NUMERICAL MODELLING OF FLOW AND DISPERSION OVER COMPLEX TERRAIN / *MODELAGEM NUMÉRICA DO ESCOAMENTO E DA DISPERSÃO EM TERRENO COMPLEXO*

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Abstract

Due to the complexity of some topography driven atmospheric flows, it is sometimes not possible to accurately predict pollutant transport on the basis of sparse wind field measurements. A possible solution is the mathematical modelling of both the flow and pollutant transport. In order to overcome shortcomings of the conventional k-ε turbulence model for this kind of flows, a more general model of environmental flows, a modified k-ε, is adopted. This non-isotropic model is derived from the algebraic stress model including wall proximity effects. The modified k-ε is implemented in a three dimensional 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. To evaluate the model, various steady state numerical solutions are compared with dispersion experiments which were conducted at the wind tunnel of Mitsubishi Heavy Industries, in Japan. Several cases of dispersion under neutrally stratified atmospheres over flat and hilly terrain are compared and discussed. Vertical profiles of concentration are shown and compared.

Keywords

Atmospheric dispersion, flow over hills, modified k-ε, numerical simulation
Dispersão atmosférica, escoamento sobre montanhas, k-ε modificado, simulação numérica

1. INTRODUCTION

The study of flow over hills (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. Dawson (1987) used 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. His results were favorably compared with experimental data, indicating that mathematical models using the eddy viscosity assumption in the turbulence model 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. Koo's model is similar to the level 2.5 model of Mellor and Yamada (1982).

Recently, 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. In Brazil, 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. 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 apply the modified k-ε model of Koo (1993), cited above, to three dimensional flows and pollutant dispersion in neutrally stratified environments.

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 viscosities to solve the concentration equation. This separation can be done as we consider that the pollutant release doesn't disturb the flow. In fact, in the wind tunnel experiment against which we compare our results, the tracer gas was released with practically no momentum nor buoyancy force.

2.1 Flow and Dispersion Modelling

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

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

$$\frac{\partial u_i}{\partial t}+u_j\frac{\partial u_i}{\partial x_j}=-\frac{1}{\rho}\frac{\partial p}{\partial x_i}+\nu\frac{\partial^2 u}{\partial x_j \partial x_j}+\frac{\partial}{\partial x_j}\left(-\overline{u_i' u_j'}\right) \tag{2}$$

$$\frac{\partial c}{\partial t}+u_j\frac{\partial c}{\partial x_j}=\frac{\partial}{\partial x_j}\left(-\overline{u_i' c'}\right) \tag{3}$$

where p is the pressure deviation with respect to the hydrostatic pressure. Primed variables denote turbulent fluctuations. As we are simulating wind tunnel flows, the Coriolis effect is neglected. In this work, only neutrally stratified flows are simulated. Modelling of fluctuation terms are described in the next section.

2.2 Turbulence Model

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. Even neutrally stratified flows feature some anisotropy. So, it's not expected that isotropic turbulence models may well reproduce the non isotropic turbulent diffusion. However, standard k-ε is successfully applied for environmental flows calculation where horizontal gradients (of velocity, temperature and turbulence variables) are smaller than the vertical gradients. In these situations, turbulent diffusion is significant only in the vertical direction, and an isotropic model can handle it appropriately. On the contrary, in the problem of pollutant dispersion from a point source, both vertical and horizontal concentration gradients are significant, so are the corresponding turbulent diffusion. For this situations, a better description of the anisotropy in turbulent exchanges is necessary.

In his Ph.D. thesis, Koo (1993) proposed a modification on the classic k-ε model, through use of algebraic stress model including wall proximity effects. The resulting model was compared to data and higher order simulations in stable, neutral and convective one dimensional atmospheric boundary layers (homogeneous horizontal flows). The modified k-ε reproduced well the observed behaviors. Also, for two dimensional flows, the model was applied to simulate the sea breeze circulation and to estimate the dispersion of pollutants by a "thermal fence" under neutral and stable conditions.

In our work we extend the application of the Koo's modified k-ε model to three dimensional flow and dispersion problems. A description of the turbulence model is given below. Detailed description of derivation of the model can be seen in Koo (1993). Following the Boussinesq's eddy viscosity concept, Reynolds stresses and turbulent mass transfer are related to the gradients of the transported quantities as

$$-\overline{u_i' u_j'}=K_m^j\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)-\frac{2}{3}k\delta_{ij} \qquad -\overline{u_j' c'}=K_c^j\frac{\partial c}{\partial x_j} \tag{4,5}$$

Where c is concentration, K_m^j and K_c^j are, respectively, turbulent eddy viscosity and turbulent eddy diffusivity of mass in the j direction.

Eddy viscosities (for momentum) and eddy diffusivities (for concentration) are expressed as function of turbulent kinetic energy and its dissipation rate. For the vertical direction:

$$K_m^z = C_m \frac{k^2}{\varepsilon} \qquad K_c^z = C_c \frac{k^2}{\varepsilon} \tag{6,7}$$

And for the horizontal directions:

$$K_m^x = K_m^y = C_\mu \frac{k^2}{\varepsilon} \qquad K_c^x = K_c^y = \frac{K_m^x}{Sc_t} \tag{8,9}$$

Sc_t=0.5 is the turbulent Schmidt number. C_m and C_c are proportionality coefficients for eddy viscosity and eddy diffusivity in the vertical direction, respectively. They are defined by functions of flow structure (from the algebraic stress model).

$$C_m = \frac{2}{3} \frac{E_7(c_1 - 1)}{E_4 - E_5 E_7 G_M} \tag{10}$$

$$C_c = \frac{2}{3} \frac{(c_1 - 1) + E_5 G_M C_m}{(c_{1T} + c'_{1T} f)E_4} \qquad f = \frac{l}{k_v z} = \frac{C_\varepsilon k^{3/2}}{k_v z \varepsilon} \tag{11,12}$$

f is the wall function which reflects the effect of the ground proximity on the Reynolds stress, l is the turbulence length scale, k_v is the von Karman constant (=0.4), z is distance from the ground and C_ε = 0.13. Other constants in equations (10) and (11) can be found in Koo (1993).

The C_m and C_h are functions of G_M, the production of turbulent kinetic energy by mean velocity shear

$$G_M = \left(\frac{k}{\varepsilon}\right)^2 \left[\left(\frac{\partial u}{\partial z}\right)^2 + \left(\frac{\partial v}{\partial z}\right)^2\right] \tag{13}$$

Turbulent kinetic energy and its dissipation rate are computed from their well known prognostic equations:

$$\frac{\partial k}{\partial t} + u_j \frac{\partial k}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\frac{K_m^j}{\sigma_k}\frac{\partial k}{\partial x_j}\right) + P - \varepsilon \tag{14}$$

$$\frac{\partial \varepsilon}{\partial t} + u_j \frac{\partial \varepsilon}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\frac{K_m^j}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial x_j}\right) + \left(C_{\varepsilon 1}P - C_{\varepsilon 2}\varepsilon\right)\frac{\varepsilon}{k} \tag{15}$$

P is the production term due to mean velocity gradient:

$$P = -\overline{u'_i u'_j}\frac{\partial u_i}{\partial x_j} = K_m^j\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\frac{\partial u_i}{\partial x_j} \tag{16}$$

Constants in equations (14) and (15) are those from the standard k-ε model and C_μ=0.09.

3. NUMERICAL TECHNIQUES

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 convection terms, except for turbulence variables where a hybrid scheme (WUDS of Raithby and Torrance, 1967) is adopted. Our own codes NAVIER and SMOKE were used to solve the flow and concentration.

As the grid used for computing the flow is not adequate for 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 1 illustrates some of the coarse grids used for flow and concentration (inflow boundary at left). Fine grids are 95x41x41 and 128x64x64 for flow and concentration, respectively. Only half domain is resolved, because of symmetry.

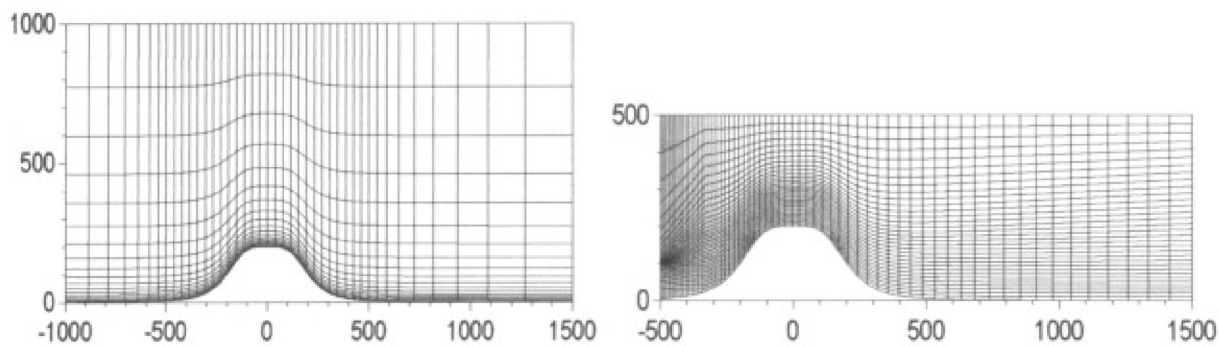

Figure 1 - Vertical view (at the xz symmetry plane) of the coarse grids, for flow (42x18x18, to the left) and concentration (64x32x32, source height 100mm, to the right)

4. TEST CASES AND BOUNDARY CONDITIONS

To verify the model performance, in a first step, the above described modified k-ε is applied to simulate wind tunnel experiments. A second series of tests, this time for a full scale experiment, will soon be performed.

4.1 The Wind Tunnel Experiment

Pollutant dispersion wind tunnel experiments were conducted at the Mitsubishi Heavy Industries, in Nagasaki, Japan, 1991. A report containing the results was obtained directly from that company. Wind tunnel test section is 2.5m wide, 1m high and 10m long. Axisymmetric hills of different heights (0, 100 and 200mm), were positioned with the top located at (x,y)=(0,0). Hill shape can be seen in fig. 1 and 2. Streamwise direction is x, lateral is y and vertical is z. Source of tracer gas was positioned at (x,y,z)=(-500 mm,0,50mm) for hill heights 0 and 100mm, and at (x,y,z)=(-500mm,0,100mm) for hill height 200mm. Cases of neutral ($\Delta T=0$, Pasquill class D) and stable atmosphere ($\Delta T=20°C$, Pasquill class E) were performed. Streamwise velocity, velocity fluctuations, temperature and concentration were measured at various locations.

4.2 Numerical experiments, boundary conditions and treatment of near source diffusivities

Three different wind tunnel experiments were simulated. They are designated with a letter - indicating stability class - followed by a number indicating hill height in mm. For the time being, only neutrally stratified flows are simulated. At the inflow boundary, velocity and turbulent kinetic energy were specified according to experimental measured values. Unitary concentration is specified at the volumes representing the source, and zero on the rest of inflow. Length scale is given by:

$$l = \frac{C_\mu^{3/4} k^{3/2}}{\varepsilon} = k_v z \tag{17}$$

Outflow conditions are that of zero-gradient for all variables. For velocity, lateral and upper boundaries are impermeable, with zero tangential stresses. For all other variables, lateral and upper boundary conditions are of zero-gradient. Wall functions are invoked to apply boundary conditions appropriate to a rough wall (z_0=1.5e-4m) at the ground. For concentration, the ground is considered impermeable (zero-gradient condition). Symmetry conditions are applied at the boundary coincident with the plane of symmetry (y=0).

After applying the modified model and computing concentrations, we constated that, for all the cases studied, there was a large unrealistic plume spread near the source and, consequently, low concentrations everywhere in the domain (specially up to 500mm downstream the source). Taking a look at the turbulence length scale near the source, we noticed that it is larger than the plume dimensions. It means that the turbulent eddy sizes present in the flow are bigger than the plume, and could not promote such a observed diffusion in the numerical simulations. Therefore, we speculate that the length scale to be applied in the eddy diffusivities for the concentration should be appropriately reduced for the initial stages of plume spread, according to local plume dimensions. Based on a Gaussian plume distribution near the source, as a first investigation, we decide to reduce linearly the eddy diffusivities computed from the flow solution, to be applied in the concentration calculations. Using this simple procedure, the quality of results improved considerably. Reduction of eddy diffusivity near the source is made taking its value (at the source location), obtained from the flow solution, and applying it in the Gaussian model for diffusion from a point source, to calculate how far from the emission point the plume width is about five times the local turbulence length scale. This value (five) was empirically determined from the analysis of the results. It was found, however, that the value is roughly the same for all the cases studied. At a given distance from the source, plume width is defined as the distance from the plume center line to the point where the concentration is 10% of its peak value. Indeed, further work is needed to better model the initial stages of plume spread, where its dimensions are smaller than the characteristic turbulence length scale of the flow.

5. RESULTS AND DISCUSSION

In order to better evaluate the modified k-ε, computations were also made using the standard model and are presented along with the experimental results in the following sections. Due to limited space, it's not possible to show all the comparisons made. Figures 3, 4 and 5 show vertical profiles of concentration on the symmetry plane (y=0) for the cases D0, D100 and D200. For this last case, it's clear that the model is overestimating the diffusion in the lee side of the hill , where there is a recirculation zone. Different inflow turbulent length scales were tested at inflow to verify a possible influence on this high diffusivity, but it was constated that the flow after the hill top is essentially determined by local conditions. An explanation for this model defect is that the pronunciated velocity gradients (see fig. 2) in this region, due to the three dimensional open recirculation zone, increase the production of turbulent kinetic energy and consequently enhance the eddy diffusivities there. Even so, the improvement of the results when compared to the standard k-ε is considerable.

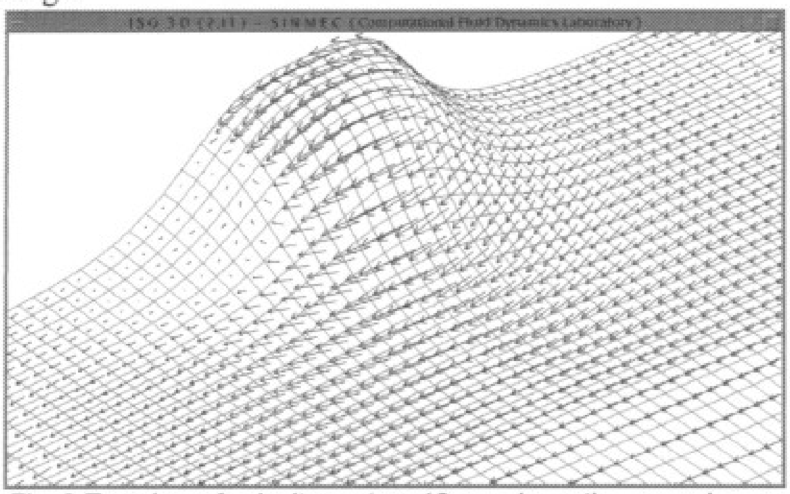

Fig. 2-Top view of velocity vectors 10mm above the ground - case D200 - hill height 200 mm

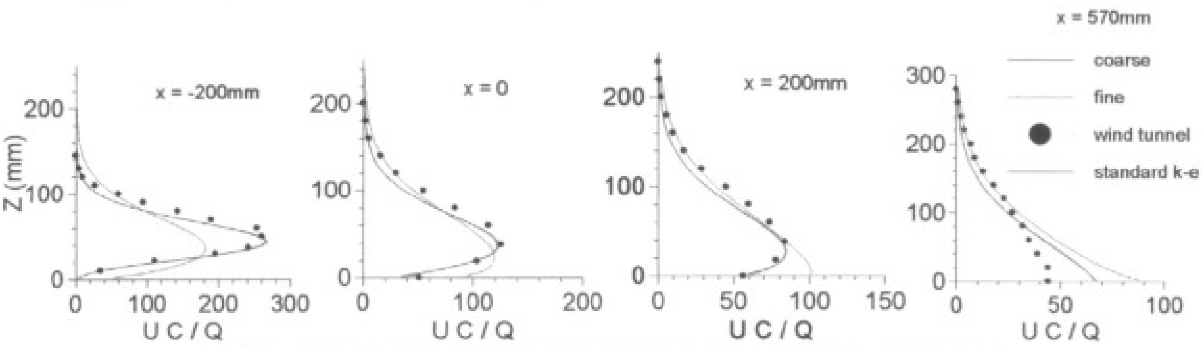

Fig. 3 - Concentration at the symmetry plane - case D0 - flat terrain

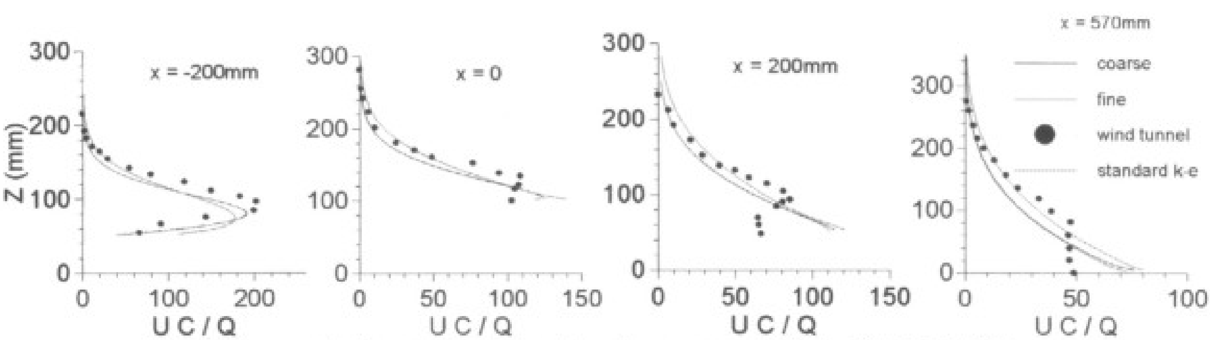

Fig. 4 - Concentration at the symmetry plane - case D100 - hill height 100 mm

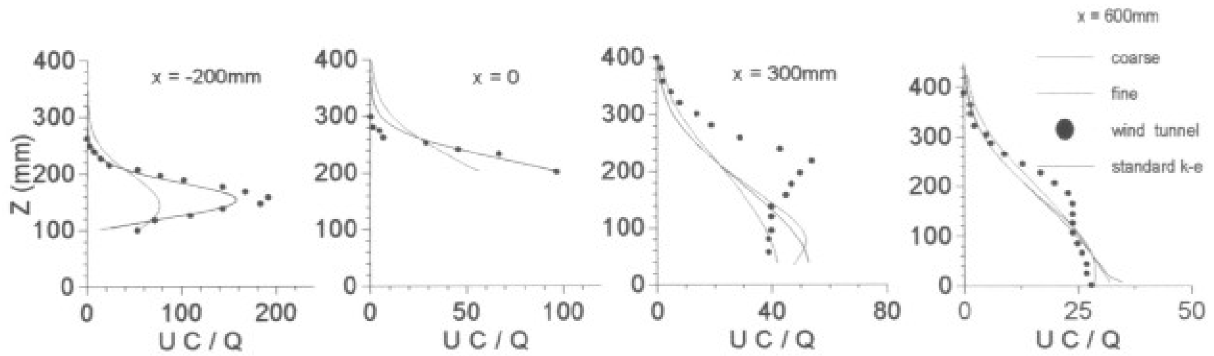

Fig. 5 - Concentration at the symmetry plane - case D200 - hill height 200 mm

6. CONCLUSIONS

A modified non-isotropic k-ε model is applied to simulate three dimensional flow and dispersion of pollutant over complex terrain. It is also proposed that the eddy diffusivities for the concentration calculation should be scaled according to the plume dimensions for the initial stages (near source). The model produces better results than the standard k-ε, when comparing with a wind tunnel dispersion experiment, although, for some cases tested, the model cannot capture the correct plume path, and only reasonable agreement is obtained against the experimental values.

7. ACKNOWLEDGMENTS

We are grateful for the support provided by CNPq and CAPES.

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