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NUMERICAL STUDY OF 3D ATMOSPHERIC POLLUTANT DISPERSION OVER REAL TERRAIN

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Abstract. *A non isotropic turbulence model is extended and applied to three dimensional stably stratified flows and dispersion calculations. The model is derived from the algebraic stress model (including wall proximity effects), but it retains the simplicity of the "eddy viscosity" concept of first order models. The "modified k-ε" is implemented in a three dimensional numerical code. Once the flow is resolved, the predicted velocity and turbulence fields are interpolated into a second grid and used to solve the concentration equation. In this work the model is evaluated against a full scale dispersion experiment. Flow and tracer dispersion over Cinder Cone Butte (USA) is computationaly simulated. The lateral divergence at low levels, a marked characteristic of stable flows, is well reproduced by the model. The plume path and its sensitivity to the approaching wind direction are well captured. Ground level concentrations are overestimated by the numerical model, probably because of large deviations of the wind direction near the ground during the field experiment, which spreaded the plume and resulted in low ground level concentrations.*

Keywords: *Atmospheric dispersion, flow over hills, modified k-ε , numerical simulation*

1. INTRODUCTION

The study of flow over complex terrain has been intense in the last two decades, aiming both the analysis of structural implications due to strong winds (neutral atmosphere) and the pollutant dispersion under neutral or stable conditions. More recently, the computational simulation has been used along with laboratory and field experiments in order to improve mathematical models which try to represent the very complex physical phenomena involved in the atmospheric boundary layer flows.

The phenomenal increase in computer power over the last two decades has led to the possibility of computing such flows by the integration of the (modelled, time-averaged)

Navier-Stokes equations and a corresponding concentration equation for the pollutant transport. Raithby *et al* (1987) employed the k-ε model (with modification in the C_μ value) to calculate the neutrally buoyant flow over the Askervein hill, and compared their numerical results with the experiment made over the real terrain in Scotland. Dawson *et al* (1991) also used the k-ε model (with some modification in the constants of the dissipation equation) to simulate the flow and dispersion over Steptoe Butte (Washington, USA) under neutrally and stably stratified atmosphere. Their results were favorably compared with experimental data, indicating that mathematical models using the eddy viscosity assumption in the turbulence closure could be used to predict the flow and pollutant dispersion over complex terrain.

Koo (1993) developed a non-isotropic modified k-ε to account for different eddy diffusivities in the lateral and vertical directions in the atmosphere. His model is derived from the algebraic stress model and was applied in one dimensional problems to predict the vertical profiles of velocity, potential temperature and turbulence variables for horizontal flow in a homogeneous boundary layer. Also, the model was applied in two dimensional problems to simulate the sea breeze circulation and the manipulation of the atmospheric boundary layer by a thermal fence

Castro and Apsley (1997) compared numerical (using a "dissipation modification" k-ε model, as named by the authors) and laboratory data for two-dimensional flow and dispersion. Also, Apsley and Castro (1997) used a finite-volume code to compute flow and dispersion in stably stratified flow over a complex topography (Cinder Cone Butte). They applied a length scale limiting strategy suitable for atmospheric boundary layer applications.

In Brazil, Dihlmann (1989) studied numerically the thermal discharge (from chimneys) into neutral and stable stratified environments. Santos *et al* (1992) applied the standard k-ε model to simulate the discharge of a chimney and the correspondent plume dispersion over a flat terrain. Queiroz *et al* (1994) applied the standard k-ε model to study (in two dimensions) the effect of heat islands in the atmospheric diffusive capacity. Netto *et al* (1997) developed a methodology to determine the atmospheric dispersive capacity in the convective atmospheric boundary layer in a given region during daytime. As a result, the Pasquill stability class and dispersion parameters are determined. Boçon and Maliska (1997a, 1997b, 1998) extended the non isotropic k-ε model of Koo (1993) to numerically simulate the flow and pollutant dispersion over complex idealized topography, under neutral and stable stratification. Computational results were compared with experimental data obtained from a wind tunnel simulation.

More sophisticated models, like the Reynolds stress model were also applied to environmental flows and pollution. Sykes and Henn (1992) applied the Large Eddy Simulation technique to simulate plume dispersion. Our view is that for the time being, because of limitations in computer resources, those more complex turbulence models (like Reynolds stress and LES) are not suitable for most engineering problems, due to large CPU time and memory required.

The main effects of topography on the dispersion of pollution result from changes to the mean flow (which affects the plume path), turbulence (which affects the plume shape and the rate of spread) and the possibility of advection into, or release within, recirculating flow regions. In the present work we extend the modified k-ε model of Koo (1993), cited above, to three dimensional flows and pollutant dispersion in neutrally stratified environments.This work is dedicated to the numerical study of flow and pollutant dispersion over a real terrain. Previous works of the present authors concerned the calculation of flow and dispersion over idealized topography and their results were compared to laboratory experiments. This time, our results are compared with the results of full scale and laboratory experiments.

2. MATHEMATICAL MODEL

The task of computing the concentration field downstream from a pollutant source is divided into two decoupled steps. Firstly we calculate the flow (velocity, temperature and turbulence variables) in the region of interest. Secondly, we use the computed velocity field and eddy diffusivities to solve the concentration equation. This separation can be done as we consider that the pollutant release does not disturb the flow. In fact, in the Cinder Cone Butte experiment, against which we compare our results, the tracer gas was released with practically no momentum nor buoyancy force.

The governing equations for the stratified flow are the conservation of mass, momentum and energy, written below in the usual tensor notation. Dispersion of a pollutant is computed from the concentration equation, after the flow is resolved.

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{1}$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial}{\partial x_i}\left(p + \frac{2}{3}\rho k\right) + \frac{\partial}{\partial x_j}\left[K^{m}_{x_j}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right] - \frac{\tilde{\rho}}{\rho} g \delta_{i3} \tag{2}$$

$$\frac{\partial \theta}{\partial t} + u_j \frac{\partial \theta}{\partial x_j} = \frac{\partial}{\partial x_j}\left(K^{h}_{x_j}\frac{\partial \theta}{\partial x_j}\right) \tag{3}$$

$$\frac{\partial c}{\partial t} + u_j \frac{\partial c}{\partial x_j} = \frac{\partial}{\partial x_j}\left(K^{h}_{x_j}\frac{\partial c}{\partial x_j}\right) + S \tag{4}$$

where u_i is velocity in x_i direction, ρ is the air density, p is the pressure deviation with respect to the hydrostatic pressure, θ is the potential temperature, c is concentration, K^j_m is the turbulent eddy viscosity in the j direction, K^j_h and K^j_c are the eddy diffusivity in the j direction, respectively for heat and concentration. As the horizontal extension of the problem is 3 km, the Coriolis force is neglected. According Meroney (1990), for distances up to 50 km this simplification may be assumed.

In environmental flows the non isotropic character of turbulence is notable, specially in the case of dispersion of a scalar (pollutant) in the flow. For the case of stably stratified flows, for instance, vertical fluctuations are much inhibited due to buoyancy forces (arising from the positive vertical temperature gradient), while horizontal fluctuations are not. The turbulence model applied is a non isotropic k-ε. Anisotropy of the turbulence is taken into account by considering different turbulent diffusivities for horizontal and vertical directions. Due to limited space, description of the turbulence model is not here presented. Details may be seen in Boçon and Maliska (1997a, 1997b, 1998).

3. EXPERIMENTAL STUDY

In 1980 the US Environmental Protection Agency (EPA) conducted a full scale dispersion experiment in Idaho, USA. The chosen site was Cinder Cone Butte (CCB), an isolated, roughly axisymetric hill about 100m high and 500m radius. Meteorological information indicated an ocurrence of very stable conditions during nightime in that region. Tracer gas was released approximately 600m upwind the hill, at 35m above the local terrain. Samples were placed at the ground level all around the hill and gas chromatography was used to determine the tracer concentrations. The results represent hour averaged values. Wind speed and direction, temperature and velocity fluctuations were measured at six meteorological towers (four of them 10m, one 30m and one 150m high). Tethersonde and minisonde systems collected some data above the heights of the towers. A complete description of the field experiment is reported by the EPA (Truppi and Holzworth, 1984).

4. NUMERICAL EXPERIMENT

Here, we report the computational simulations of one particular case study (experiment 206, 05:00-06:00 local time).This case was chosen because it is representative of very stable atmospheric conditions, which is generally the worst situation from the view of atmospheric pollution. Also, this case was already numerically studied by Apsley and Castro (1997), and was object of a laboratory (towink tank) experiment conducted by the EPA (Snyder, 1990). Figure 1 sketches the problem as it was computationally simulated for the flow calculation. For the flow, the domain extends 3km in the lateral (horizontal crosswind) direction. For the concentration, the grid is 1500m long in the main flow direction (x), begining 50m upwind the source. Laterally it extends 1200m in the crosswind direction, and is 300m high.

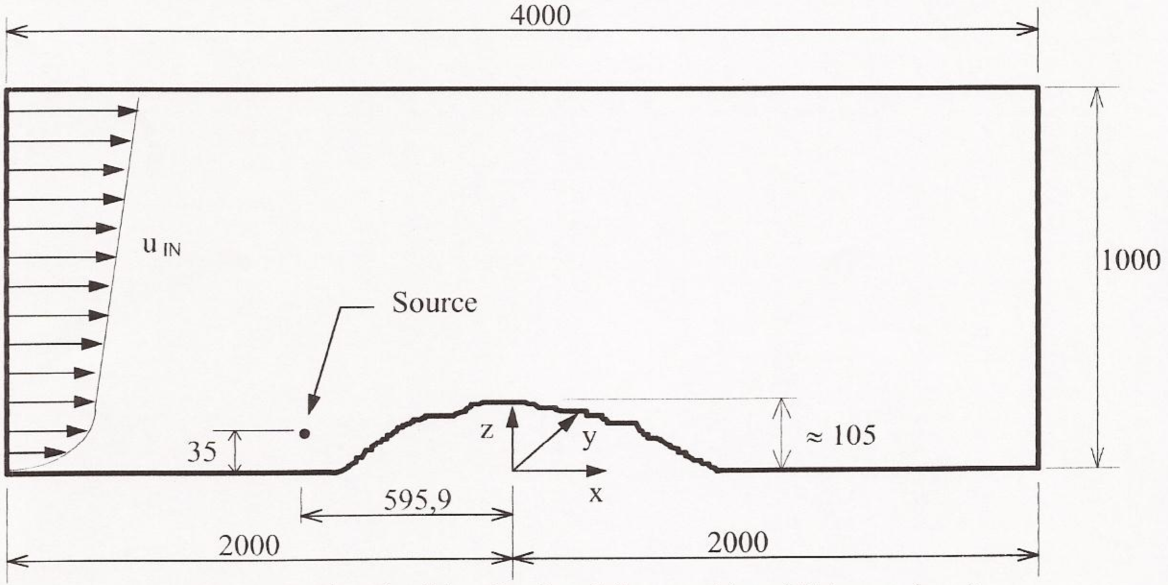

Figure 1- Sketch of the simulated flow problem (distances in m)

As the grid used for computing the flow is not adequate for the concentration calculation, a second grid (refined near the source) is used for the last purpose. Velocities and eddy diffusivities obtained from the flow solution are interpolated into the second grid for the concentration calculation. Also, in order to verify grid dependent errors, the computations are made in a coarse and in a fine grid. Figure 2 illustrates the grid used for flow (inflow boundary at left). Coarse grids have half the number of volumes in each direction, with respect to the fine grids. Flow grids are 35x32x18 and 70x64x35, concentration grids are 49x49x27 and 98x97x55. The grids were algebrically generated by our code TOPOGRID, which takes the digitised topography and produces grids aligned with the upwind direction, allowing local refinement where it is necessary.

The average upwind direction is 127° (with respect to the W-E direction) and the average speed at the tracer source is 1,1 m/s. The potential temperature gradient of the approaching flow is 2,1 K / 100 m. The finite volume method is employed to solve the governing equations, in a non orthogonal, generalized curvilinear coordinate system. Co-located arrangement is used for variables storage in the grid, and the QUICK interpolation scheme with source deferred correction term (Lien, 1994) is applied on the convective terms, except for turbulence variables where a hybrid scheme (WUDS) is adopted. Our own codes NAVIER (1991) and SMOKE (1997) are used to solve the governing equations, respectively, for the flow and concentration.

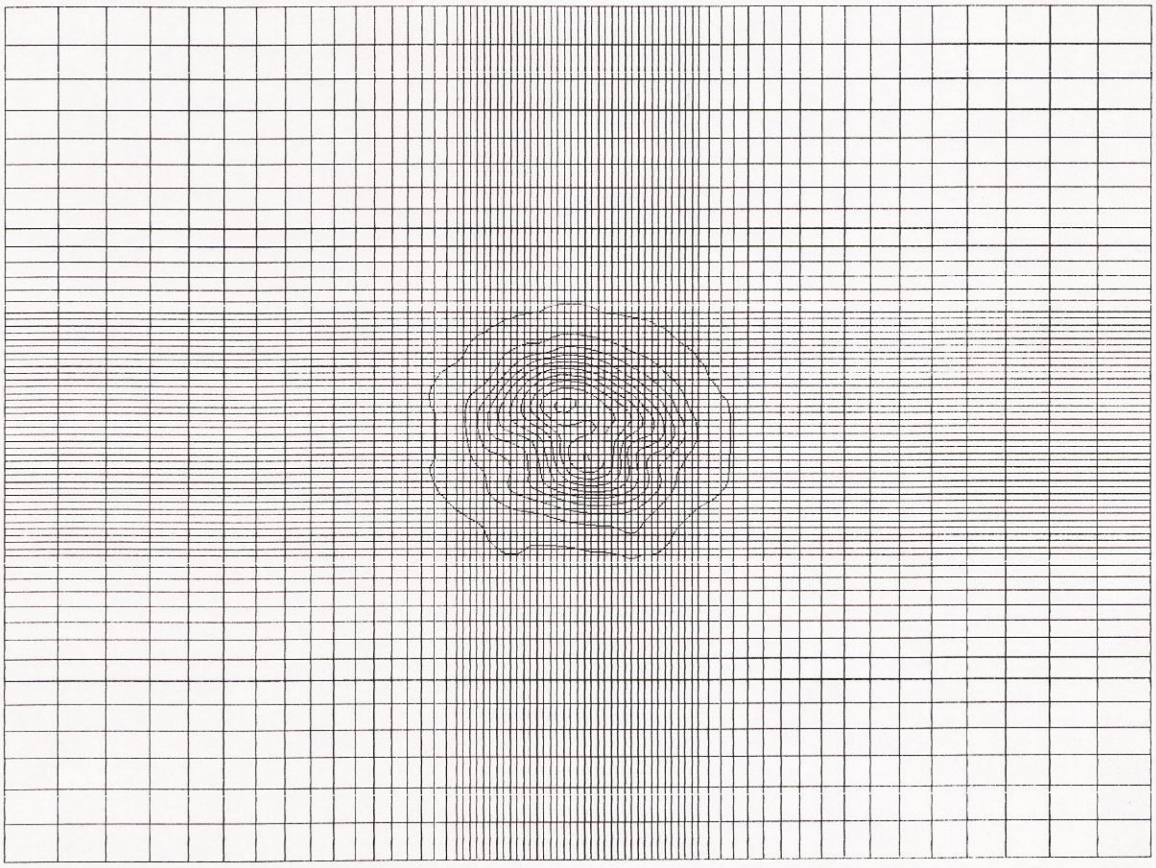

Figure 2- Top view of the fine grid for the flow calculation over CCB

5. BOUNDARY CONDITIONS

Velocity and potential temperature at the upwind boundary were adjusted from the experimental data. As the turbulence intensity was not measured, turbulent kinetic energy and its dissipation rate at the inflow were determined by solving the one dimensional counterparts (in the vertical direction) of the governing equations for the flow, using the velocity and temperature inflow profiles.

$$u = \begin{cases} u_0\left(\dfrac{z}{80}\right)^{0.8} & (z \leq 106\ \text{m}) \\ u_0\left(\dfrac{z-95}{80}\right)^{1/7} + 3 & (z > 106\ \text{m}) \end{cases} \qquad (5)$$

$$\theta = \theta_0 + \frac{T_*}{k_v}\left(\ln\frac{z}{z_0} + \frac{5z}{L}\right) \quad (6)$$

where u_0=6m/s, $\theta_0 = 279$ K , $T_* = 0.053$ K e L = 33 m (comprimento de Monin-Obukhov).

At the ground, the law of the wall suitable for atmospheric flows is applied. Velocity and temperature at the volumes adjacent to the ground are related to momentum and heat fluxes by

$$V_p = \frac{u_*}{k_v}\left[\ln\frac{h_p}{z_0} + \Psi_m\left(\frac{h_p}{L}\right)\right] \quad (7)$$

$$\theta_p - \theta_0 = \frac{-H}{k_v \rho C_p u_*}\left(\ln\frac{h_p}{z_0} + \frac{5h_p}{L}\right) \quad (8)$$

where V_p, θ_p and h_p are velocity, temperature and height of the volumes adjacent to the ground, u_* is the friction velocity, θ_0 is the ground temperature, H is the heat flux and z_0 is the surface roughness (=0,1m). For the turbulence variables it is assumed local equilibrium at the ground, and for concentration the ground is considered impermeable (null mass flux). All fluxes of momentum, heat and pollutant at the lateral and upper boundaries are null. Diffusive flux of all variables are neglected at the outflow boundary.

6. FLOW RESULTS

An interesting feature of stable stratified flows is the fact that, in presence of an obstacle, at low levels the flow does not have enough energy to overpass the hill. This lower layer has significant lateral divergence with the flow following the countours of the hill. According to Snyder et al (1985), there is an upstream height - the dividing streamline height - below which flow has insufficient energy to attain the summit of the hill and must pass around the sides. The calculated height of the so called dividing streamline for the present case study is 32m. In the numerical simulation, however, there is not a clear separation between the lower (almost horizontal) and the upper (passing over the hill) layers. It was found that for heights up to ≈10m the flow is essentially horizontal, passing around the hill. Above ≈20m the flow overpasses the hill with no lateral divergence. The numerical dividing streamline height of ≈15m may be assumed, considerably less than the theoretical height of 32m.

7. CONCENTRATION RESULTS

A plume released in stable atmosphere over flat terrain demands longer distances to reach the ground, because of relative small turbulent diffusion, in contrast with releases under neutral or unstable flows. Over irregular terrain the plume reaches the ground much closer the source (compared with flat terrain) due to the topography. In the present case of CCB the plume reached the ground on the upwind slope of the hill, roughly 400m downwind the source. Other important feature is the lateral deviation, caused by the divergence of the flow, which turns around the hill at low levels (up to 15m, as explained in the previous section). Concentration results at the ground (1m above local terrain) are shown in fig. 4. Numerical results are overestimated, when compared with the experimental values. This can be explained by the large variation of the flow direction near the ground (20° to 240°, 127° average), as plotted in fig. 3. Changes in the wind direction drive the plume from one side of the hill to another, alternately. That causes a large spread of the real plume and, hence, lower concentrations at the ground.

As cited in the introduction section, Apsley and Castro (1997) numerically studied the flow and dispersion over CCB. Due to the limited space it is not possible to present their results in this work to better compare them with ours . We verified that the plume path was similarly predicted by their model (comparing with our results), while the concentration values obtained by those authors were even more overestimated than our results, when compared with the experimental concentrations.

To verify the influence of the wind direction (WD), two different cases were numerically studied. Deviations of 5° and 10° with respect to the observed mean wind direction (127°) were considered. Boundary conditions were the same as for the case WD=127°. Fig. 5 shows ground level concentration contours for WD=127°, 122° and 117°. Our numerical and the EPA's laboratory small scale experiment (Snyder 1990) results may be compared. It can be noticed that in the physical experiment the influence of the approaching wind direction is more significant. Also, the towing tank concentrations are clearly overestimated. As the approaching flow wind direction changed by a mere 10°, the region of high ground level concentrations switched from one side of the hill to the other, consistent with the large spread of concentration encountered over the hour during the field experiment.

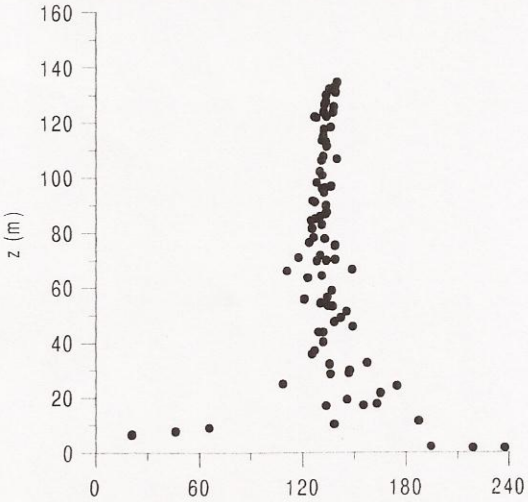

Figure 3 - Upwind mean direction (deg)

Due to the great sensitivity of the plume path to the wind direction, along with the large variation of the last near the ground, we conclude that the plume dispersion, and hence the concentrations, may not be quantitatively well predicted by computational or laboratory experiments in which the upstream conditions remain constant. Inspecting the ground level concentration results we noted that the best concordance between computational and experimental concentrations is attained for WD=127°, which is the measured mean wind direction during the field experiment. It means that the numerical model has satisfactory hability to predict the plume path , while the concentration values are overestimated.

8. CONCLUSION

A modified non isotropic k-ε model is applied to simulate three dimensional stably stratified atmospheric flow (Pasquill class E) and dispersion over real terrain (Cinder Cone Butte - CCB). Anisotropy of the turbulence is taken into account by considering different turbulent diffusivities for horizontal and vertical directions. Once the flow is calculated, the variables are interpolated into a second grid and the concentration equation is resolved. The finite volume method is employed to solve the differential model equations. Results show the characteristic of lateral divergence of the low levels of the flow, which contour the hill horizontally. This lateral divergence causes the plume to be convected to one side of the hill. The predicted plume path is in concordance with the experimental data from CCB. Numerical concentrations at the ground are overestimated, much possibly because of large changes in the upwind mean direction during the field experiment, which enhanced the spread of the real plume and resulted in lower concentrations.

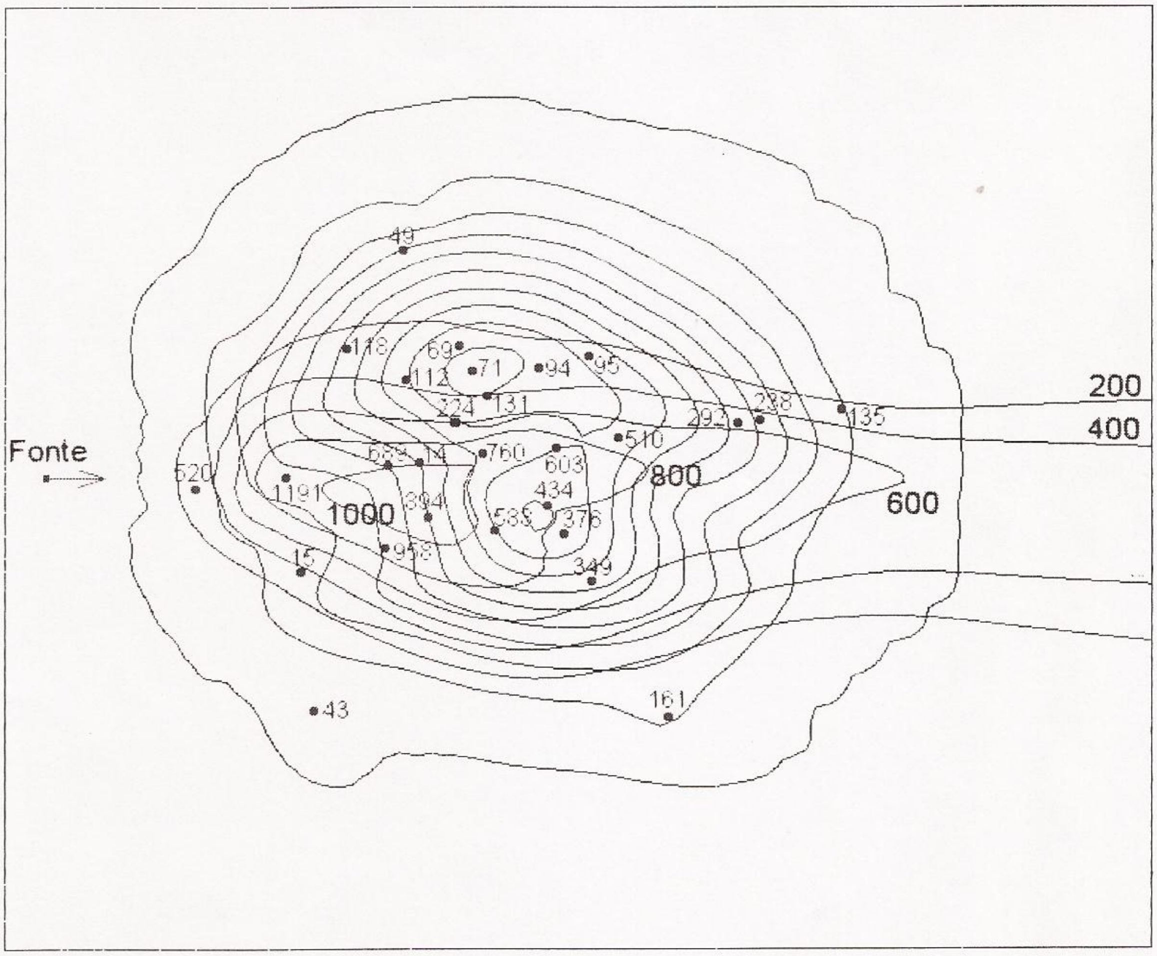

Figure 4 - Ground level concentration contours for WD=127° (dotted values are experimental)

9. ACKNOWLEDGMENTS

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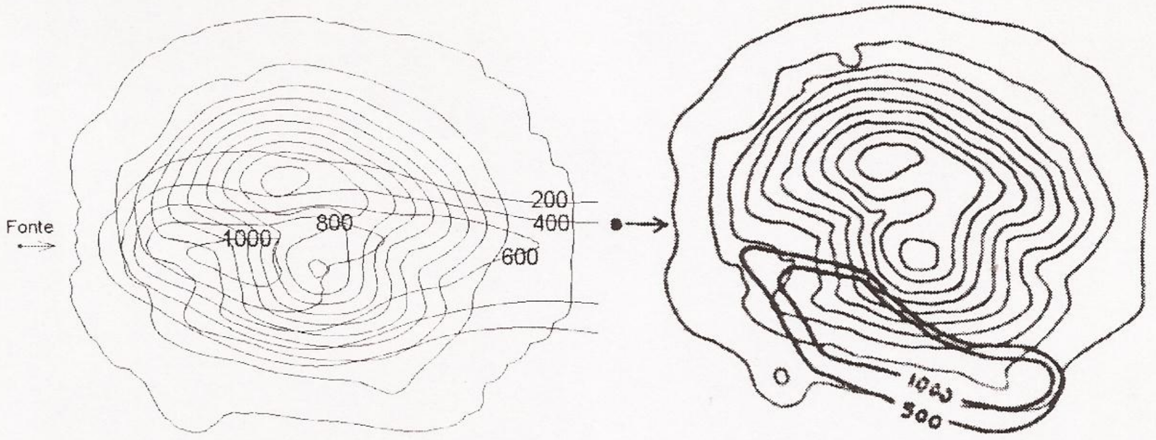
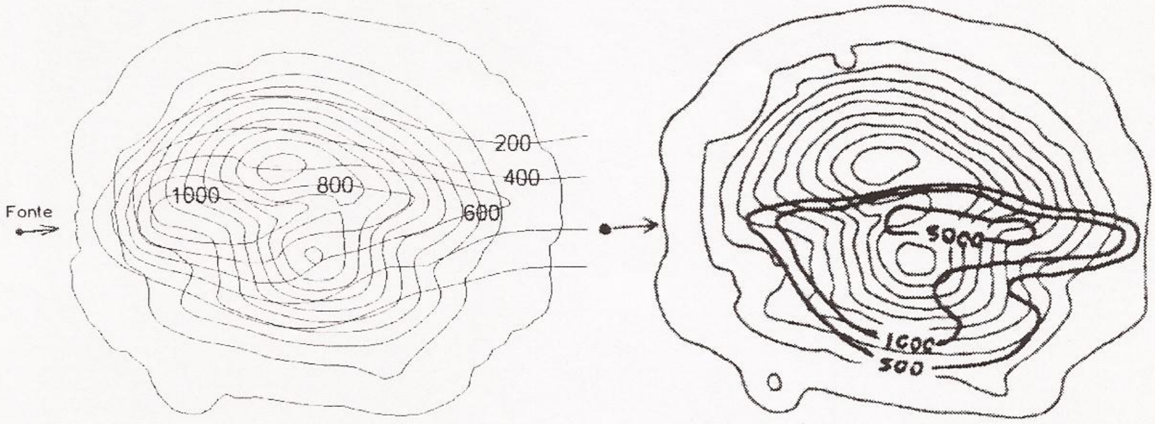
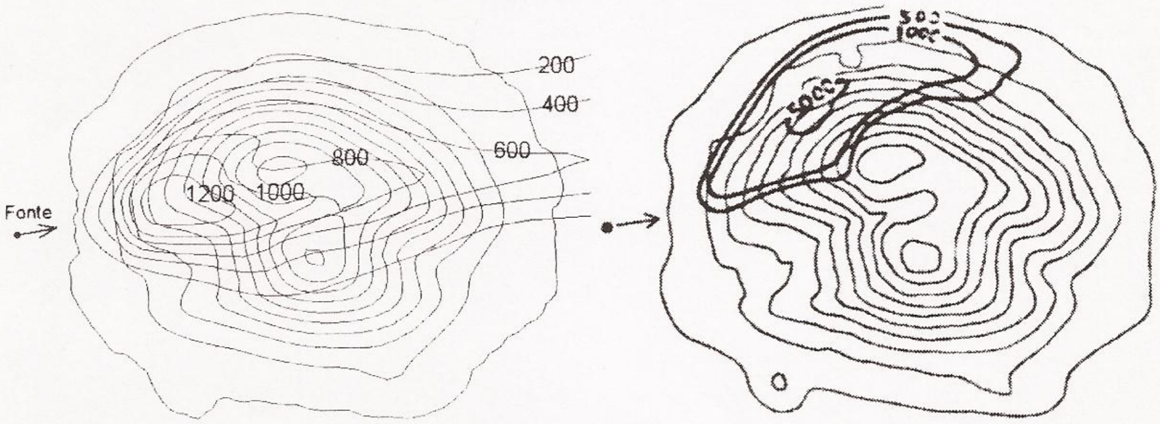


(a) WD = 127°



(b) WD = 122°



(c) WD = 117°

Figure 5 - Sensitivity to wind direction (WD).
Numerical (left) and laboratory (towing tank) results (right) - values in ppt

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