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Mathematical modelling and numerical simulation of an air pollution problem and its local effects

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Abstract

Second order finite elements are applied to a Diffusion-Advection Equation to model and simulate the presence of air pollutants produced by local sources. Simplifications in the domain are presented and permit visualization of this presence. Some of these numerical results are presented.

1 Introduction

In recent years an effort has been made by State Authorities to locate a thermoelectric plant for the generation of electricity in the region close to the Campinas State University. Although much attention was given to the daily amounts of pollutants this plant would generate (70-80 daily tons of aerosols), little or no discussion was held on *where* this pollution would end up. Legal decisions on the location of such plants are at present taken at county level. This study indicates that these decisions should be at least regional including several affected counties.

The problem we model here with the purpose of undertaking numerical approximations and consequent computational simulations (in spite of no reliable data) includes the following phenomena:

(i) diffusion - the diffusive effect of the polluting particles in air;

(ii) advection - the transport of the particles by predominant wind currents in the region.

(iii) degradation - some of the particles react either with other components or with air bacteriae

The problem of simulating the environmental impact of the presence of this type of plant in a certain region in terms of the transport of aerosol pollutants becomes one of studyng the diffusive/advective problem with a localized source of this pollutant in a domain Ω.

2 The Models

According to 1., the model must be of the following kind (cf Marchuk [3])

$$\frac{\partial p}{\partial t} = \{\text{diffusion}\} - \{\text{advection}\} - \{\text{degration}\} + \{\text{source}\} \tag{2.1}$$

for $p = p(\boldsymbol{x}, t)$, $\boldsymbol{x} \in \Omega \subset I\!R^n$, $t \in [0, T]$.

Classic results give ([3], [4]), for (2.1)

$$\frac{\partial p}{\partial t} = \operatorname{div}(\alpha \nabla p) - \operatorname{div}(p.W) - \sigma p + f(\boldsymbol{x}, t), \tag{2.2}$$

where we have

α: the diffusivity of p in the domain Ω,

W: the direction and magnitude of predominant wind situation in the domain Ω and during the period $(0, T]$,

σ: the degradation parameter for p in $\Omega \times (0, T]$, and

f: the source(s) of p in $\Omega \times (0, T]$.

Even though the domain Ω is a limited subset of $I\!R^3$, considering a relatively large region, a "box" with a base meausuring 100 km $\times$ 50 km and height of 1 km, for example, leads us to a first approximation, by considering the domain simply as the rectangular base, so Ω becomes a domain of $I\!R^2$, and diffusivity becomes constant, $\alpha(x,t) = \alpha_0$, and we obtain instead of eqn(2.2):

$$(2.3) \quad \frac{\partial p}{\partial t} - \alpha_0 \Delta p + \operatorname{div}(W, p) + \sigma p = f \qquad \text{in } \Omega \subset I\!R^2 \text{ and } (0,T],$$

where $W = (V_1, V_2)$ represents wind magnitude and direction, σ is the decay of p, and f its source. Boundary conditions are of Dirichlet type (which explains the "distant" boundaries), and Initial Conditions are known:

$$(2.4) \qquad p(\boldsymbol{x}, t) = 0, \qquad \boldsymbol{x} \in \partial\Omega \text{ and } t \in (0,T],$$

$$(2.5) \qquad p(\boldsymbol{x}, 0) = p_0(\boldsymbol{x}), \qquad \boldsymbol{x} \in \Omega.$$

Instead of the classical formulation given by eqns(2.3)-(2.5), the weak or variational formulation is chosen, for several reasons. One of them is the source, which may, in fact, be non-zero only at one point. We therefore get:

$$p \in \mathcal{V},$$

$$(2.6) \quad \left(\frac{\partial p}{\partial t} | v\right) + \alpha_0 (\nabla p | \nabla v) + (\operatorname{div}(Wp)|v) + \sigma(p|v) = (f|v), \forall v \in \mathcal{V}, \text{ for}$$

$$(2.7) \quad \mathcal{V} = \{v \in L^2((0,T), H_0^1(\Omega))\} \text{ and}$$

$$(2.8) \quad p(\boldsymbol{x}, 0) = p_0(\boldsymbol{x}) \qquad \text{on } \Omega.$$

For this formulation existence and uniqueness results can be derived, Lions [2] and Palomino-Castro [5], and with the use of second order finite elements, the obtained results are in the first figure (note that the source is located in the center of the domain, and that the x-axis was chosen in the direction of predominant wind current).

Another possible approach is that of considering a vertical plane (in the x and z axes), cutting the original three-dimensional domain in such a way that it contains the predominant wind current and the source. Several differences from the previous case must be mentioned.

In this new situation the diffusivity is no longer constant and is considered as a linear function in z, the height:

$$\alpha(z) = \alpha_0 + \beta z. \tag{2.9}$$

Equation (2.2) becomes, consequently,

$$\frac{\partial p}{\partial t} - \alpha_0 \Delta p - \beta \frac{\partial p}{\partial z} + V_1 \frac{\partial p}{\partial x} + V_3 \frac{\partial p}{\partial z} + \sigma p = f, \quad \text{for} \quad \boldsymbol{x} \in \Omega \subset I\!R^2 \text{ and } t \in (0,T]. \tag{2.10}$$

Here, V_1 and V_3 are the components of W in the x and z directions, respectively. Boundary conditions are also different. Naming the four sides of the rectangular domain as Γ_0 (the "ground" side), Γ_2 (the "sky" side), Γ_1 and Γ_3 (the "lateral" sides of Ω), with $\partial\Omega = \Gamma_0 \cup \Gamma_1 \cup \Gamma_2 \cup \Gamma_3$, we get:

$$p(\boldsymbol{x}, t) = 0 \tag{2.11}$$

$\boldsymbol{x} \in \Gamma_1 \cup \Gamma_3$, $t \in (0,T]$, for Γ_1 and Γ_3 taken as distant from the source as necessary, and

$$\frac{\partial p}{\partial \eta}(\boldsymbol{x}, t) = 0 \tag{2.12}$$

$\boldsymbol{x} \in \Gamma_0 \cup \Gamma_2$, $t \in (0,T]$, indicating that no pollutant leaves the domain neither by the sky side nor by the ground side.

As previously, the initial conditions are known:

$$p(\boldsymbol{x}, 0) = p_0(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega. \tag{2.13}$$

Also as previously, the variational formulation is used:

$$p \in \mathcal{V},$$

$$\left(\frac{\partial p}{\partial t}\middle| v\right) + \alpha_0 (\nabla p)|\nabla v) + V_1 \left(\frac{\partial p}{\partial n}\middle| v\right) + \\ +(V_3 - \beta)\left(\frac{\partial p}{\partial z}\middle| v\right) + \sigma(p|v) = (f|v), \forall v \in \mathcal{V}. \tag{2.14}$$

The space $\mathcal{V}$ is now a subspace of the chosen space in the previous example:

$$\mathcal{V} = \left\{v \in L^2((0,T), H^1(\Omega)) : v|_{\Gamma_1 \cup \Gamma_3} = 0, \left.\frac{\partial v}{\partial n}\right|_{\Gamma_0 \cup \Gamma_2} = 0\right\}. \tag{2.15}$$

Existence and uniqueness results still hold.. First order finite elements were chosen in this case, and the resulting numerical simulations are illustrated in the last two figures.

3 Conclusions

In spite of not being able to use precise data, the parameters used in the numerical calculations were suggested by the Nucleus for the Study of Environmental Problems (NEPAM) of the University [6], results clearly indicate what common sense states in an imprecise but truthfull manner: wind spreads pollutants all over. But more directly, these simulations show that even if pollutants already exist, and a source is present, prevailing wind currents may cause greater pollution elsewhere, accross the county line, so to say. The conclusion is that legislation permitting local decisions in installing polluting plants must be modified. These decisions must be at least regional if not at state level.

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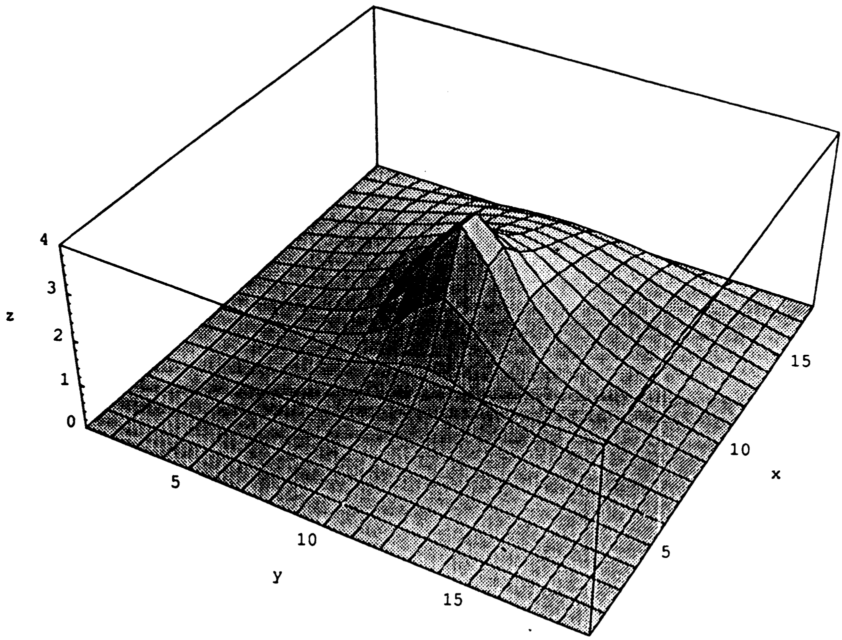
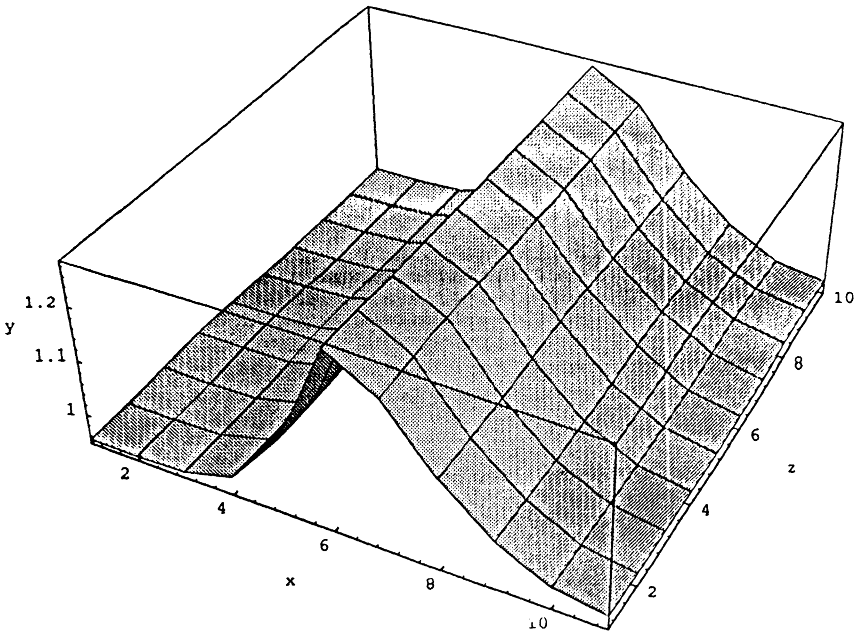


Figure 1: Horizontal Domain, Constant Diffusivity



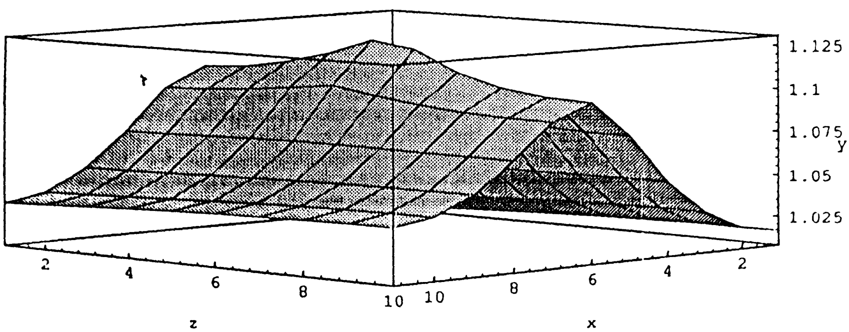


Figure 2: Vertical Domain, Variable Diffusivity