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Fall-out estimation by lagrangian random walk model

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Abstract

The purpose of this paper is an estimation of the concentration of pollutants above the terrain surface based on lagrangian random walk model. Firstly, an estimation of wind fields in a region of interest using the continuity equation, known vertical profile of wind (modelled by an Ekman spiral and ground parametrized modulus profile) and known density is presented. A diagnostic model[1] based on a proposed merit function which uses the conservation of mass and knowledge of *n* measurements of the wind field within the region is derived. The model, of reduced order, is then solved by using variational calculus and finite differences. In the second section a Lagrangian model is presented. It is based on stochastic differential equations[2]. It is necessary to relate the parameters of the stochastic differential equation to the diffusion parameters. The Briggs' parametrization with open-country conditions is used[4,6]. The Carson and Moses equations are used here to model the plume rise[7]. Dry deposition and inversion layer are also modelled[3,5,6]. This model has been applied at the hypothetical electrical generation plant at Valdecaballeros, in the North East of the province of Badajoz (Spain), where meteorological and topographic measurements are available.

1 Estimation of wind fields

The estimate of wind fields is performed by the calculation of the horizontal and vertical velocities neglecting frictional effects. Afterwards, planetary boundary layer effects are modelled by an Ekman spiral and ground parametrized modulus profile.

This estimation is based on continuity equation, known profile of wind and known density, yielding (appendix I),

$$\vec{\nabla}_{(x,y)} \cdot \int_{h(x,y)}^{\infty} \left[\rho \vec{V}_{(x,y)}\right] dz = 0 \quad (1)$$

where ρ is the density and $\vec{V}_{(x,y)}$ is the horizontal wind velocity vector.

The wind vector, neglecting frictional effects, may be written as a function of its components in the previous reference system $\vec{V}^{\infty} = u^{\infty}\vec{i} + v^{\infty}\vec{j} + w^{\infty}\vec{k}$. The superscript "∞" is used since layer friction in the planetary boundary layer is not considered; this occurs at heights greater than 1 *km* above the earth's surface.

To introduce the planetary boundary layer effects, the Ekman spiral will be used to model the rotation $\alpha(z)$ of the wind and typical established profiles $n(z)$ used to calculate its modulus (appendix II).

The horizontal wind at height z may be written as,

$$\begin{pmatrix} u(z) \\ v(z) \end{pmatrix} = n(z) \begin{pmatrix} \cos\alpha(z) & -\operatorname{sen}\alpha(z) \\ \operatorname{sen}\alpha(z) & \cos\alpha(z) \end{pmatrix} \begin{pmatrix} u^{\infty} \\ v^{\infty} \end{pmatrix}$$

and its vertical component as (appendix III),

$$w = m\left(\vec{V}_{(x,y)} \cdot \nabla h\right) = m\left(u\frac{\partial h}{\partial x} + v\frac{\partial h}{\partial y}\right)$$

The above integral (1) is evaluated considering Ekman spiral $G[\alpha(z)]$.

$$\begin{bmatrix} u \\ v \end{bmatrix}_{(x,y)} = n(z)G[\alpha(z)] \begin{bmatrix} u^{\infty} \\ v^{\infty} \end{bmatrix}_{(x,y)} \Rightarrow$$

$$\Rightarrow \int_{h}^{\infty} \rho n(z) G[\alpha(z)] \begin{bmatrix} u^{\infty} \\ v^{\infty} \end{bmatrix}_{(x,y)} dz = \left[\rho_o \int_{h}^{\infty} e^{-\frac{z}{H}} n(z) G[\alpha(z)] dz\right] \begin{bmatrix} u^{\infty} \\ v^{\infty} \end{bmatrix}_{(x,y)} = M_{(x,y)} \begin{bmatrix} u^{\infty} \\ v^{\infty} \end{bmatrix}_{(x,y)}$$

We are interested in the principle direction of contamination diffusion and therefore require knowledge of the most stationary wind. Many merit functions may exist to calculate it but one of the form $\vec{V}^{\infty}_{(x,y)} \cdot \vec{V}^{\infty}_{(x,y)}$ is proposed.

The problem is transformed into the minimization of the auxiliary functional (appendix IV):

$$F=\left[\frac{1}{2}\iiint_{\tau}\left(\vec{V}^{\infty}_{(x,y)}\cdot\vec{V}^{\infty}_{(x,y)}\right)d\tau\right]+\sum_{i=1}^{n}\bar{\lambda}_i\cdot\left[\vec{V}^{\infty}_{(x,y)}(p_i)-\vec{V}^{\infty}_{(x,y)_i}\right]+\iiint_{\tau}\mu\left(\nabla\cdot m\vec{V}^{\infty}_{(x,y)}\right)d\tau$$

where n is the number of wind measurements taken at n different positions transformed to ∞.

Using the current function ψ, it may be written as,

$$F=\frac{1}{2}\iiint_{\tau}\frac{1}{m^2}\left[\left(\frac{\partial\psi}{\partial x}\right)^2+\left(\frac{\partial\psi}{\partial y}\right)^2\right]d\tau+\sum_{i=1}^{n}\bar{\lambda}_i\cdot\left[\left(\frac{1}{m}\frac{\partial\psi}{\partial y},-\frac{1}{m}\frac{\partial\psi}{\partial x}\right)-\vec{V}^{\infty}_{(x,y)_i}\right]$$

The solution to the above equation is computed using finite differences.

2 The Random Walk Lagrangian Model

The particle movement is modelled by an stochastic linear differential equation. It can be shown that the probability distribution associated to these kind of equations is the solution of an advection - diffusion equation[2] (appendix V).

$$\begin{pmatrix}\Delta x\\ \Delta y\\ \Delta z\end{pmatrix}=\begin{pmatrix}u\\ v\\ w\end{pmatrix}T+\begin{pmatrix}\sigma_h w_x^*\\ \sigma_h w_y^*\\ \sigma_v w_z^*\end{pmatrix}$$

where the Brownian processes $\vec{\omega}^*$ are generated according to a normal distribution $N(0,1)$.

The linear deterministic term of the stochastic equation is related to the advection term. It is equal to the estimated wind velocity. The stochastic term is related to the diffusion term. It is obtained by a Briggs' parametrization with open-country conditions.

The equation is solved by simulation. The time increment is chosen in order to the displacements to be of the order of the resolution of the mesh.

The deposition probability of a particle is proportional to the deposition velocity V_d. It is calculated by (appendix VI),

$$P_{dep}=\frac{V_d}{w}$$

The Carson and Moses equations (see Wark[7]) are used for plume rise modelling.

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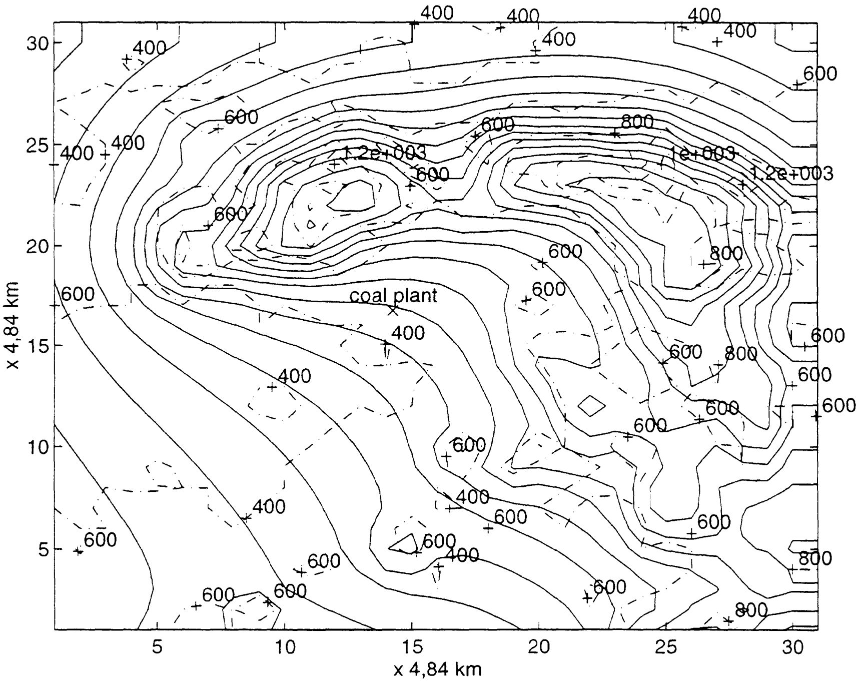

Figure 1: Results from the simulation. Dashed line represents topographic measurements. Solid line represents concentration of particles above the terrain surface.

3 Example

The hypothetical coal plant is located in the municipal district of Valdecaballeros, in the North East of the province of Badajoz (Spain), almost bordering on the province of Cáceres.

The thermal plant consists of three groups with an installed electric power of 350 MW each one. The emission rates of SO_2 and particles were estimated to be 1010.3 kg/h and 257 kg/h, respectively. The exit gas velocity and temperature was assumed to be 25 m/s and $170° C$. The stack height and outlet diameter were 343 m and 12 m, respectively.

The Cartesian grids used are 150×150 km with 31×31 nodes. The coal plant is located 8.48 km from the centre of the grid in Northwest direction.

A total of 40,000 particles were simulated. Concentrations are computed by dividing the number of particles within each square of the grid between the total particles simulated.

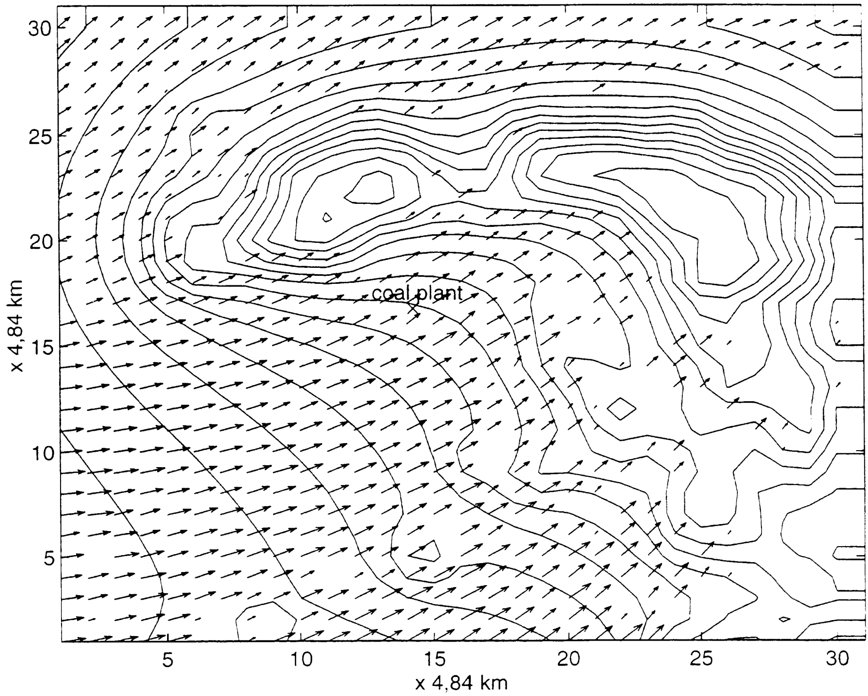

Figure 2: Concentration of particles above the terrain surface vs. direction of the wind. Estimation of wind field has been performed on: height of 460 m, measured point at the coal plant is located and horizontal velocity measured (1,1) m/s.

Acknowledgments

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Appendix I

The continuity equation shows that

$$\vec{\nabla}_{(x,y)} \cdot \left[\rho \vec{V}_{(x,y)}\right] + \frac{\partial}{\partial z}\left(\rho V_z\right) = 0$$

where ρ is the density and $\vec{V}$ is the wind velocity vector.

Combining the hydrostatic equation with the state-equation for a perfect gas yields,

$$\rho(x,y,z) = \rho_o(x,y) e^{-\frac{z}{H}}$$

where H is the scale height. An intermediate value is $H = 7.25\ \text{km}$. For air: $\rho_o = 1.229\ \text{kg/m}^3$.

Let consider a column of air at an altitude of $h(x,y)$ and integrating under the constrains $V_z\left[x,y,h(x,y)\right] = 0$ y $\rho(x,y,\infty) = 0$ is shown that:

$$\int_{h(x,y)}^{\infty} \vec{\nabla}_{(x,y)} \cdot \left[\rho \vec{V}_{(x,y)}\right] dz + \left[\rho V_z\right]_{h(x,y)}^{\infty} = 0 \Rightarrow \vec{\nabla}_{(x,y)} \cdot \int_{h(x,y)}^{\infty} \left[\rho \vec{V}_{(x,y)}\right] dz = 0$$

Appendix II

The rotation angle α will be given by,

$$\alpha = \operatorname{arctg}\frac{1-e^{-\gamma z}\cos(\gamma z)}{e^{-\gamma z}\operatorname{sen}(\gamma z)} \quad \text{where} \quad \gamma = \sqrt{\frac{f}{2K}}$$

f is the Coriolis parameter ($7\cdot10^{-5}$ rad/s for average latitude) and K is a diffusivity coefficient; $K \in (10\ ,\ 100)\ \mathrm{m}^2/s$.

Typical profiles considered here are:

$$n(z) = \begin{cases} \left(\dfrac{z}{z_1}\right)^{\frac{1}{2}} & \text{si} \quad z < z_1(m) \\ 1 & \text{si} \quad z \geq z_1(m) \end{cases}$$

- Above city: $z_1 = 500$; $\beta = \frac{1}{2}$
- Above wood: $z_1 = 400$; $\beta = \frac{1}{3.5}$
- Above plain: $z_1 = 300$; $\beta = \frac{1}{7}$

Appendix III

From the continuity equation and mass conservation, it may shown that,

$$div\left(\rho_o e^{-\frac{z}{H}}\vec{V}^{\infty}\right) = 0 \Rightarrow \frac{\partial u^{\infty}}{\partial x} + \frac{\partial v^{\infty}}{\partial x} + \frac{\partial w^{\infty}}{\partial x} - \frac{1}{H}w^{\infty} = 0$$

Alternatively, the constraint $\nabla\cdot m\vec{V}^{\infty}_{(x,y)} = 0$ yields,

$$\frac{\partial u^{\infty}}{\partial x} + \frac{\partial v^{\infty}}{\partial y} = -\frac{1}{m}\left(u^{\infty}\frac{\partial m}{\partial x} + v^{\infty}\frac{\partial m}{\partial y}\right)$$

which may be substituted into the above equation yielding,

$$\frac{\partial w^{\infty}}{\partial z} - \frac{1}{H}w^{\infty} = \frac{1}{m}\left(u^{\infty}\frac{\partial m}{\partial x} + v^{\infty}\frac{\partial m}{\partial y}\right) \Rightarrow \frac{\partial}{\partial z}e^{-\frac{z}{H}}w^{\infty} = \frac{e^{-\frac{z}{H}}}{m}\left(u^{\infty}\frac{\partial m}{\partial x} + v^{\infty}\frac{\partial m}{\partial y}\right)$$

Integrating with respect to z under the restriction $w^{\infty}(\infty) = 0$ yields,

$$w^{\infty} = m\left(\vec{V}^{\infty}_{(x,y)}\cdot\nabla h\right)$$

Appendix IV

Many merit functions of this type exist but we require the function to minimize

$$J = \frac{1}{2}\iiint_\tau \left(\vec{V}^{\infty}_{(x,y)} \cdot \vec{V}^{\infty}_{(x,y)}\right) d\tau$$

under the constraints,

$$\nabla \cdot m\vec{V}^{\infty}_{(x,y)} = 0$$

$$\vec{V}^{\infty}_{(x,y)}(p_i) = \vec{V}^{\infty}_{(x,y)_i} \quad i = 1,\ldots,n$$

Using Lagrange multipliers, the problem is transformed into the minimization of the auxiliary functional:

$$F = \left[\frac{1}{2}\iiint_\tau \left(\vec{V}^{\infty}_{(x,y)} \cdot \vec{V}^{\infty}_{(x,y)}\right) d\tau\right] + \sum_{i=1}^{n} \bar{\lambda}_i \cdot \left[\vec{V}^{\infty}_{(x,y)}(p_i) - \vec{V}^{\infty}_{(x,y)_i}\right] + \iiint_\tau \mu\left(\nabla \cdot m\vec{V}^{\infty}_{(x,y)}\right) d\tau$$

Since flow divergent to the horizontal is not considered, the field $m\vec{V}^{\infty}_{(x,y)}$ may be written using the current function ψ,

$$u^{\infty} = \frac{1}{m}\frac{\partial \psi}{\partial y} \qquad\qquad v^{\infty} = -\frac{1}{m}\frac{\partial \psi}{\partial x}$$

The auxiliary functional may be written as,

$$F = \frac{1}{2}\iiint_\tau \frac{1}{m^2}\left[\left(\frac{\partial \psi}{\partial x}\right)^2 + \left(\frac{\partial \psi}{\partial y}\right)^2\right] d\tau + \sum_{i=1}^{n} \bar{\lambda}_i \cdot \left[\left(\frac{1}{m}\frac{\partial \psi}{\partial y}, -\frac{1}{m}\frac{\partial \psi}{\partial x}\right) - \vec{V}^{\infty}_{(x,y)_i}\right]$$

Appendix V

Since the velocity vector is known at each point within the region, every particle in the region may be written as a function of this velocity. Modelling of turbulence effects (chaotic/random movements) is performed by the introduction of a random term,

$$\begin{pmatrix} dx \\ dy \\ dz \end{pmatrix} = \begin{pmatrix} u \\ v \\ w \end{pmatrix} dt + \begin{pmatrix} b_x(t)dw_x \\ b_y(t)dw_y \\ b_z(t)dw_z \end{pmatrix}$$

w_x, w_y, w_z representing independent Brownian Motion. For this type of motion, the state of the variable $x(t=t_0)$ at the new time $x(t=t_1)$ will change according to the random variable X having the distribution $X : N(x_0, t_1 - t_0)$.

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Each component is represented by a unidimensional, homogeneous in time, stochastic differential equation of the form

$$dx(t) = a(t)dt + b(t)dw(t)$$

where $x(0) = x_o$; $a(t)$ and $b(t)$ are deterministic functions.

The solution is given by,

$$p(x,t_o,y,t) = \left[2\pi\int_{t_o}^{t} b^2(u)du\right]^{-\frac{1}{2}} \exp\left[\frac{-\left(y - x - \int_{t_o}^{t} a(u)du\right)^2}{2\int_{t_o}^{t} b^2(u)du}\right]$$

The problem, therefore, reduces to one of relating the parameters of the stochastic differential equation with the diffusion parameters. It is known that $a(t)$ is the velocity component in the direction of interest and represents the transformation from the stationary Gaussian system to the non-stationary Lagrangian system. We will concentrate on the Gaussian model (steady-state solution of the diffusion equation) which also may be studied as the product of two normal distributions; one horizontal and the other vertical.

Equating terms from the horizontal density function yields,

$$\sigma_h^2 = \int_0^T b^2 dt \Rightarrow b = \frac{\sigma_h}{\sqrt{T}}$$

where T is the increment in time. The same may be applied to vertical density function with a typical deviation σ_v.

From the above equations, we can write:

$$\begin{pmatrix} dx \\ dy \\ dz \end{pmatrix} = \begin{pmatrix} u \\ v \\ w \end{pmatrix} dt + \begin{pmatrix} \frac{\sigma_h}{\sqrt{T}} dw_x \\ \frac{\sigma_h}{\sqrt{T}} dw_y \\ \frac{\sigma_v}{\sqrt{T}} dw_z \end{pmatrix}$$

Which when integrated at each increment in time yields $\Rightarrow$

$$\begin{pmatrix} \Delta x \\ \Delta y \\ \Delta z \end{pmatrix} = \begin{pmatrix} u \\ v \\ w \end{pmatrix} T + \begin{pmatrix} \frac{\sigma_h}{\sqrt{T}} w_x \\ \frac{\sigma_h}{\sqrt{T}} w_y \\ \frac{\sigma_v}{\sqrt{T}} w_z \end{pmatrix}$$

where w_x, w_y, w_z are independent Brownian processes with a distribution described by $W{:}N(0,T)$. Tipification may be performed using the transformation $W^* = \frac{W}{\sqrt{T}}$ yielding,

$$\begin{pmatrix}\Delta x\\ \Delta y\\ \Delta z\end{pmatrix}=\begin{pmatrix}u\\ v\\ w\end{pmatrix}T+\begin{pmatrix}\sigma_h w_x^{::}\\ \sigma_h w_y^{::}\\ \sigma_v w_z^{::}\end{pmatrix}$$

where the Brownian processes are generated according to $N(0,1)$.

Appendix VI

Let C_o be the concentration of particles, typically one meter, above the terrain surface. Consider a volume τ close to the surface of the terrain. The quantity of particles contained in this volume is

$$m_v = C_o\tau = C_o Sw\Delta t$$

where S is the base surface and Δt the time interval considered.

Also, the mass of the deposited particles will be

$$m_{dep} = C_o\tau = C_o SV_d\Delta t$$

The deposition probability for a particle is calculated by

$$P_{dep} = \frac{m_{dep}}{m_w} = \frac{C_o SV_d\Delta t}{C_o Sw\Delta t} = \frac{V_d}{w}$$

The median deposition velocity for iodine and sulphur dioxide species is about $0.01\frac{m}{s}$. This value also appears to be a reasonable estimate for many other species in the absence of detailed information on the micrometeorology and surface characteristics.