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Adaptive finite element simulation of stack pollutant emissions over complex terrains

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ABSTRACT

A three-dimensional finite element model for the pollutant dispersion is presented. In these environmental processes over a complex terrain, a mesh generator capable of adapting itself to the topographic characteristics is essential. The first stage of the model consists on the construction of an adaptive tetrahedral mesh of a rectangular region bounded in its lower part by the terrain and in its upper part by a horizontal plane. Once the mesh is constructed, an adaptive local refinement of tetrahedra is used in order to capture the plume rise. Wind measurements are used to compute an interpolated wind field, that is modified by using a mass-consistent model and perturbing its vertical component to introduce the plume rise effect. Then, we use an Eulerian convection–diffusion–reaction model to simulate the pollutant dispersion. In this work, the transport of pollutants is considered and dry deposition is formulated as a boundary condition. The discretization of the stack geometry allows to define the emissions as boundary conditions. The proposed model uses an adaptive finite element space discretization, a Crank-Nicolson time scheme, and a splitting operator. This approach has been applied in La Palma island. Finally, numerical results and conclusions are presented.

1. Introduction

Numerical simulation of pollutant transport and reaction on atmosphere has been the result of important advances in the last thirty years. However, nowadays it remains as a scientific challenge. Key analysis is related to acid rain, ozone, particle matter and toxic emissions [1]. Air quality modelling systems mainly involve three components: emissions, meteorology and transport–chemistry. The first component characterizes different emission sources of chemical compounds [2], the second one determines the atmospheric phenomena as wind and temperature fields, and the third one simulates the transport of pollutants (convection and diffusion) and their chemical reactions.

Environmental Protection Agency (www.epa.gov) classifies Air Quality Modelling Systems as Dispersion, Photochemical and Receptor models. Dispersion models estimate pollutant concentrations at ground level near a punctual source. Photochemical models consider all the sources in a large area. Receptor models identify and characterize the emission sources using receptor measures.

Main dispersion models include Gaussian plume models [3], particle tracking models [4], and puff models [5–7]. The two latters models are based on a Lagrangian approach and usually include first order chemistry reactions or linearised photochemical-reaction models. Versions with complex non-linear photochemical-reaction models have been also developed [8].

In contrast with dispersion models, photochemical ones follow an Eulerian description of the coupled transport and hydrodynamic problem. Most of these Eulerian models approximate the solution to this problem by using finite difference schemes. The modelling domains usually vary from about few thousands to tens of kilometres, and the grid spatial discretization varies from about tens of kilometres to 1 km using nested sub-grids [9–11]. The height of the computational domain usually varies from 4 up to 10 km with a non-uniform vertical discretization between 10 and 20 levels.

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Vertical spatial resolution ranges from few tens metres close to the ground level to one thousand metres above 2 km over the terrain. The number of grid points in this kind of problems can vary from tens to hundreds thousand. The most advanced photochemical models consider local emissions and are known as Plume in Grid (PIG). For this purpose, CAMx [12] and CMAQ [13] include a puff model, and UAM-V [14] uses a plume model.

In environmental management, dispersion and photochemical models have very different applications. The first ones are usually applied to local emission impact assessments, and the second ones to regional planning and monitoring. Both models have a clearly different application scale and photochemical reaction complexity. However, because of the great coupling among key components as ozone, nitrogen compounds, and Volatile Organic Components [15,16], and due to the awareness about the socio-economic impacts of their immission [17–19], some references about the need of coupling local emissions using regional planning with Plume in Grid photochemical models can be found [9,10,20]. Although Plume in Grid models can couple local scales (up to a resolution of 1 km) with regional scales, several limitations have been reported [9]. For example, it is clear that this local high resolution can be insufficient for complex terrains. Thus, the search of alternatives is justified.

In this paper, we present a new methodology for local scale air quality simulations by using a non-steady finite element method with unstructured and adaptive tetrahedral meshes. The aim of this proposal is to introduce an alternative to the standard implementation of current models, improving the computational cost of methods that use structured meshes [21].

Three remarkable uses of unstructured meshes in atmospheric pollution problems are the two-dimensional regional–global examples presented in Lagzi et al., [22], Ahmad et al. [23], the three-dimensional regional examples, including local refinement with element sizes of 2 km, presented in Tomlin et al. [24], and the three-dimensional tetrahedral meshes for local wind field analysis with element sizes ranging from 2 m up to 2 km, see Montenegro et al. [25], Montero et al. [26]. The ideas of this last approach are considered to determine the wind field, that includes the effect of the plume rise, used in the air quality problem.

The wind field is crucial for the pollutant transport, specially in complex terrain areas. In order to simulate it, we have used a mass-consistent model. Several two-dimensional [27] and three-dimensional [28–30] adaptive finite element solutions have been developed by the authors.

The convection, diffusion and reaction problem is usually solved using splitting schemes [31,32] and specific numerical solvers for time integration of photochemical reaction terms [23,33,34]. A non-steady and non-linear transport model is presented in this paper. A stabilized finite element formulation, specifically Least-Squares, with a Crank-Nicolson temporal integration is proposed to solve the problem [35,36]. The chemistry is simulated by using the RIVAD/ARM3. This is a very simplistic empirical chemistry model used in codes such as CALPUFF [37] and is employed here as a proof of concept. More complete chemistry models will be included in future work. The transport and chemical terms are treated separately with Strang splitting operators [38]. The non-linear chemical part is solved node by node with a second order Rosenbrock method [39]. A previous description of the proposed procedure can be found in Pérez-Foguet et al. [40].

In the second Section of the paper we describe the proposed methodology. It mainly involves the following steps: an automatic tetrahedral mesh generator, the wind field simulation, the plume rise approximation and the air pollution simulation. In the third Section we apply the proposed air quality model in La Palma island (Canary Islands, Spain).

2. Wind and air pollution modelling

In this section we introduce the models to simulate the wind field and the transport and reaction of pollutants. The evaluation of the wind field is based on a mass-consistent model, while the transport of pollutant is calculated by a convection–diffusion–reaction PDE by using a non-linear chemical model. The proposed methodology is summarized in Algorithm 1.

Algorithm 1. Wind and air pollution modelling.

1: Construct an adaptive tetrahedral mesh of the domain
  1.1: Adaptive discretization of the terrain surface
  1.2: Vertical spacing function and 3D distribution of points
  1.3: Three-dimensional mesh generation
  1.4: Mesh optimisation
2: Wind field simulation from experimental or forecasting data
  2.1: Construction of the initial interpolated wind field
  2.2: Approximation of the wind field with a mass-consistent model
3: Wind field modification including the plume rise effect
  3.1: Compute a plume rise trajectory
  3.2: Mesh refinement along the plume rise trajectory
  3.3: Simulate a wind field in the new mesh (applying step 2)
  3.4: Modify vertical components of the wind field along the plume rise
4: Air pollution simulation from stack emission data

The paper is organised as follows. In Section 2 we describe the main steps of the proposed methodology. Results are shown in Section 3, and finally the conclusions and future work are presented in Section 4.

2.1. Automatic tetrahedral mesh generation

The studied domain is limited at the bottom by the terrain and at the top by a horizontal plane. The lateral walls are formed by four vertical planes. A uniform distribution of nodes is defined on the upper boundary. A refinement/derefinement algorithm [41] is applied on this uniform mesh to construct a node distribution adapted to the terrain surface and stacks. Once the node distribution is defined both on the terrain and the upper boundary, we distribute the nodes located between both layers by using a vertical spacing function. Next, a three-dimensional mesh generator based on Delaunay triangulation [42] is applied. Finally, the untangling and smoothing procedure described in [43] is used to get a valid mesh and to improve its quality. A detailed description of the mesh generation procedure can be seen in [44,45].

2.2. Wind field simulation

Once the tetrahedral mesh is constructed, we consider a mass-consistent model [28–30] to compute a wind field u in the three-dimensional domain Ω, with a boundary $\Gamma = \Gamma_a \cup \Gamma_b$, that verifies the continuity equation (mass conservation) for constant density and the impermeability condition on the terrain Γ_a,

$$\begin{aligned} \nabla\cdot\mathbf{u} &= 0 \quad \text{in} \quad \Omega \\ \mathbf{n}\cdot\mathbf{u} &= 0 \quad \text{on} \quad \Gamma_a \end{aligned} \tag{1}$$

where n is the outward-pointing normal unit vector.

The model formulates a Least-Squares problem in the domain Ω to find a wind field $\mathbf{u} = (u,v,w)$, such that it is adjusted as much as possible to an interpolated wind field $\mathbf{u}_0 = (u_0,v_0,w_0)$. The wind field u verifies the Euler–Lagrange equation,

$$\mathbf{u} = \mathbf{u}_0 + \mathbf{P}^{-1}\nabla\phi \tag{2}$$

where ϕ is the Lagrange multiplier, $\mathbf{P}$ is a 3×3 diagonal matrix with $P_{1,1} = P_{2,2} = 2\alpha_1^2$ and $P_{3,3} = 2\alpha_2^2$, being α_1 and α_2 constant in Ω.