MODELIZACIÓN DE LA CONTAMINACIÓN ATMOSFÉRICA EN EL ENTORNO DE CENTRALES TÉRMICAS

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Contents

- Mesh generation
- Velocity field of the fluid
- Air pollution model
- Numerical experiments
- Conclusions

Mesh generation (1)

- 2-D initial coarse mesh corresponding to the discretization of the top
- 2-D Adaptive mesh generation of the terrain surface and chimneys
- Generation of points inside the 3-D domain
- 3-D Delaunay triangulation
- Simultaneous untangling and smoothing of the 3-D mesh
- Local refinement of the tetrahedral mesh

Velocity field of the fluid (1)

Mass consistent models are diagnostic models for constructing wind velocity fields:

- The physical laws of an incompressible fluid
- The empirical design of the wind profiles
- The values of velocities measured at the stations

Based on the continuity equation with constant air density in the domain Ω

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

and *no-flow-through* conditions on the terrain (and the top)

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

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Velocity field of the fluid (2)

A least square problem:
to adjust a velocity field $\vec{u}(\widetilde{u}, \widetilde{v}, \widetilde{w})$ *to another* $\vec{v}_0(u_0, v_0, w_0)$ *which is obtained from experimental measurements*

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

Equivalent to find the saddle point $(\vec{v}(u, v, w), \phi)$ of L

$$L\left(\vec{u}, \lambda\right) = E\left(\vec{u}\right) + \int_\Omega \lambda \vec{\nabla} \cdot \vec{u} \, d\Omega$$

Lagrange multiplier technique leads to the Euler-Lagrange equations

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

Diagonal transmissivity tensor: $T = (T_h, T_h, T_v)$, $T_h = \frac{1}{2\alpha_1^2}$, $T_v = \frac{1}{2\alpha_2^2}$

Velocity field of the fluid (3)

Euler-Lagrange equations yield the following elliptic problem

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

with zero Dirichlet conditions on *flow-through* boundaries and Neumann conditions on the terrain and the top.

$$\begin{aligned}\phi &= 0\ \text{ en }\ \Gamma_a\\ \vec{n}\cdot T\,\vec{\nabla}\mu &= -\vec{n}\cdot\vec{v}_0\ \text{ en }\ \Gamma_b\end{aligned}$$

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Velocity field of the fluid (4)

Construction of the initial wind $\vec{v}_0(u_0, v_0, w_0)$

Horizontal Interpolation

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

$$0 \leq \varepsilon \leq 1$$

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Velocity field of the fluid (5)

Vertical Extrapolation

Friction velocity: $\vec{v}^* = \frac{k\ \vec{v}_0(z_m)}{\log\frac{z_m}{z_0} - \Phi_m}$

Height of the planetary boundary layer: $z_{pbl} = \frac{\gamma\,|\vec{v}^*|}{f}$

$f = 2\omega\ \sin\varphi$ is the Coriolis parameter

ω is the Earth rotation and φ the latitude

γ is a parameter depending on the atmospheric stability

Mixing height:

- $h = z_{pbl}$ in neutral and unstable conditions
- $h = \gamma' \sqrt{\frac{|\vec{v}^*|\,L}{f}}$ in stable conditions

γ': parameter of proportionality.

Height of surface layer: $z_{sl} = \frac{h}{10}$

Velocity field of the fluid (6)

Log-linear profi le of wind velocities

$$\vec{v}_0(z) = 0 \qquad z \leq z_0$$

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

$\Phi_m = 0$ (Neutral atmosphere)

$\Phi_m = -5\frac{z}{L}$ (Stable atmosphere)

$\Phi_m = \log\left[\left(\frac{\theta^2+1}{2}\right)\left(\frac{\theta+1}{2}\right)^2\right] - 2\arctan\theta + \frac{\pi}{2}$ (Unstable atmosphere)

$\theta = (1 - 16\frac{z}{L})^{1/4}$, $\frac{1}{L} = az_0^b$ (a, b, are dependent of the Pasquill stability class)

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

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

$$\vec{v}_0(z) = \vec{v}_g \qquad z > z_{pbl}$$

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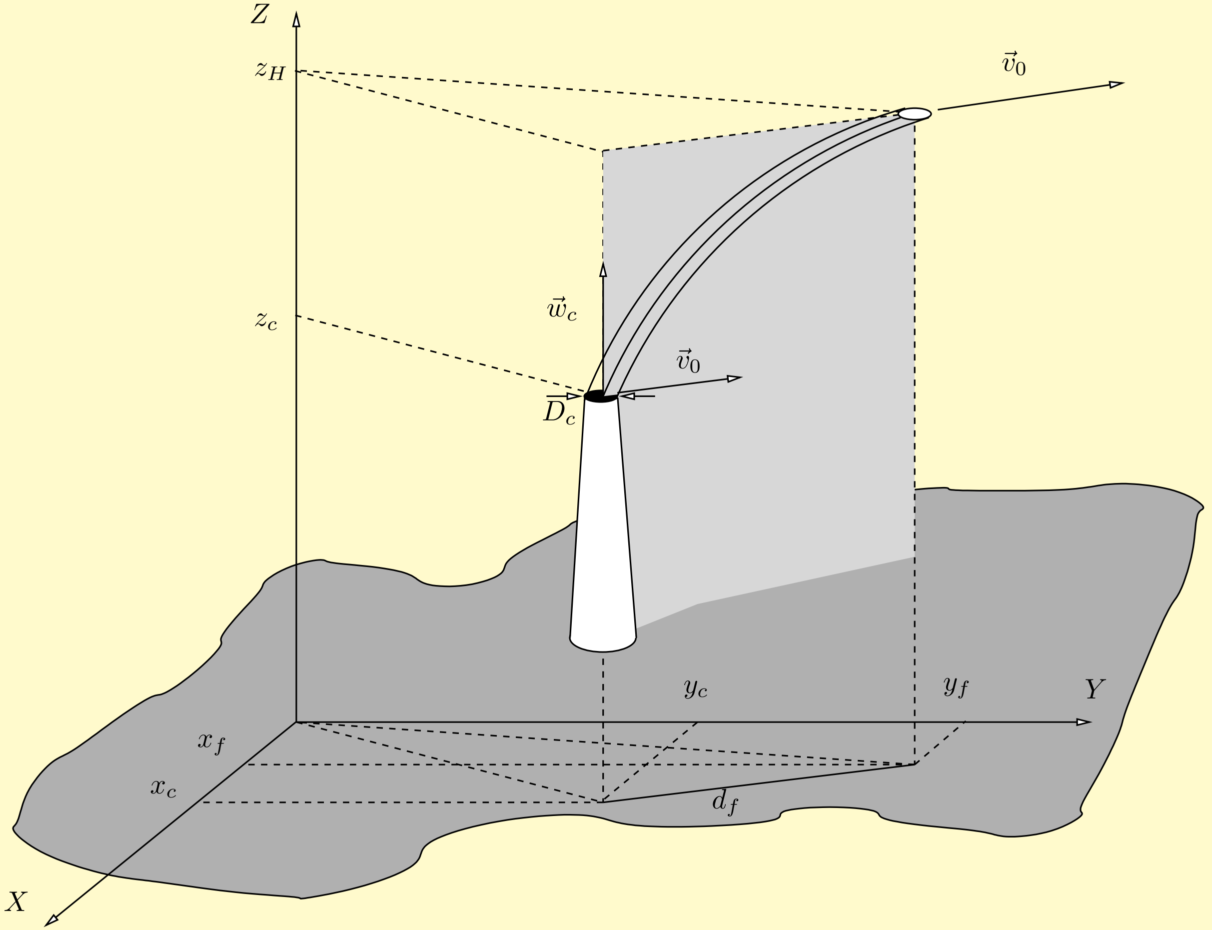
Velocity field of the fluid (7)

Vertical correction in the plume



Correction of vertical velocity by buoyancy rise

Velocity field of the fluid (7)

Vertical correction in the plume

Plume models approximate z_H and d_f in function of the emission characteristics, the wind and the atmospheric stability. In practice, the real height of the chimney z_c is replaced by z'_c,

$$
\begin{aligned}
z'_c &= z_c && \text{if } w_c \geq 1.5\,|\vec{v}_0\,(x_c, y_c, z_c)| \\
z'_c &= z_c \quad + 2D_c\left[(w_c / |\vec{v}_0\,(x_c, y_c, z_c)|) - 1.5\right] && \text{if } w_c < 1.5\,|\vec{v}_0\,(x_c, y_c, z_c)|
\end{aligned}
$$

(x_c, y_c, z_c): center of chimney top, D_c: diameter of chimney top

$$F = g w_c D_c^2 \frac{T_c - T}{4T_c}$$

F: Buoyancy flux parameter, T_c: Temperature of gases in chimney in K,
T: Environment temperature in K

$$s = \frac{g}{T}\frac{\Delta\theta}{\Delta z}$$

s: Stability parameter, $\dfrac{\Delta\theta}{\Delta z}$: Potential temperature variation with height

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Velocity field of the fluid (7)

Vertical correction in the plume

Buoyancy rise: $\dfrac{w_c}{|\vec{v}_0\,(x_c, y_c, z_c)|} \leq 4$

Unstable and neutral conditions

$$z_H = z'_c + 21.425 \frac{F^{3/4}}{|\vec{v}_0\,(x_c, y_c, z_c)|} \qquad d_f = 49F^{5/8} \qquad \text{if } F < 55$$

$$z_H = z'_c + 38.71 \frac{F^{3/5}}{|\vec{v}_0\,(x_c, y_c, z_c)|} \qquad d_f = 119F^{2/5} \qquad \text{if } F \geq 55$$

Stable conditions

$$z_H = z'_c + 2.6 \left(\frac{F}{s\,|\vec{v}_0\,(x_c, y_c, z_c)|} \right)^{1/3} \qquad d_f = 2.07\,|\vec{v}_0\,(x_c, y_c, z_c)|\,s^{-1/2}$$

$$\text{if } |\vec{v}_0\,(x_c, y_c, z_c)| \geq 0.2746 F^{1/4} s^{1/8}$$

$$z_H = z'_c + 4F^{1/4} s^{-3/8} \qquad d_f = 0$$

$$\text{if } |\vec{v}_0\,(x_c, y_c, z_c)| < 0.2746 F^{1/4} s^{1/8}$$

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Velocity field of the fluid (7)

Vertical correction in the plume

Value of parameter t (elapsed time) at d_f

$$t_f = \frac{-|\vec{v}_0(x_c, y_c, z_c)| + \sqrt{|\vec{v}_0(x_c, y_c, z_c)|^2 + 2a_d d_f}}{a_d}$$

Parametrisation of vertical acceleration, velocity and position,

$$\begin{aligned}
a_0(t) &= \frac{-4w_c t_f + 6(z_H - z_c')}{t_f^2} + \frac{6w_c t_f - 12(z_H - z_c')}{t_f^3} t \\
w_0(t) &= w_c + \frac{-4w_c t_f + 6(z_H - z_c')}{t_f^2} t + \frac{3w_c t_f - 6(z_H - z_c')}{t_f^3} t^2 \\
x(t) &= x_c + u_0(x_c, y_c, z_c)t + \frac{1}{2} a_{dx} t^2 \\
y(t) &= y_c + v_0(x_c, y_c, z_c)t + \frac{1}{2} a_{dy} t^2 \\
z(t) &= z_c' + w_c t + \frac{-2w_c t_f + 3(z_H - z_c')}{t_f^2} t^2 + \frac{w_c t_f - 2(z_H - z_c')}{t_f^3} t^3
\end{aligned}$$

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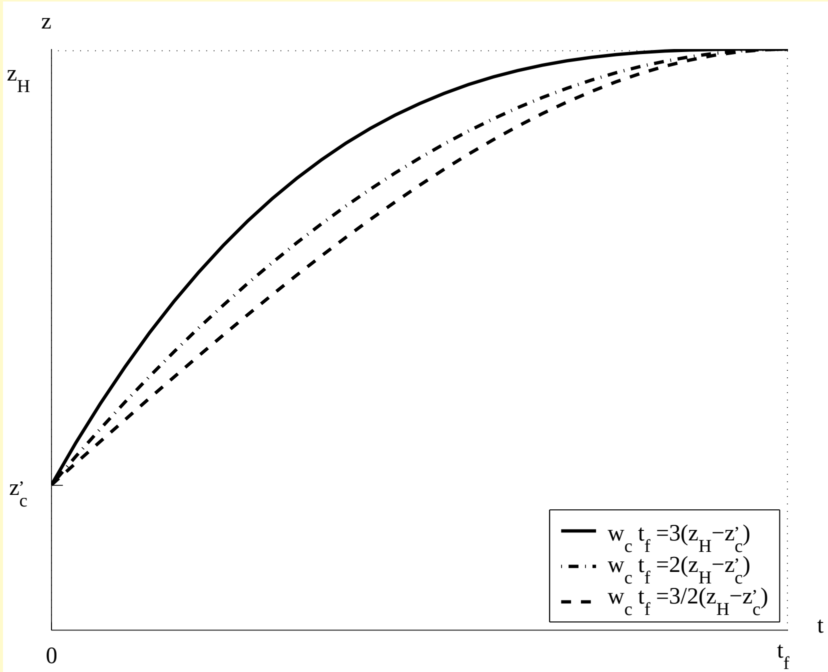
Velocity field of the fluid (8)

Vertical correction in the plume

Since the movement is linearly unaccelerated,

$$\frac{3}{2} \le \frac{w_c t_f}{(z_H - z_c')} \le 3 \quad \Rightarrow \quad a_d = (1+\delta)\frac{2w_c}{3(z_H - z_c')}\left[(1+\delta)\frac{w_c}{3(z_H - z_c')}d_f - |\vec{v}_0(x_c, y_c, z_c)|\right]$$

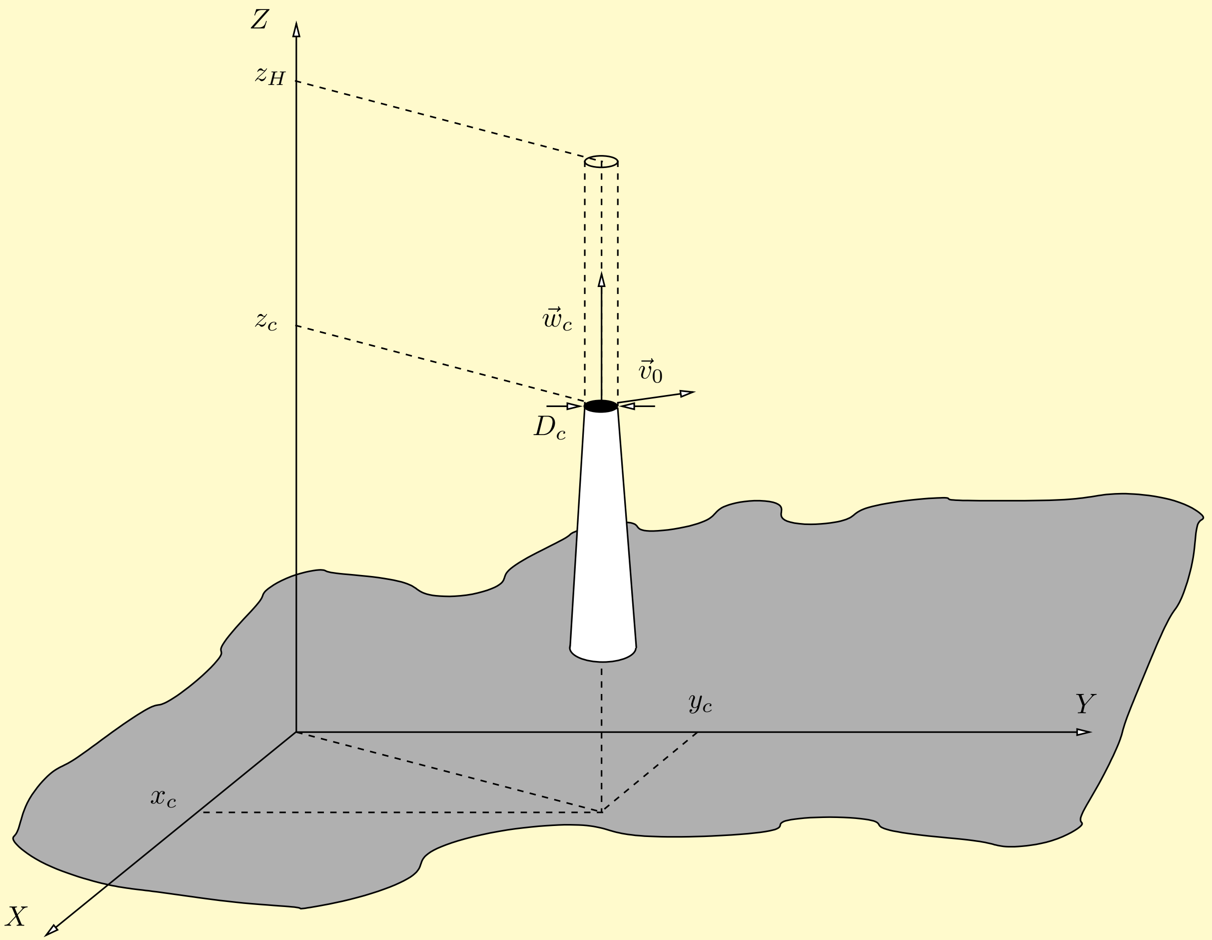
$$0 \le \delta \le 1.$$



Family of curves for $z(t)$ in $[0, t_f]$

Velocity field of the fluid (7)

Vertical correction in the plume



Correction of vertical velocity by momentum rise

Velocity field of the fluid (7)

Vertical correction in the plume

Momentum rise: $$\frac{w_c}{\left|\vec{v}_0\left(x_c, y_c, z_c\right)\right|} > 4$$

For unstable or neutral conditions $$z_H = z_c' + \frac{3 D_c w_c}{\left|\vec{v}_0\left(x_c, y_c, z_c\right)\right|}$$

For stable conditions $$z_H = z_c' + 1.5\left[\frac{D_c^2 w_c^2 T}{4 T_c \left|\vec{v}_0\left(x_c, y_c, z_c\right)\right|}\right]^{1/3} s^{-1/6}$$

$$\begin{aligned} t_f &= \frac{2\left(z_H - z_c'\right)}{w_c} \\ a_0 &= \frac{-w_c}{t_f} \\ t &= t_f\left(1 - \sqrt{1 - \frac{2\left(z - z_c'\right)}{w_c t_f}}\right) \end{aligned}$$

$$w_0(t) = w_c\left(1 - \frac{t}{t_f}\right)$$

$$z = z_c + w_c t\left(1 - \frac{1}{2}\frac{t}{t_f}\right)$$

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Air pollution model (1)

Convection-diffusion-reaction equation

In an Eulerian model, the convection-diffusion-reaction equation may be written for a pollutant specie i, as

$$\frac{\partial c_i}{\partial t} + \vec{v} \cdot \vec{\nabla} c_i - \vec{\nabla} \cdot (K_i \vec{\nabla} c_i) = f_i \qquad i = 1, ..., p, \qquad \text{in} \quad \Omega$$

p: is the number of pollutant species

$c_i = c_i(x, y, z, t)$: the average concentration of pollutant i

$\vec{v}$: the (adjusted) velocity fi eld of the fluid

$K_i = [K_{i1}(x, y, z), K_{i2}(x, y, z), K_{i3}(x, y, z)]$: diagonal diffusivity tensor of pollutant i

$f_i = f_i(c_1, c_2, ..., c_p)$: the external sources of pollutant i

Air pollution model (2)

Initial conditions

$$c_i(x,y,z,0) = c_i^0(x,y,z) \qquad i = 1,...,p, \qquad \text{in} \quad \Omega$$

Boundary conditions

In open boundaries we asume the conservation of the flow along a time step. For in-flow and out-flow we have

$$\vec{n}\cdot\left[\vec{v}c_i^{n+1} - K_i\vec{\nabla}c_i^{n+1}\right] = \vec{n}\cdot\left[\vec{v}c_i^{n} - K_i\vec{\nabla}c_i^{n}\right] \qquad i = 1,...,p, \qquad \text{on} \quad \Gamma_{a_0}(\vec{n}\cdot\vec{v} \neq 0)$$

where $\vec{n}$ is the out normal vector to the corresponding boundary and c_i^n the concentration of pollutant i on Γ_{a_0} at time t_n.
In open boundaries with tangent velocity, the condition is simplifi ed as

$$-\vec{n}\cdot K_i\vec{\nabla}c_i^{n+1} = -\vec{n}\cdot K_i\vec{\nabla}c_i^{n} \qquad i = 1,...,p, \qquad \text{on} \quad \Gamma_{a_1}(\vec{n}\cdot\vec{v} = 0)$$

Air pollution model (3)

Boundary conditions

For an emission source in Γ_{b_0}, we impose in-flow

$$\vec{n} \cdot \left[\vec{v} c_i^{n+1} - K_i \vec{\nabla} c_i^{n+1}\right] = -E_i^{n+1} \qquad i = 1, ..., p, \qquad \text{on} \quad \Gamma_{b_0}$$

where E_i^{n+1} is the $i-th$ pollutant in-flow at $t = t_{n+1}$.

Dry deposition consists of two phenomena, the pollutant transport to the terrain surface and physical and chemical interactions between the surface and the pollutant.

In the terrain (Γ_{b_1}) the dry deposition is considered as,

$$-\vec{n} \cdot K_i \vec{\nabla} c_i^{n+1} = v_{di} c_i^{n+1} - e_i^{n+1} \qquad i = 1, ..., p, \qquad \text{on} \quad \Gamma_{b_1}$$

where v_{di} is the dry deposition velocity and e_i^{n+1} is $i-th$ pollutant in-flow due to superficial sources on the terrain.

Pollutant	V_{di} in m/s
SO_2	0.0044
$SO_4^=$	0.0026
NO_x	0.0013
NO_3^-	0.0054

Air pollution model (4)

Source term

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

$R_i(x, y, z, t)$: creation or elimination of specie i by chemical reactions

$P_i(x, y, z, t)$: elimination of specie i due to precipitation

Chemical reactions

Primary species: SO_2 and NO_x (NO, NO_2) $R_{ij} = \overline{\alpha}_{ij} \cdot c_j \qquad i, j = 1, 2, ..., N$

Secondary species: H_2SO_4 and HNO_3 $\overline{\alpha}_{ij}$: Kinetic constants of specie i reactions

The velocities of reaction are,

$$NO_2 + h \cdot v \xrightarrow{1} NO + O\cdot \qquad \frac{dc_{NO_x}}{dt} = -2 \cdot k_1 \cdot k_2 \cdot c_{NO_x}$$

$$OH \cdot + NO_2 \xrightarrow{2} HNO_3 \qquad \frac{dc_{HNO_3}}{dt} = 2 \cdot k_1 \cdot k_2 \cdot c_{NO_x}$$

$$OH \cdot + SO_2 \xrightarrow{3} HOSO_2 \cdot \qquad \frac{dc_{SO_2}}{dt} = -2 \cdot \frac{k_1 \cdot k_3}{k_2} \cdot c_{SO_2}$$

$$\frac{dc_{H_2SO_4}}{dt} = 2 \cdot \frac{k_1 \cdot k_3}{k_2} \cdot c_{SO_2}$$

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Air pollution model (5)

$$W_g = v_{wi} I c(x, y, z_t, t)$$

I: intensity of precipitation

v_{wi}: washout velocity given by $v_{wi} = \dfrac{C(aq)}{c(x, y, z_t, t)}$

$C(aq)$: concentration of product precipitated in the surface layer

We consider constant precipitation from the terrain to z_{sl},

$$P_i = -\frac{v_{wi}}{z_{sl}} I c_i, \qquad w_h = \frac{v_{wi}}{z_{sl}}$$: modifi ed coeffi cient of washout

So, in the equation of source terms, we have

$\alpha_{ij} = \overline{\alpha}_{ij}$ if $j \neq i$

and $\alpha_{ii} = \overline{\alpha}_{ii} - w_h I$

Pollutant	Modifi ed coeffi cient of washout w_h
SO_2	6.00×10^{-2}
$SO_4^{=}$	3.00×10^{-2}
NO_x	0.40×10^{-2}
NO_3^{-}	0.39×10^{-2}

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Air pollution model (6)

Hight order time accuracy scheme

From the governing equation, first and second time derivatives of c_i,

$$\begin{aligned} c^n_{i_t} &= -\vec{v}.\vec{\nabla} c^n_i + K_i \nabla^2 c^n_i + f_i \\ c^n_{i_{tt}} &= -\vec{v}_t \cdot \vec{\nabla} c^n_i - \vec{v} \cdot \vec{\nabla} c^n_{i_t} + K_i \nabla^2 c^n_{i_t} + f_{i_t} \end{aligned}$$

Taylor span yields,

$$\frac{c^{n+1}_i - c^n_i}{\Delta t} = -\vec{v} \cdot \vec{\nabla} \left[c^n_i + \frac{\Delta t}{2} c^n_{i_t} + \frac{\Delta t^2}{6} c^n_{i_{tt}} + O(\Delta t^3) \right] + K_i \nabla^2 \left[c^n_i + \frac{\Delta t}{2} c^n_{i_t} + O(\Delta t^2) \right] + f_i$$

Using these equations we obtain

$$\begin{aligned} \frac{c^{n+1}_i - c^n_i}{\Delta t} = -\vec{v} \cdot \vec{\nabla} \Big[c^n_i &+ \frac{\Delta t}{2} \left(-\vec{v} \cdot \vec{\nabla} c^n_i + K_i \nabla^2 c^n_i + f_i \right) \\ &+ \frac{\Delta t^2}{6} \left(-\overrightarrow{v}_t \cdot \vec{\nabla} c^n_i - \overrightarrow{v} \cdot \vec{\nabla} c^n_{i_t} + K_i \nabla^2 c^n_{i_t} + f_{i_t} \right) + O(\Delta t^3) \Big] \\ &+ K_i \nabla^2 \left[c^n_i + \frac{\Delta t}{2} c^n_{i_t} + O(\Delta t^2) \right] + f_i \end{aligned}$$

Air pollution model (7)

Scheme of hight order time accuracy

Finally, ordering, applying the properties of derivation and eliminating hight order derivatives, the equation for each family of pollutant specie results

$$\left[1-\frac{\Delta t^2}{6}\left((\vec{v}\cdot\vec{\nabla})\vec{v}\cdot\vec{\nabla}+\vec{v}\cdot(\vec{v}\cdot\vec{\nabla})\vec{\nabla}\right)-\Delta t K_i\nabla^2\right]\left(\frac{c_i^{n+1}-c_i^n}{\Delta t}\right)$$

$$-\left[\frac{\Delta t}{2}\alpha_{i1}-\frac{5}{12}\Delta t^2\alpha_{i1}\vec{v}\cdot\vec{\nabla}\right]\left(\frac{c_1^{n+1}-c_1^n}{\Delta t}\right)-\left[\frac{\Delta t}{2}\alpha_{i2}-\frac{5}{12}\Delta t^2\alpha_{i2}\vec{v}\cdot\vec{\nabla}\right]\left(\frac{c_2^{n+1}-c_2^n}{\Delta t}\right)$$

$$=-\vec{v}\cdot\vec{\nabla}c_i^n+\frac{\Delta t}{2}\left[(\vec{v}\cdot\vec{\nabla})\vec{v}\cdot\vec{\nabla}c_i^n+\vec{v}\cdot(\vec{v}\cdot\vec{\nabla})\vec{\nabla}c_i^n-\left(K_i\nabla^2\vec{v}\right)\cdot\vec{\nabla}c_i^n\right]+K_i\nabla^2c_i^n$$

$$+\frac{\Delta t^2}{6}\vec{v}\cdot\vec{\nabla}\left(\vec{v}_t\cdot\vec{\nabla}c_i^n\right)-\frac{\Delta t}{2}\alpha_{i1}\left[K_i\nabla^2c_1^n+\alpha_{11}c_1^n+\alpha_{12}c_2^n\right]+\alpha_{i1}c_1^n+\alpha_{i2}c_2^n$$

$$-\frac{\Delta t}{2}\alpha_{i2}\left[K_i\nabla^2c_2^n+\alpha_{21}c_1^n+\alpha_{22}c_2^n\right]-\frac{\Delta t}{2}K_i\nabla^2f_i+O(\Delta t^3,\|K_i\|\,\Delta t^2,\|K_i\|^2\,\Delta t)$$

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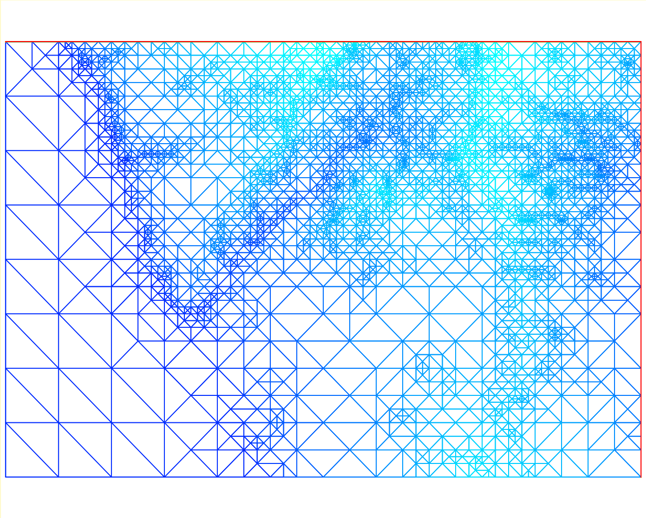
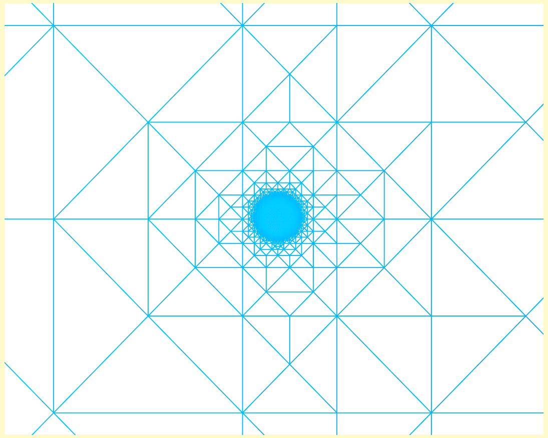
Numerical experiments (1)

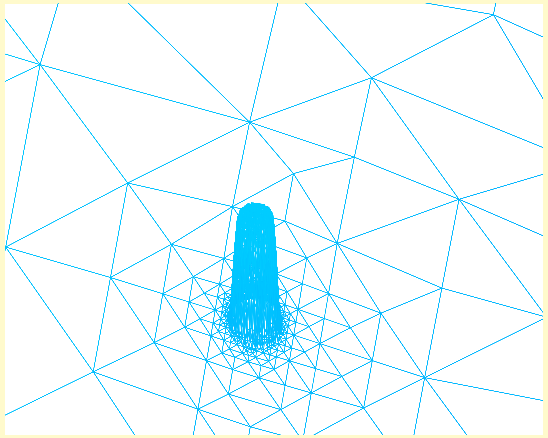


Terrain discretization

Velocity fi eld in La Palma with a chimney

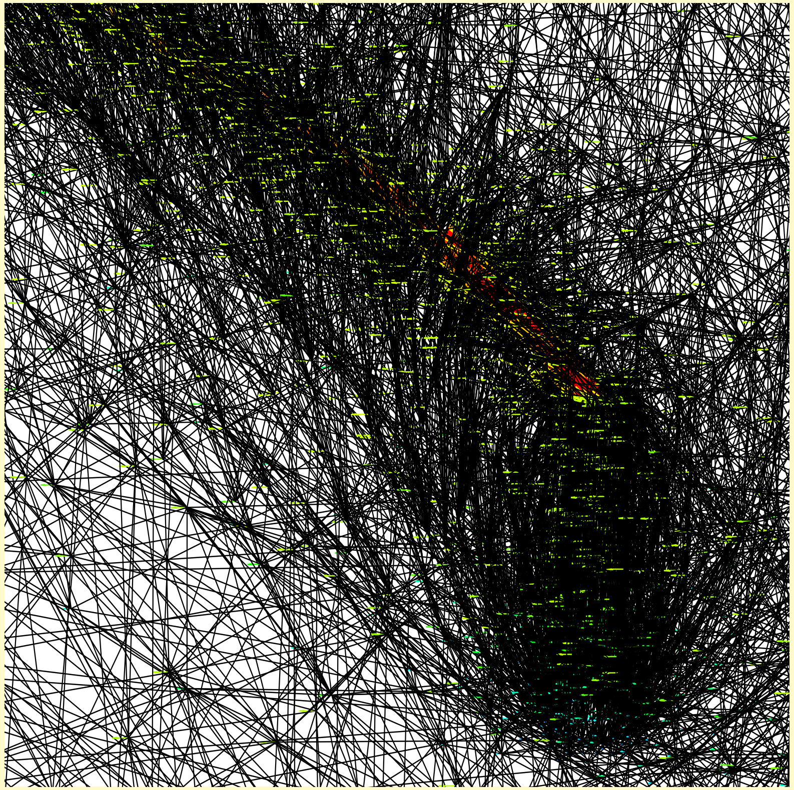
- ⋆ $22803 \times 15600 \times 9000\ m^3$
- ⋆ 4 Stations
- ⋆ Chimney: $r_i = 20m$, $r_e = 40m$, $h = 200m$





Details of the mesh (chimney)

Numerical experiments (2)

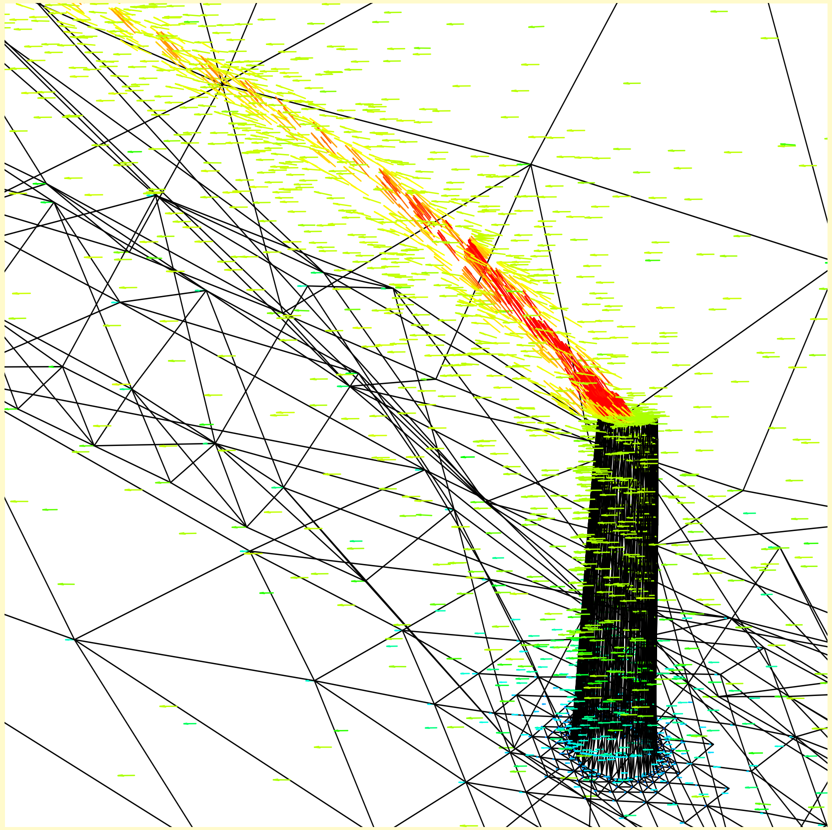


Detail of the mesh in the chimney
(All edges)

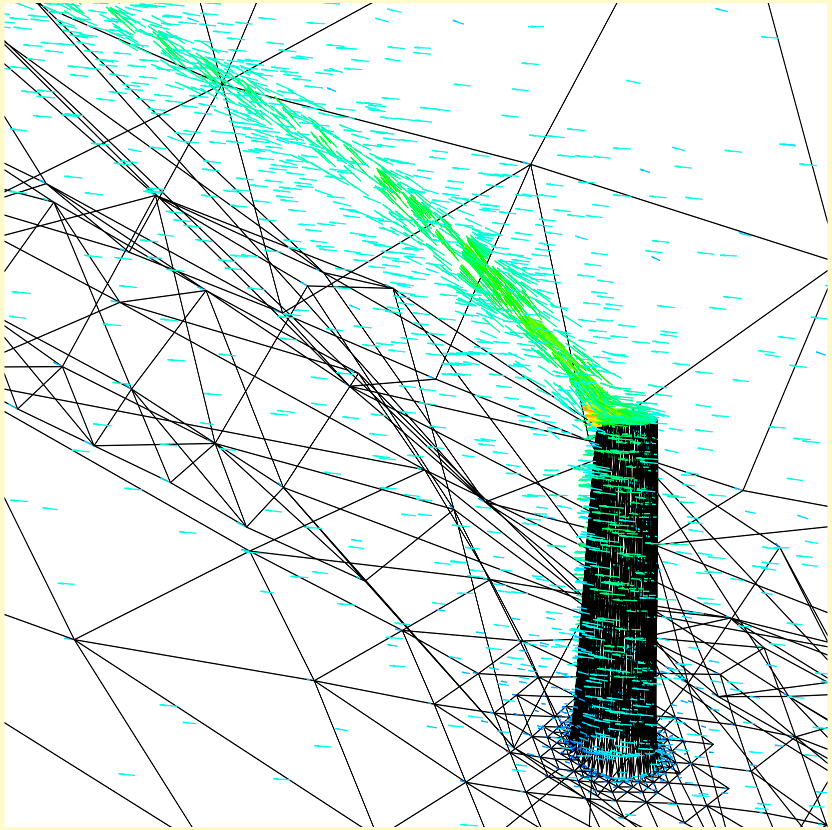
Local refinement in the plume cylinder

Mesh	Nodes	Tetrahedra
0	28387	153085
1	28652	154595
2	29996	160960
3	33277	177473
4	33322	177685
5	34551	183659
6	34626	184017

Numerical experiments (3)



Initial velocity fi eld



Adjusted velocity fi eld

Conclusions

- The efficient generation of the mesh, including the discretization of the emission source, has allowed us to formulate different boundary conditions in the chimney.
- A refinement algorithm has been used in order to discretize efficiently the trajectory of the plume.
- The correction of the observed velocity field has allowed to go on working with an adjusted velocity field related an incompressible fluid which takes into account the plume evolution.