A 3-D high-order accurate time-stepping scheme for air pollution modelling

N. Sanín[1] G. Montero[1]

Abstract

In this work a 3-D model for pollutant transport in the atmosphere is proposed. We consider a set of coupled convection-diffusion equations including the reactions of the pollutant species. In particular, the modelling of oxidation and hydrolysis of sulphur and nitrogen oxides released to the surface layer is studied. The convective phenomenon is mainly produced by the wind field which is obtained from a 3-D mass consistent model. The dry deposition process is represented by the so-called deposition velocity, which is proportional to the degree of absorptivity of the surface, and it is assumed as constant along the vertical flow, and thus, it is introduced as a boundary condition. The wet deposition is simulated by a source term in the convection-diffusion equations using the washout coefficient. To obtain a numerical solution, first, the problem is transformed using a conformal coordinates system. This allows us to work with a simpler domain in order to build a mesh that provides high consistency for finite difference schemes. Then, the convection-diffusion equations are solved using a high order time discretization with a finite differences scheme.

1 Wind field approach

The continuity equation and the impermeability conditions on the terrain Γ_b are,

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

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

assuming that the air density is constant in the whole domain. We formulate a least-square problem in the domain Ω with the wind $\vec{u}(\tilde{u}, \tilde{v}, \tilde{w})$ to be adjusted and the observed wind $\vec{v}_0(u_0, v_0, w_0)$,

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

with α_1 and α_2 being the Gauss precision moduli. The solution $\vec{v}\,(u, v, w)$ is equivalent to find a saddle point $(\vec{v}, \phi)$ of Lagrangian [13]

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

Lagrange multiplier technique is used to minimize problem (4), whose minimum comes to form the Euler-Lagrange equations,

$$u = u_0 + T_h \frac{\partial \phi}{\partial x}, \quad v = v_0 + T_h \frac{\partial \phi}{\partial y}, \quad w = w_0 + T_v \frac{\partial \phi}{\partial z}, \tag{5}$$

where ϕ is the Lagrange multiplier and $T = (T_h, T_h, T_v)$ is the diagonal transmission tensor, with $T_h = \frac{1}{2\alpha_1^2}$ and $T_v = \frac{1}{2\alpha_2^2}$. As α_1 and α_2 are constant in Ω, the variational approach results in an elliptic equation in ϕ, by substituting (5) in (1),

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{T_v}{T_h}\frac{\partial^2 \phi}{\partial z^2} = -\frac{1}{T_h}\left(\frac{\partial u_0}{\partial x} + \frac{\partial v_0}{\partial y} + \frac{\partial w_0}{\partial z}\right) \quad \text{in } \Omega \tag{6}$$

The boundary conditions result as follows (Dirichlet condition on permeable boundaries and Neumann condition on terrain and top),

$$\phi = 0 \quad \text{on} \quad \Gamma_a \tag{7}$$

$$\vec{n} \cdot T \vec{\nabla} \mu = -\vec{n} \cdot \vec{v}_0 \quad \text{on } \Gamma_b \tag{8}$$

1.1 Terrain conformal coordinates

We propose the following conformal coordinate transformation which reduces the tridimensional domain to an unitary cube Ω', where the terrain is now a horizontal plane,

$$\xi = \frac{x}{x_l}, \quad \eta = \frac{y}{y_l}, \quad \sigma = \frac{z - z_s}{z_t - z_s} \tag{9}$$

Here, $z_s(x, y)$ is the function which define the terrain topography, z_t is the maximum height and both x_l, y_l are the maximum horizontal dimensions of the domain. Let denote $\pi = z_t - z_s$. Then equation (6) becomes to

$$\begin{aligned}
&\frac{\pi}{x_l^2}\frac{\partial^2 \phi}{\partial \xi^2} + \frac{\pi}{y_l^2}\frac{\partial^2 \phi}{\partial \eta^2} + \left[\frac{(\sigma-1)^2}{\pi}\left(\left(\frac{\partial z_s}{\partial x}\right)^2 + \left(\frac{\partial z_s}{\partial y}\right)^2\right) + \frac{1}{\pi}\frac{T_v}{T_h}\right]\frac{\partial^2 \phi}{\partial \sigma^2} \\
&+2(\sigma - 1)\left[\frac{1}{x_l}\frac{\partial z_s}{\partial x}\frac{\partial^2 \phi}{\partial \xi \partial \sigma} + \frac{1}{y_l}\frac{\partial z_s}{\partial y}\frac{\partial^2 \phi}{\partial \eta \partial \sigma}\right] \\
&+(\sigma - 1)\left[\frac{\partial^2 z_s}{\partial x^2} + \frac{\partial^2 z_s}{\partial y^2} + \frac{2}{\pi}\left(\left(\frac{\partial z_s}{\partial x}\right)^2 + \left(\frac{\partial z_s}{\partial y}\right)^2\right)\right]\frac{\partial \phi}{\partial \sigma} \\
= &-\frac{\pi}{T_h}\left(\frac{1}{x_l}\frac{\partial u_0}{\partial \xi} + \frac{1}{y_l}\frac{\partial v_0}{\partial \eta}\right) \qquad (10) \\
&-\frac{1}{T_h}\left[(\sigma - 1)\left(\frac{\partial u_0}{\partial \sigma}\frac{\partial z_s}{\partial x} + \frac{\partial v_0}{\partial \sigma}\frac{\partial z_s}{\partial y}\right) + \frac{\partial w_0}{\partial \sigma}\right] \quad \text{in } \Omega' \qquad (11)
\end{aligned}$$

With the conformal transformation, the boundary conditions (7) and (8) yield

$$\phi = 0 \quad \text{on } \Gamma'_a \tag{12}$$

$$\frac{\partial \phi}{\partial \sigma} = 0 \text{ on } \Gamma'_{b1} \tag{13}$$

$$\frac{\partial \phi}{\partial \sigma} = \frac{\frac{\pi}{T_h}\left[\left(u_0 + \frac{1}{x_l}\frac{\partial \phi}{\partial \xi}\right)\frac{\partial z_s}{\partial x} + \left(v_0 + \frac{1}{y_l}\frac{\partial \phi}{\partial \eta}\right)\frac{\partial z_s}{\partial y} - w_0\right]}{\left[\left(\frac{\partial z_s}{\partial x}\right)^2 + \left(\frac{\partial z_s}{\partial y}\right)^2\right] + \frac{T_v}{T_h}} \text{ on } \Gamma'_{b0} \tag{14}$$

Γ'_a being to the vertical faces of the boundary, Γ'_{b1} ($\sigma = 1$) the top and Γ'_{b0} ($\sigma = 0$) the bottom.

1.2 Initial wind profile

The most common technique of horizontal interpolation is formulated as a function of the inverse of the squared distance between the point and the station [8].

$$\vec{\mathbf{v}}_0(z_m) = \varepsilon \frac{\sum_{n=1}^{N} \frac{\vec{\mathbf{v}}_n}{d_n^2}}{\sum_{n=1}^{N} \frac{1}{d_n^2}} + (1-\varepsilon) \frac{\sum_{n=1}^{N} \frac{\vec{\mathbf{v}}_n}{|\Delta h_n|}}{\sum_{n=1}^{N} \frac{1}{|\Delta h_n|}} \tag{15}$$

The value of $\vec{v}_n$ is the velocity observed at station n, N is the number of stations considered in the interpolation, d_n is the horizontal distance from station n to the point of the domain where we are computing the wind velocity, $|\Delta h_n|$ is the height difference between station n and the studied point, and ε is a weighting parameter ($0 \leq \varepsilon \leq 1$), which allows to give more importance to one of these criteria.

In this work, a log-linear wind profile is considered [3] in the surface layer, which takes into account the horizontal interpolation [8] and the effect of roughness on the wind intensity and the direction. These values also depend on the air stability (neutral, stable or unstable atmosphere) according to the Pasquill stability class. Above the surface layer, a linear interpolation is carried out using the geostrophic wind. The logarithmic profile is given by,

$$\vec{\mathbf{v}}_0(z) = \frac{\vec{\mathbf{v}}^*}{k}\left(\log\frac{z}{z_0} - \Phi_m\right) \qquad z_0 < z \leq z_{sl} \tag{16}$$

where $\vec{v}^*$ is the friction velocity, k is von Karman's constant, z_0 is the roughness length [5] and z_{sl} is the height of the surface layer. Φ_m depends on the air stability,

$$\begin{aligned} \Phi_m &= 0 && \text{(neutral atmosphere)} \\ \Phi_m &= -5\frac{z}{L} && \text{(stable atmosphere)} \\ \Phi_m &= \log\left[\left(\frac{\theta^2+1}{2}\right)\left(\frac{\theta+1}{2}\right)^2\right] - 2\arctan\theta + \frac{\pi}{2} && \text{(unstable atmosphere)} \end{aligned} \tag{17}$$

where, $\theta = (1 - 16\frac{z}{L})^{1/4}$ and $\frac{1}{L} = a z_0^b$, with a, b, depending on the Pasquill stability class (see e.g. [14]). The friction velocity is obtained at each point from the interpolated measurements at the height of the stations(horizontal interpolation),

$$\vec{\mathbf{v}}^* = \frac{k\ \vec{\mathbf{v}}_0(z_m)}{\log \dfrac{z_m}{z_0} - \Phi_m} \tag{18}$$

The height of boundary layer z_{pbl} above the ground is chosen such that the wind intensity and direction are constant at that height,

$$z_{pbl} = \frac{\gamma\ |\vec{\mathbf{v}}^*|}{f} \tag{19}$$

where $f = 2\Omega \sin\phi$ is the Coriolis parameter (Ω is the earth rotation and ϕ the latitude), and γ is a parameter depending on the atmospheric stability, and being between 0.15 and 0.3. The height of the mixed layer h is considered to be equal to z_{pbl} in neutral and unstable conditions. In stable conditions, it is approximated by

$$h = \gamma' \sqrt{\frac{|\vec{\mathbf{v}}^*|\ L}{f}} \tag{20}$$

where $\gamma' = 0.4$. The height of surface layer is $z_{sl} = \frac{h}{10}$. From z_{sl} to z_{pbl}, a linear interpolation with geostrophic wind $\vec{v}_g$ is carried out,

$$\vec{\mathbf{v}}_0(z) = \rho(z)\,\vec{\mathbf{v}}_0(z_{sl}) + [1-\rho(z)]\vec{\mathbf{v}}_g \qquad z_{sl} < z \leq z_{pbl} \tag{21}$$

$$\rho(z) = 1 - \left(\frac{z - z_{sl}}{z_{pbl} - z_{sl}}\right)^2 \left(3 - 2\frac{z - z_{sl}}{z_{pbl} - z_{sl}}\right) \tag{22}$$

Finally, this model assumes $\vec{v}_0(z) = \vec{v}_g$ if $z > z_{pbl}$ and $\vec{v}_0(z) = 0$ if $z \leq z_0$.

2 Air pollution modelling

In an Eulerian model, the transport-diffusion equation for a pollutant specie i is formulated as (see e.g. [2]),

$$\frac{\partial c_i}{\partial t} + \vec{\mathbf{v}}\cdot\vec{\nabla} c_i - \vec{\nabla}\cdot(\mathbf{K}_i\vec{\nabla} c_i) = f_i \qquad i = 1,...,p, \qquad \text{in } \Omega \tag{23}$$

where p is the number of pollutant species, $c_i = c_i(x_1, x_2, x_3, t)$ represents the average concentration of pollutant i, $\vec{v}$ is the wind speed arising from the previous model, $K_i = [K_{i1}(x_1,x_2,x_3),\ K_{i2}(x_1,x_2,x_3),\ K_{i3}(x_1,x_2,x_3)]$ is the diagonal tensor of diffusivity and $f_i = f_i(c_1, c_2, ..., c_p)$ is the source term. We suppose that the initial value of c_i, $i = 1, ..., p$, is known in Ω,

$$c_i(x_1,x_2,x_3,0) = c_i^0(x_1,x_2,x_3) \qquad i = 1,...,p, \qquad \text{in } \Omega \tag{24}$$

as well as the boundary conditions on Γ_a and Γ_b,

$$c_i = C_i(x_1,x_2,x_3,t) \qquad i = 1,...,p, \qquad \text{en } \Gamma_a \tag{25}$$

$$-\vec{\mathbf{n}}\cdot\mathbf{K}_i\vec{\nabla} c_i = 0 \qquad i = 1,...,p, \qquad \text{en } \Gamma_{b1} \tag{26}$$

$$-\vec{\mathbf{n}}\cdot\mathbf{K}_i\vec{\nabla} c_i = v_{di}\, c_i \qquad i = 1,...,p, \qquad \text{en } \Gamma_{b0} \tag{27}$$

where v_{di} is the velocity of dry deposition on the terrain. In general, C_i will be considered equal to zero or to the environmental value.

2.1 The source of pollutants

If the chemistry of the species and the wet deposition are taken into account in the model, the source term of equation (23) becomes to [12],

$$f_i = E_i + R_i + P_i = E_i + \sum_{j=1}^{p} \alpha_{ij}\, c_j \tag{28}$$

where $E_i(x_1, x_2, x_3, t)$ is the direct emission of specie i, $R_i(x_1, x_2, x_3, t)$ represents the variation of the concentration of specie i due to chemical reactions and $P_i(x_1, x_2, x_3, t)$ its elimination by the precipitations (wet deposition). This model assumes that R_i and P_i are lineal. The emission of a chimney located at (x_{01}, x_{02}, x_{03}) has been approached by,

$$E_i = \frac{e_{i_0}(t)}{s_1 s_2 s_3 \sqrt{(2\pi)^3}} \exp\left[-\frac{1}{2}\left(\left(\frac{x_1 - x_{01}}{s_1}\right)^2 + \left(\frac{x_2 - x_{02}}{s_2}\right)^2 + \left(\frac{x_3 - x_{03}}{s_3}\right)^2\right)\right] \tag{29}$$

We have considered NO_x, HNO_3, SO_2 and H_2SO_4 as significant species, and simplified the nonlinear module of reactions [10]. This leads to linear terms (see e.g. [7]),

$$R_{NO_x} = \overline{\alpha}_{NO_x,NO_x}\, c_{NO_x} \tag{30}$$

$$R_{HNO_3} = -\overline{\alpha}_{NO_x,NO_x}\, c_{NO_x} \tag{31}$$

$$R_{SO_2} = \overline{\alpha}_{SO_2,SO_2}\, c_{SO_2} \tag{32}$$

$$R_{H_2SO_4} = -\overline{\alpha}_{SO_2,SO_2}\, c_{SO_2} \tag{33}$$

with $\overline{\alpha}_{NO_x,NO_x} = -2\,k_1\,k_2$ and $\overline{\alpha}_{SO_2,SO_2} = -2\,\frac{k_1 k_3}{k_2}$, where k_1, k_2 and k_3 are kinetic parameters corresponding to,

1. $NO_2 + h \cdot v \rightarrow NO + O\cdot$
2. $OH \cdot + NO_2 \rightarrow HNO_3$
3. $OH \cdot + SO_2 \rightarrow HOSO_2$

The wet deposition is a linear term too,

$$P_i = -\frac{v_{wi}}{h}\, c_i \tag{34}$$

being h the average mixed layer and v_{wi} the velocity of wet deposition defined by

$$v_{wi} = w_{ri}\, p_0 \tag{35}$$

where w_{ri} is the proportion between the concentration of precipitated materia and the concentration of materia in the air on the surface, and p_0 is the intensity of precipitation. Thus, the coefficients of equation (28) become to,

$$\alpha_{ij} = \overline{\alpha}_{ij} \text{ if } j \neq i \quad \text{and } \alpha_{ii} = \overline{\alpha}_{ii} - \frac{v_{wi}}{h} \tag{36}$$

2.2 Taylor Galerkin formulation

Following the technique developed by Lax and Wendroff [4], a general formulation for the convection-diffusion-reaction equation is proposed. It is based on a high order time discretization by means of the Taylor's span. Thus, we have for the specie i,

$$c_i^{n+1} = c_i^n + \Delta t \left.\frac{\partial c_i}{\partial t}\right|_n + \frac{\Delta t^2}{2} \left.\frac{\partial^2 c_i}{\partial t^2}\right|_{n+\theta} + O(\Delta t^3) \qquad 0 \leq \theta \leq 1 \tag{37}$$

From equation (23), the first time derivative $\frac{\partial c_i}{\partial t}$ may be expressed in terms of spatial derivatives, and also $\frac{\partial^2 c_i}{\partial t^2}$ may be approached from the time derivation of equation (23) (see e.g. [1]). The new formulation of equation (37) results,

$$\begin{aligned}
&\left[1 - \tfrac{\Delta t^2}{6}\left((\vec{v}\cdot\vec{\nabla})\vec{v}\cdot\vec{\nabla} + \vec{v}\cdot(\vec{v}\cdot\vec{\nabla})\vec{\nabla}\right) - \Delta t \mathbf{K}_i \nabla^2\right] \\
&\left(\tfrac{c_i^{n+1}-c_i^n}{\Delta t}\right) - \left[\tfrac{\Delta t}{2}\alpha_{i1} - \tfrac{5}{12}\Delta t^2 \alpha_{i1}\vec{v}\cdot\vec{\nabla}\right]\left(\tfrac{c_1^{n+1}-c_1^n}{\Delta t}\right) \\
&- \left[\tfrac{\Delta t}{2}\alpha_{i2} - \tfrac{5}{12}\Delta t^2 \alpha_{i2}\vec{v}\cdot\vec{\nabla}\right]\left(\tfrac{c_2^{n+1}-c_2^n}{\Delta t}\right) \\
= \; & -\vec{v}\cdot\vec{\nabla}c_i^n + \tfrac{\Delta t}{2}(\vec{v}\cdot\vec{\nabla})\vec{v}\cdot\vec{\nabla}c_i^n + \tfrac{\Delta t}{2}\vec{v}\cdot(\vec{v}\cdot\vec{\nabla})\vec{\nabla}c_i^n \\
&- \tfrac{\Delta t}{2}\left(\mathbf{K}_i\nabla^2\vec{v}\right)\cdot\vec{\nabla}c_i^n + \tfrac{\Delta t^2}{6}\vec{v}\cdot\vec{\nabla}\left(\vec{v}_t\cdot\vec{\nabla}c_i^n\right) + \mathbf{K}_i\nabla^2 c_i^n \\
&- \tfrac{\Delta t}{2}\vec{v}\cdot\vec{\nabla}E_i - \tfrac{\Delta t}{2}\alpha_{i1}\mathbf{K}_i\nabla^2 c_1^n - \tfrac{\Delta t}{2}\alpha_{i1}E_1 - \tfrac{\Delta t}{2}\alpha_{i1}\alpha_{11}c_1^n \\
&- \tfrac{\Delta t}{2}\alpha_{i1}\alpha_{12}c_2^n - \tfrac{\Delta t}{2}\alpha_{i2}\mathbf{K}_i\nabla^2 c_2^n - \tfrac{\Delta t}{2}\alpha_{i2}E_2 - \tfrac{\Delta t}{2}\alpha_{i2}\alpha_{21}c_1^n \\
&- \tfrac{\Delta t}{2}\alpha_{i2}\alpha_{22}c_2^n - \tfrac{\Delta t^2}{6}\vec{v}\cdot\vec{\nabla}E_{it} + E_i + \alpha_{i1}c_1^n + \alpha_{i2}c_2^n \\
&+ O(\Delta t^3, \|\mathbf{K}_i\|\,\Delta t^2, \|\mathbf{K}_i\|^2\,\Delta t)
\end{aligned} \tag{38}$$

3 Finite differences discretization

Before applying finite differences for the spatial discretization, equation (38) is transformed using the conformal coordinate system (9). The selected finite difference scheme depends on the node location. We heave related to each location by a reference number, as shown in figure 1. In the following, a mesh with regular horizontal spacing is considered. However, in the vertical direction, the spacing may be variable.

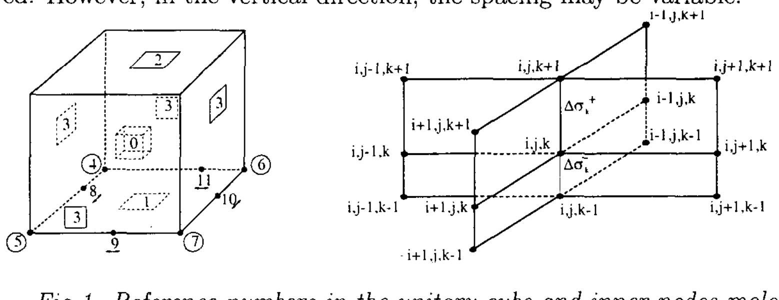

Fig 1. Reference numbers in the unitary cube and inner nodes molecule.

For the inner points, of which reference number is 0, the schemes proposed for derivatives of $c(x_{1i}, x_{2j}, x_{3k}, t)$ are,

$$
\begin{aligned}
\frac{\partial c}{\partial \xi} &= \frac{c_{i+1,j,k} - c_{i-1,j,k}}{2\Delta\xi} + O(\Delta\xi^2) \\
\frac{\partial c}{\partial \eta} &= \frac{c_{i,j+1,k} - c_{i,j-1,k}}{2\Delta\eta} + O(\Delta\eta^2) \\
\frac{\partial c}{\partial \sigma} &= \frac{\lambda_k^2 c_{i,j,k+1} - \left(\lambda_k^2 - 1\right) c_{i,j,k} - c_{i,j,k-1}}{\Delta\sigma_k^+ \left(\lambda_k + \lambda_k^2\right)} + O(\lambda_k \Delta\sigma_k^{+^2}) \\
\frac{\partial^2 c}{\partial \xi^2} &= \frac{c_{i-1,j,k} - 2c_{i,j,k} + c_{i+1,j,k}}{\Delta\xi^2} + O(\Delta\xi^2) \\
\frac{\partial^2 c}{\partial \eta^2} &= \frac{c_{i,j-1,k} - 2c_{i,j,k} + c_{i,j+1,k}}{\Delta\eta^2} + O(\Delta\eta^2) \\
\frac{\partial^2 c}{\partial \sigma^2} &= 2\frac{c_{i,j,k-1} - (1+\lambda_k) c_{i,j,k} + \lambda_k c_{i,j,k+1}}{\Delta\sigma_k^{+^2}\left(\lambda_k + \lambda_k^2\right)} \\
&\quad -\tfrac{1}{3}\left(\Delta\sigma_k^+ - \Delta\sigma_k^-\right)\frac{\partial^3 c}{\partial \sigma^3} + O(\Delta\sigma_k^{+^2} - \Delta\sigma_k^-\Delta\sigma_k^+ + \Delta\sigma_k^{-^2}) \\
\frac{\partial^2 c}{\partial \xi \partial \eta} &= \frac{c_{i+1,j+1,k} - c_{i-1,j+1,k} - c_{i+1,j-1,k} + c_{i-1,j-1,k}}{4\Delta\xi\Delta\eta} + O(\Delta\xi^2, \Delta\eta^2) \\
\frac{\partial^2 c}{\partial \xi \partial \sigma} &= \frac{\lambda_k^2 c_{i+1,j,k+1} - \lambda_k^2 c_{i-1,j,k+1} - c_{i+1,j,k-1} + c_{i-1,j,k-1}}{2\Delta\sigma_k^+\left(\lambda_k + \lambda_k^2\right)\Delta\xi} \\
&\quad + \frac{\left(\lambda_k^2 - 1\right) c_{i-1,j,k} - (\lambda_k^2 - 1) c_{i+1,j,k}}{2\Delta\sigma_k^+\left(\lambda_k + \lambda_k^2\right)\Delta\xi} + O(\Delta\xi^2, \lambda_k\Delta\sigma_k^{+^2}) \\
\frac{\partial^2 c}{\partial \eta \partial \sigma} &= \frac{\lambda_k^2 c_{i,j+1,k+1} - \lambda_k^2 c_{i,j-1,k+1} - c_{i,j+1,k-1} + c_{i,j-1,k-1}}{2\Delta\sigma_k^+\left(\lambda_k + \lambda_k^2\right)\Delta\eta} \\
&\quad + \frac{\left(\lambda_k^2 - 1\right) c_{i,j-1,k} - (\lambda_k^2 - 1) c_{i,j+1,k}}{2\Delta\sigma_k^+\left(\lambda_k + \lambda_k^2\right)\Delta\eta} + O(\Delta\eta^2, \Delta\sigma_k^-\Delta\sigma_k^+)
\end{aligned}
$$

being $\lambda_k = \frac{\Delta\sigma_k^-}{\Delta\sigma_k^+}$. All the schemes are second order, except the one corresponding to $\frac{\partial^2 c}{\partial \sigma^2}$. However, if the mesh is also regular in vertical spacing $\left(\Delta\sigma_k^+ = \Delta\sigma_k^-\right)$, or even if we define $\Delta\sigma_k^+$ such that the difference $\Delta\sigma_k^+ - \Delta\sigma_k^-$ is second order, e.g.,

$$\Delta\sigma_k^+ = \Delta\sigma_k^- + \Delta\sigma_0^{+^2} \quad (39)$$

$$\Delta\sigma_k^+ = \Delta\sigma_k^- + \Delta\sigma_k^-\ \Delta\sigma_0^+ \quad (40)$$

$$\Delta\sigma_k^+ = \Delta\sigma_k^- + \Delta\sigma_k^{-^2} \quad (41)$$

where $\Delta\sigma_0^+$ is the vertical spacing at the bottom, this scheme becomes second order too. The expressions (39) and (40) define the vertical spacing such that the σ coordinate of nodes are given by arithmetical and geometrical progressions, respectively. The approach (41) produces more concentration of points near the terrain. Also second order schemes are proposed for first order derivatives of c on the boundary for each reference number, and the schemes for the derivatives of z_s and for the boundary conditions are obtained by using the same technique (see[9]). The elliptic equation arising from the wind problem is also discretized with the schemes shown in the above table.

As the resulting system of equations $Ax = b$ is non-symmetric, a suitable linear solver should be applied. Here, the biorthogonalization algorithm of Bi-CGSTAB [11] has been used, since this method has proved its efficiency for solving this type of linear systems of equations which arises from the finite difference discretization. To improve its convergence, several classical preconditioners, like $diag(A)$, $SSOR(w)$ and $ILU(0)$ [6], have been implemented.

4 Conclusions

In this work a consistent mass model has been developed to adjust 3-D wind fields. From these fields, we construct an air pollution model to approach the concentration of two set of coupled species: NO_x, HNO_3, and SO_2, H_2SO_4. The use of a terrain conformal coordinate system allows a simple construction of the mesh, due to the elimination of the irregular surface of the terrain. Though, in general, the variable vertical spacing leads to schemes of first consistence order, some strategies, here proposed, lead to second order schemes. Thus, the proposed formulation for the convection-diffusion-reaction problem provides interesting properties of consistence and stability. The model does not only allow to generate wind maps from the measurements obtained in few stations, but to obtain the history of a pollution episode for the considered species.

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1. Department of Mathematics. University of Las Palmas de Gran Canaria.

Edifice de Informática y Matemáticas, Campus Universitario de Tafira,

35017-Las Palmas de Gran Canaria.