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Coupling regional and local air quality models for short-time prediction around punctual pollutant sources using finite elements

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ABSTRACT

Most Air Quality models are able to simulate the local influence of punctual pollutant emissions as those emitted from chimneys. This paper takes as a reference the CMAQ (Community Multiscale Air Quality) model, one of the most used. CMAQ model includes a Plume-in-Grid (PinG) model to simulate local emission sources. When CMAQ is coupled with a predictive meteorological model as MM5, it becomes a predictive tool for air quality. Therefore, the PinG model embedded with CMAQ can be used in order to predict air quality at local scale, however an improved approach is proposed here. CMAQ model is coupled with a Finite Element local air quality model. These kind of models approximate wind velocity field from provided data and simulates transport and reaction with a convection – diffusion – reaction finite element model. Here, a simplified version of that presented in [1] is used. Results of embedded local air quality models in regional ones can be useful for short-term predictions from few tens of meters to tens of kilometers around punctual emissions, including reaction with background substances or coupling between plumes of different punctual sources.

CMAQ model simulates transport and reaction of pollutants with the chemical – transport modeling system CCTM. It uses three different finite volume methods (Yamartino-Blackman cubic scheme, Bott scheme, and piecewise parabolic method) to solve pollutant transport and two models (CB4, RADM2) to represent chemical reactions. Domain is decomposed in a regular grid. Horizontal element size is in the range 8 to 32 kilometers, for square domains up to one thousand of kilometers each side. Total height, from 10 to 18 kilometers, is discretized in an unequally spaced sequence of 12 to 20 layers. Results of CMAQ simulations are mean values of unknows in central cell points of these volumes. Meteorological predictions from models as MM5 are used to feed CMAQ simulations. Standard time interval is one hour.

CMAQ model incorporate local effects throughout a PinG model. It adds the influence of local emissions to the regional scale. PinG model uses the Plume Dynamics Model (PDM) as a preprocessor of velocities at the local scale. PDM is used within CMAQ model to interpolate the wind field and to calculate which nodes will be crossed by the plume. To improve accuracy close to punctual pollutant sources, here, local scale is modeled by a Finite Element local air quality model. In order to couple CMAQ model with it, first of all, the role of the PDM is substituted by an interpolated three-dimensional wind velocity field covering all the domain. A tetrahedral mesh is computed, and the wind field is interpolated on all mesh nodes. Same mesh will be used to compute the transport and reaction part of the local model.

To mesh the atmospheric volume of interest, the following strategy, based on discretization by layers, is proposed:

- To start with a Digital Terrain Model (DTM) of the area of interest
- To follow the CMAQ layer approach as a guide to cover all height of the domain
- To smooth curvature on layers depending on height
- To calculate mesh element size distribution in each layer as function of curvature
- To mesh the three dimensional domain based on layer discretizations

Mean curvature in a layer is approximated by the Laplacian of the height field (by central differences with regular grid data or other techniques as quadratic fitting with non-regular mesh data [2]). Element size is computed from mean curvature and desired precision as explained in [3]. Layers above terrain are computed recursively with an iterative method which smoothes curvature. Smoothing curvature is important in order to increase appropriately element size in top layers.

Wind velocity field can be interpolated from CMAQ data following three major strategies: A linear interpolation, a consistent mass model approximation [4], and a 2.5 Navier-stokes approximation [5]. The linear interpolation is used here. 2-D Meterological data of the (CMAQ) coarse regular grid has been interpolated using linear shape functions. Once the data is know in the unknow nodes of the Finite Element tetrahedra mesh the typical log-linear equation is used to compute the wind velocity in all nodes. Final correction to project wind field to terrain surface is needed.

With wind velocity field known, a finite element model is used to simulate convection, diffusion and reaction of emitted pollutants on the area of interest. Concentrations given by CMAQ model are used as initial conditions of the Finite Element transport – reaction problem. As a first option, initial conditions are interpolated with a discontinuous approach, with the same value of the CMAQ central cell point for all the mesh nodes that are inside the cell. Diffusion rates, and deposition velocities are also interpolated from those used in CMAQ. At this point transport – reaction evolution is computed with the finite element model. Transport – reaction splitting is implemented in order to uncouple both processes following work presented in [1].

Proposed approach has been implemented with data from the example presented in the CMAQ model tutorial. Several time steps has been simulated with CMAQ model and then data is used to compute influence at the local scale of a fictitious chimney emission: A three-dimensional mesh is created, wind field, initial conditions and other data is interpolated, and transport and reaction is computed. First comparison of obtained result with those of PinG approach is encouraging.

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