urban scale processes has been achieved and recommendations on best modelling practices have

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being formulated. Examples of state-of-the-art integrated multi-scale models include the MECTM system that couples the macro-scale model CTM2 with the air flow model METRAS, the multiscale French SUBMESO system for calculating the dispersion and transport-diffusion-transformations of reactive pollutants within an urban area, the EMEP Eulerian photochemistry model coupling regional scale models to global modelling systems and the US EPA's Models-3 Air Quality modelling systems which provides the software framework for utilising different models in a single case study.

The European project ATREUS was focused on investigating thermal effects and wind flow modifications caused by urban structures on the street canyon and building level, as well as assessing the impact of heating and cooling loads of the buildings on the urban microclimate. To this end, a cascaded model infrastructure has been developed integrating different modelling techniques, from Numerical Weather Prediction models for providing the synoptic conditions, continuing to mesoscale models that provide the upper boundary conditions to microscale models, using appropriate interfaces. These microscale models, in turn, are coupled with available street canyon simulation codes in order to study the energy behaviour of the buildings. A one-way coupling method between the microscale model MIMO and mesoscale model MEMO aiming to provide the microscale model with accurate initial and boundary conditions as a means to improve flow computations within and around elements of the urban canopy (Ehrhard et al., 2000). The main limitation of such approaches lies in their inability to incorporate fully bidirectional interaction between scales, i.e. the effect of microscale domains on the mesoscale calculations.

A full two-way mesoscale–microscale coupling scheme would ideally be able to account for the effect of small scale urban structures, to the extent represented by the microscale calculations, on the dispersion and chemical transformation of pollutants within the mesoscale domain. In this way, the influence of proposed interventions in the urban, local and street scales (e.g. land use changes, modification of local traffic patterns or interventions in the geometry of urban canopy) would all be accurately represented and incorporated in a multiscale assessment.

More recent modelling efforts to resolve obstacle-induced influences on the mesoscale structure of the urban atmospheric boundary layer, including one- and two-way mesoscale–microscale coupling, have been reviewed by Schlünzen et al. (2011). In its most advanced form, this kind of coupling involves an online interaction between the mesoscale and the microscale models during each mesoscale integration step, while the integration time of the microscale steady-state solution is kept to a minimum. In addition, the spatial interfaces between interacting models/scales still need to be carefully isolated by means of non-uniform grids, in order to prevent spurious reflections (Schroeder and Schlünzen, 2009). The use of non-uniform grids and differing integration timescales, however, comes with a significant computational cost that can become forbidding when trying to simulate extended urban agglomerations. Moreover, the interpretation of calculated fields over non-uniform grids in coupled multiscale applications can become extremely problematic, especially in the calculation of spatial or temporal spectra (Schlünzen et al., 2011).

Aiming to address the limitations which arise as a result of the physical disparities between the modelling scales affecting the urban canopy, a two-way scheme has been introduced for coupling the mesoscale model MEMO (Moussiopoulos et al., 1993) and the microscale model MIMO (Ehrhard et al., 2000), utilising a collection of interpolating metamodelling. The coupled system was evaluated in simulations of meteorological fields and the dispersion of air pollutants over the Greater Paris area during a multi-day wintertime case study.

## 2. Methodology

### 2.1. Interpolating metamodelling methodology

A set of interpolating functions (the so-called *metamodels*) is used to implement a two way coupling between the mesoscale model MEMO and the microscale model MIMO. The disturbances induced by the urban canopy on the mesoscale flow are represented as vertical profiles of perturbations of the wind and turbulent kinetic energy fields. For each mesoscale grid cell and in each simulation timestep, these perturbation profiles are re-calculated by means of a metamodel comprising of vertically stacked multi-dimensional interpolating functions (Tsegas et al., 2011). A radial-basis-function (RBF) neural-network formulation (Nabney, 2001) is used to implement each of the interpolating functions. Hence, the metamodel can be viewed as an interpolation scheme that given a state of “input” condition profiles  $x=(u_{in}^i, \alpha_{in}^i, E_{in}^i)$  provides the perturbed “output” state profiles  $y=(u_{out}^i, \alpha_{out}^i, E_{out}^i)$  which consist of the wind velocity ( $u$ ), wind direction ( $\alpha$ ) and turbulent kinetic energy (TKE,  $E$ ) vertical profiles. Both “input” and “output” profiles are discretised along the vertical direction on the mesoscale grid, with  $j$  denoting the corresponding vertical mesoscale layer. The “input” and “output” (perturbed) profiles are thought of as representing area averages of the corresponding parameters over the lateral inflow and outflow boundaries of a given microscale domain. Each of the six lateral boundaries is denoted by a “in” or “out” index, depending on the net sign of mass flow across that boundary, as shown in Fig. 1.

The metamodels are initially calibrated on the basis of explicit MIMO calculations. A set of  $N_{cal}$  microscale flow conditions is explicitly simulated with MIMO, each state representing a different combination of urban geometry and wind conditions. From the  $N_{cal}$  microscale simulations, a set of input and output calibration profiles  $(x_k^i, y_k^i)$ ,  $k=1..N_{cal}$  is obtained, which in turn is then used to calibrate the interpolating functions of each metamodel. The calibration process involves “training” the neural-network interpolators to provide the  $y_k^i$  profile when the corresponding  $x_k^i$  profile is given to them as input.

During the coupled operation of the model, the calibrated metamodel receives new “input” profiles  $(u_{in}^i, \alpha_{in}^i, E_{in}^i)$ . These new “input” profiles are interpolated based on values obtained from the neighbouring vector grid points of the eight nearest mesoscale

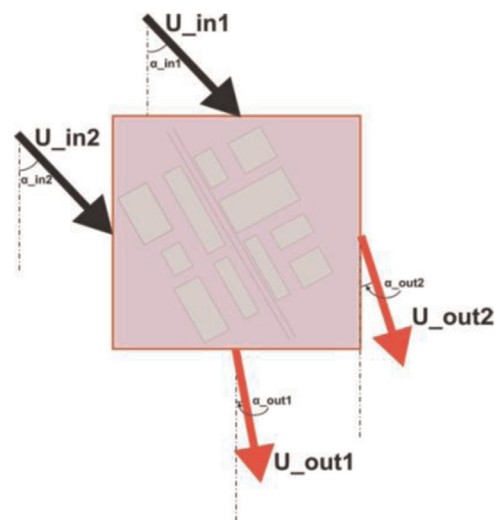


Fig. 1. Definition of the  $u_{in}$ ,  $u_{out}$  (scalar flow speed) and  $\alpha_{in}$ ,  $\alpha_{out}$  (flow deflection angle) of the corresponding metamodel “input” and “output” condition vectors, defined for a simple case of 2 inflow and 2 outflow lateral boundaries (cross-flow case). TKE components (not shown) are defined in an analogous fashion.

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