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A finite difference model for air pollution simulation

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Abstract

A 3-D model for atmospheric pollutant transport is proposed considering a set of coupled convection–diffusion–reaction equations. The convective phenomenon is mainly produced by a wind field obtained from a 3-D mass consistent model. In particular, the modelling of oxidation and hydrolysis of sulphur and nitrogen oxides released to the surface layer is carried out by using a linear module of chemical reactions. The dry deposition process, represented by the so-called deposition velocity, is introduced as a boundary condition. Moreover, the wet deposition is included in the source term of the governing equations using the washout coefficient. Before obtaining a numerical solution, the problem is transformed using a terrain conformal coordinate system. This allows to work with a simpler domain in order to build a mesh that provides finite difference schemes with high spatial accuracy. The convection–diffusion–reaction equations are solved with a high order accurate time-stepping discretization scheme which is constructed following the technique of Lax and Wendroff. Finally, the model is tested with a numerical experiment in La Palma Island (Canary Islands).

Keywords: Wind modelling; Mass consistent models; Air pollution modelling; Eulerian model; Finite differences; Accurate time-stepping

1. Introduction

The difficulty for developing a complete understanding of environmental impacts taking into account few measures of atmospheric phenomena arises from the complexity of atmospheric physical and chemical processes, the spatial dimension of the atmosphere and the time scaling of the episodes. Numerical simulations of the atmosphere play an important role in reaching a more complete understanding of environmental impacts. In this paper, a numerical model for wind and air pollution simulation is proposed. On the one hand, the wind computation is carried out using a mass consistent model which is based on the mass conservation law, several measures of wind velocities at different points of the domain and the physics of the atmosphere [1]. More details about the general procedure and mathematical supports for this kind of models, with particular reference to the approximations that characterize them, may be seen in [2]. On the other hand, an Eulerian model is proposed for the resolution of pollutant concentrations. This model is based on the convection–diffusion–reaction equation of pollutant species and includes emission sources, dry and wet depositions and chemical reactions; see, e.g. [3].

In this paper, we have used the finite difference method in spite of other discretization techniques, like finite element or finite volume methods, are also suitable. The finite difference method is based on local approximations of the partial derivatives in a PDE, which are derived by low order Taylor series expansions. In general, this method is quite simple to define and rather easy to implement. Also, it is particularly appealing for simple regions, such as the cube obtained in our model after a terrain conformal coordinate transformation. In addition, it is profitable if meshes are uniform, e.g., the structured meshes used here with regular horizontal and variable vertical discretization. The matrices that result from this technique are often well structured and they typically consist of a few nonzero diagonals. Another advantage is that there are a number of *fast solvers* for constant coefficient problems, which can deliver the solution in logarithmic time per grid point, i.e., the

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total number of operations is of the order of $n\log n$, being n the total number of discretization points. Finally, the finite difference method has been chosen since the advantage of other discretization techniques, in terms of accuracy, for structured meshes is not considerable. Nevertheless, for unstructured and adaptive meshes the finite element method is preferred. We have obtained preliminary results with this method related to wind modelling [4,5].

In Section 2, the mass consistent model for wind field adjustment is summarized, including the governing equations, the transformation to a terrain coordinate system and the construction of the interpolated wind. Section 3 is devoted to the air pollution model. In addition to the convection–diffusion–reaction equation, a detailed study of the emissions, chemical reactions and wet deposition is presented. Also a high order accurate time-stepping scheme is proposed in Section 3. The finite difference schemes for the spatial discretization is defined in Section 4. In order to illustrate the performance of the model, in Section 5 a numerical experiment is carried out. Finally, conclusions are presented in Section 6.

2. Wind field approach

We look for a wind velocity field that satisfies the continuity equation and non-flow-through conditions on the terrain Γ_b, respectively

$$\vec{\nabla}\cdot\vec{u} = 0 \quad \text{in } \Omega \tag{1}$$

$$\vec{n}\cdot\vec{u} = 0 \quad \text{on } \Gamma_b \tag{2}$$

assuming that the air density is constant in the whole domain. In addition, the computed wind field $\vec{u}(\widetilde{u},\widetilde{v},\widetilde{w})$ must be as close to an observed one $\vec{v}_0(u_0,v_0,w_0)$ as possible. So a least-square problem is formulated in the domain Ω, such that the wind field is adjusted to an initial wind field obtained from experimental measures,

$$E(\tilde{u},\tilde{v},\tilde{w}) = \int_\Omega [\alpha_1^2((\tilde{u}-u_0)^2+(\tilde{v}-v_0)^2)+\alpha_2^2(\tilde{w}-w_0)^2]\mathrm{d}\Omega \tag{3}$$

where α_1 and α_2 are the Gauss precision moduli which are the weights of the horizontal and vertical adjustments of the wind velocity components. In fact, if $\alpha_1 \gg \alpha_2$, flow adjustment in the vertical direction predominates, so that wind is more likely to go over a terrain barrier rather than around it. However, if $\alpha_1 \gg \alpha_2$, flow adjustment occurs primarily in the horizontal plane, so that air is more likely to go around a terrain barrier rather than over it. See for example [5,7].

To solve problem (3) is equivalent to find a saddle point $(\vec{v},\phi)$ of Lagrangian [6],

$$\Upsilon(\vec{v}) = \min_{\vec{u}\in K} E(\vec{u}) + \int_\Omega \phi\vec{\nabla}\cdot\vec{u}\mathrm{d}\Omega \tag{4}$$

The technique of Lagrange multipliers allows to solve problem (4) and yields the Euler–Lagrange equations,

$$u = u_0 + T_h\frac{\partial\phi}{\partial x} \tag{5}$$

$$v = v_0 + T_h\frac{\partial\phi}{\partial y} \tag{6}$$

$$w = w_0 + T_v\frac{\partial\phi}{\partial z} \tag{7}$$

where ϕ is the Lagrange multiplier and $T=(T_h,T_h,T_v)$ is the diagonal transmissivity tensor,

$$T_h = \frac{1}{2\alpha_1^2} \quad \text{and} \quad T_v = \frac{1}{2\alpha_2^2} \tag{8}$$

As α_1 and α_2 are constant in Ω, the variational approach results in an elliptic equation by substituting Eqs. (5)–(7) in (1),

$$\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}+\frac{T_v}{T_h}\frac{\partial^2\phi}{\partial z^2} = -\frac{1}{T_h}\left(\frac{\partial u_0}{\partial x}+\frac{\partial v_0}{\partial y}+\frac{\partial w_0}{\partial z}\right) \tag{9}$$

with Dirichlet boundary conditions on flow-through boundaries and Neumann boundary conditions on the terrain and top,

$$\phi = 0 \quad \text{on } \Gamma_a \tag{10}$$

$$\vec{n}\cdot T\vec{\nabla}\phi = -\vec{n}\cdot\vec{v}_0 \quad \text{on } \Gamma_b \tag{11}$$

2.1. Terrain conformal coordinates

We propose the following conformal coordinate transformation which reduces the three-dimensional domain to a $1\times1\times1$ cube Ω', where the terrain is now represented as a horizontal plane,

$$\xi = \frac{x}{x_l}, \quad \eta = \frac{y}{y_l} \quad \text{and} \quad \sigma = \frac{z-z_s}{z_t-z_s} = \frac{z-z_s}{\pi} \tag{12}$$

Here, $z_s(x,y)$ is a function which defines the terrain topography, z_t is the maximum height and both x_l and y_l are the maximum horizontal lengths of the domain. Denoting $\pi = z_t - z_s$, Eq. (8) becomes to

$$\begin{aligned}
&\frac{\pi}{x_l^2}\frac{\partial^2\phi}{\partial\xi^2}+\frac{\pi}{y_l^2}\frac{\partial^2\phi}{\partial\eta^2}+\left[\frac{(\sigma-1)^2}{\pi}\left(\left(\frac{\partial z_s}{\partial x}\right)^2+\left(\frac{\partial z_s}{\partial y}\right)^2\right)+\frac{T_v}{T_h}\frac{1}{\pi}\right]\frac{\partial^2\phi}{\partial\sigma^2}\\
&\quad+2(\sigma-1)\left[\frac{1}{x_l}\frac{\partial z_s}{\partial x}\frac{\partial^2\phi}{\partial\xi\partial\sigma}+\frac{1}{y_l}\frac{\partial z_s}{\partial y}\frac{\partial^2\phi}{\partial\eta\partial\sigma}\right]\\
&\quad+(\sigma-1)\left[\frac{\partial^2 z_s}{\partial x^2}+\frac{\partial^2 z_s}{\partial y^2}+\frac{2}{\pi}\left(\left(\frac{\partial z_s}{\partial x}\right)^2+\left(\frac{\partial z_s}{\partial y}\right)^2\right)\right]\frac{\partial\phi}{\partial\sigma}\\
&\quad=-\frac{1}{T_h}\left[\pi\left(\frac{1}{x_l}\frac{\partial u_0}{\partial\xi}+\frac{1}{y_l}\frac{\partial v_0}{\partial\eta}\right)+(\sigma-1)\left(\frac{\partial u_0}{\partial\sigma}\frac{\partial z_s}{\partial x}+\frac{\partial v_0}{\partial\sigma}\frac{\partial z_s}{\partial y}\right)+\frac{\partial w_0}{\partial\sigma}\right]
\end{aligned} \tag{13}$$

Finally, using the conformal transformation, boundary conditions (10) and (11) result

$$\phi = 0 \quad \text{on } \Gamma_a \tag{14}$$

$$\frac{\partial\phi}{\partial\sigma} = 0 \quad \text{on } \Gamma_{b_1} \tag{15}$$

$$\frac{\partial\phi}{\partial\sigma} = \frac{\frac{\pi}{T_h}\left[\left(u_0+T_h\frac{1}{x_l}\frac{\partial\phi}{\partial\xi}\right)\frac{\partial z_s}{\partial x}+\left(v_0+T_h\frac{1}{y_l}\frac{\partial\phi}{\partial\eta}\right)\frac{\partial z_s}{\partial y}-w_0\right]}{\left(\frac{\partial z_s}{\partial x}\right)^2+\left(\frac{\partial z_s}{\partial y}\right)^2+\frac{T_v}{T_h}} \quad \text{on } \Gamma_{b_0} \tag{16}$$

where Γ_a is related to the vertical faces of the cube, $\Gamma_{b_1}(\sigma=1)$ is the top and $\Gamma_{b_0}(\sigma=0)$ is the bottom.