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DISPERSION MODELING OF ATMOSPHERIC CONTAMINANTS IN THE ANGRA NUCLEAR POWER PLANT USIN LES AND A NEW MODEL FOR THE CBL GROWTH

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ABSTRACT

In the present work we report a comparison between experimental data and GILTT approach to simulate radioactive contaminant dispersion in the Atmospheric Boundary Layer using micrometeorological parameters generated by LES (Large Eddy Simulation) in the area around the Angra dos Reis Nuclear Power Plant. Furthermore, starting from the evolution equation for the turbulent energy density spectrum (EDS), we develop a new model for the growth of the turbulence in Convective Boundary Layer (CBL). We apply dimensional analysis to parameterize the unknown inertial transport and convective source term in the dynamic equation for the three-dimensional (3-D) spectrum. The non linear integro-differential equation is solved by Adomian decomposition method. The one-dimensional vertical spectrum is derived from the 3-D spectrum, employing a weight function. This allows us to select the magnitude of the vertical spectral component for the construction of the growing 3-D. Using the micrometeorological parameters generated by LES, for the first time, we employ the vertical component of the energy spectrum to calculate the eddy diffusivity (required in dispersion models). This new eddy diffusivity is used in the simulations of the ground-level concentrations considering experimental data of the Nuclear Power Plant.

1. INTRODUCTION

Pollutants that enter the atmosphere become subject to various meteorological processes that determine their transport and distribution characteristics. In the event of a radioactive effluent release, say, from a nuclear power station, it would be essential to predict the trajectory of the plume and the downwind concentrations. In addition to meteorological processes, factors such as emission rates and half-lives of the pollutants will also be crucial in determining their concentration in the air and when deposited on the ground. Other factors, including terrain characteristics, also play a crucial role in influencing the transport of radionuclides through the atmosphere.

The primary process that is responsible for dispersion is advection (flow the wind) and hence wind speed and direction are critical parameters in predicting the transport of radioactive pollutants in the atmosphere. The pollutants also suffer dispersion through processes such as diffusion and turbulence which dilute the pollutant concentration. Other important variables include, for example, mixing depth, friction velocity and convective velocity scale, which also need to be known in order to estimate the concentration of radionuclides in the air.

The prediction of the dispersion of contaminants released into various turbulent flows is of practical importance in a number of applications ranging from industrial mixing problems to the analysis of nuisance and hazard in air quality, pollution and combustion problems involving the release of toxic, radioactive or flammable materials. In this sense, the safety has been an important consideration from the very beginning of the development of nuclear reactors. The main safety concern has always been the possibility of an uncontrolled release of radioactive material, leading to contamination and consequent radiation exposure off-site.

The potential danger from an accident at a nuclear power plant is exposure to radiation. This exposure could come from the release of radioactive material from the plant into the environment, usually characterized by a plume formation. The area the radioactive release may affect is determined by the amount released from the plant, wind direction and speed and weather conditions which would swiftly drive the radioactive material to the ground. In consequence, much effort has been expended on the development of mathematical models to predict mean concentrations of contaminants for a given emission-source distribution. In fact, models are instruments for control strategies and contaminants emissions. Moreover, the formulation of emergency plans is based on the possible scenarios of concentration in the air and, therefore, with tools (as the mathematical models of dispersion in atmosphere) able to tie the causes (the sources) of pollution with the relative effects (the concentrations of contaminants) and to foresee the concentrations to the ground and in different heights.

The evolution of the heat flux in the Earth's surface during the morning produces an increase of turbulence in the Convective Boundary Layer (CBL). This creates a variation in all scales that characterize the state of CBL. The dispersion of contaminants in the lower atmosphere is influenced by variation of the properties of turbulence during the growth of the CBL. In the diffusion-advection equation, used in models of Eulerian dispersion, the physical properties of the turbulent field are described by the eddy diffusivity. This quantity can be obtained of the energy density spectrum from the classical statistical diffusion theory [1]. Recently [2] published a study proposing a model to describe the evolution of the properties of turbulence during the growth of the CBL. Some results of this study will be used in this work to estimate the ground-level concentration in the Angra I Nuclear Power Plant.

In this context, recently was proposed a mathematical model for radioactive contaminant dispersion in atmosphere: the GILTT (Generalized Integral Laplace Transform Technique) method. In a recent work, to evaluate this model with radioactive dispersion, the experimental data used in the simulations were of controlled releases of radioactive tritiated water vapour from the meteorological tower close to the power plant at Itaorna Beach, Brazil, in 1985. In the model the wind profile was determined using experimental meteorological data and the micrometeorological parameters were calculated from semi-empirical equations obtained in the literature. In the present work, we step forward reporting a numerical and statistical comparison between experimental data and GILTT approach to simulate radioactive contaminant dispersion in the Atmospheric Boundary Layer using micrometeorological parameters generated by LES (Large Eddy Simulation) in the area around the Angra dos Reis Nuclear Power Plant. Furthermore, starting from the evolution equation for the turbulent energy density spectrum (EDS), we develop a new model for the growth of the turbulence in CBL. We apply dimensional analysis to parameterize the unknown inertial transport and convective source term in the dynamic equation for the three-dimensional (3-D) spectrum. The non linear integro-differential equation is solved by Adomian decomposition method. The one-dimensional vertical spectrum is derived from the 3-D spectrum, employing a weight function. This allows us to select the magnitude of the vertical spectral component for the construction of the growing 3-D. Using the micrometeorological parameters generated by LES, for the first time, we employ the vertical component of the energy spectrum to calculate the eddy diffusivity (required in dispersion models). This new eddy diffusivity is used in the simulations of the ground-level concentrations considering experimental data of the Nuclear Power Plant.

To reach our objective we organize this paper as follows: in section 2.1 we report the model for the growth of the Convective Boundary Layer from the Energy Density Spectrum equation. In section 2.2 we report advection-diffusion equation solution by the GILTT method. In section 3, experimental data e numerical results are presented, and finally in section 4, the conclusions.

2. THE MODELS

2.1. The model for the growth of the Convective Boundary Layer from the Energy Density Spectrum equation

From the Navier-Stokes equations is obtained an equation for the Energy Density Spectrum (EDS) in a homogeneous turbulent field [3]:

$$\frac{\partial}{\partial t}E(k,t;z)=T(k,t;z)+\frac{g}{T_0}H(k,t;z)-2\nu k^2E(k,t;z) \qquad (1)$$

where t is time, k is the wave-number, $E(k,t;z)$ is the 3-D EDS, $\frac{g}{T_0}H(k,t)$ is buoyancy term, z is the height above the ground, $T(k,t;z)$ is the inertial transport of energy term and the last term on the r.h.s. of equation (1) is the energy loss due to viscous dissipation.

A turbulent flow contains eddies of different size or different wavelengths. The small eddies are subjected to the stress generated by large eddies. This field increases the vorticity of small eddies and, consequently, their kinetic energy. Thus, turbulent kinetic energy is transferred from large eddies towards smaller and smaller eddies until the Kolmogorov micro-scale is reached, where the energy is dissipated as heat. This process is represented by the term $T(k,t;z)$ of equation (1). This term was parameterized according to [4] for a turbulent homogeneous flow on the basis of dimensional analysis, as follows:

$$T(k,t;z)=-\left[\frac{\partial}{\partial k}\left(\alpha^{-1}\varepsilon^{1/3}k^{5/3}E(k,t;z)\right)+\frac{\partial}{\partial k}\left(\frac{m_2}{w_* z_i}\varepsilon^{2/3}k^{1/3}E(k,t;z)\right)\right] \qquad (2)$$

where m_2 in a dimensionless constant, α is the Kolmogorov constant, w_* is the convective velocity scale, z_i is the height of the CBL and ε is the rate of molecular dissipation of turbulent kinetic energy. The buoyancy effect was parameterized by [2] from dimensional analysis,

$$\frac{g}{T_0} H(k,t,z) = m_1 \frac{w_*^3}{\left(\overline{w\theta}\right)_0 z_i} \frac{\partial \theta}{\partial z} \varepsilon^{-1/3} k^{-2/3} E_0(k;z) \sin\left(\Omega t\right) \tag{3}$$

where m_1 is a dimensionless constant, $\left(\overline{w\theta}\right)_0$ is surface heat flux, $\frac{\partial \theta}{\partial z}$ is the temperature gradient and Ω is the Earth's angular velocity. Substituting (3) and (2) in (1) is obtained the 3-D energy density spectrum. To calculate the vertical component of the spectrum we consider that for a particular time instant *t* there is a relationship between the 1-D spectra and the 3-D average spectrum given by the following expression:

$$F_w(k,t;z) = a(k) \frac{\frac{1}{T}\int_0^t F_w(k,t;z)dt}{\frac{1}{T}\int_0^t E(k,t;z)dt} E(k,t;z) \tag{4}$$

where the ratio between the two integrals is a weight function that indicates as the *w* component takes part in the construction of the 3-D spectrum and $a(k)$ is the proportionality constant. The solution of Equation (4) provides the vertical component as a function of the 3-D spectrum:

$$F_w(k,t,z) = F_w(k,0,z) \exp[\int_0^t Q'(k,s)ds] \tag{5}$$

In this case $F_w(k,0,z) = F_w(k,z)$ is given by equation,

$$F_w(k,z) = \frac{0.16 z_i \psi_\varepsilon^{2/3} \left(1 - e^{-4z/z_i} - 0.0003 e^{8z/z_i}\right) w_*^2}{(1 + 0.43\left(1 - e^{-4z/z_i} - 0.0003 e^{8z/z_i}\right) z_i k)^{5/3}} \tag{6}$$

where ψ_ε is the dimensionless rate dissipation.

$$Q'(k,s) = a(k)Q(k,s) + \frac{1}{Q(k,s)} \frac{\partial Q(k,s)}{\partial s} \tag{6a}$$

and $Q(k,s)$ given by:

$$Q(k,s) = \frac{E(k,s)}{\int_0^t E(k,s)ds} \tag{6b}$$

During the growth of the CBL the length scale (z_i) and velocity scale (w_*) vary from zero up to the maximum value that occurs when the CBL reaches its steady-state. An expression for the height variation of the CBL was suggested by [5],

$$z_i^2 = \frac{2(1+2A)\overline{(w\theta)}_0}{\gamma(0)(\beta^2+\Omega^2)} \exp(-2\beta t)\left[\exp(\beta t)(\beta \sin(\Omega t) - \Omega\cos(\Omega t) + \Omega)\right] \tag{7}$$

where $\overline{(w\theta)}_0$ is the heat flux in the Earth's surface, $\gamma(0) = 18\text{x}10^{-3}\,Km^{-1}$, $\beta = 0.6\text{x}10^5 s^{-1}$ and $A = 0.5$. The velocity scale (w_*) is calculated for definition,

$$w_*(t) = \left[\frac{g}{T_0} z_i(t)\overline{(w\theta)}_0 \sin(\Omega t)\right]^{1/3} \tag{8}$$

where g/T_0 is the buoyancy parameter.
The eddy diffusivity is the obtained from the classical statistical diffusion theory ([1], [6]):

$$K_z(t,z) = \frac{\sigma_w^2(z)\beta_w F_w(z)}{4} \tag{9}$$

Where $F_w(z)$ is the vertical component of the 3-D spectrum, calculated in origin ($k=0$), σ_w^2 is the wind velocity variances calculated by,

$$\sigma_w^2(t,z) = \int_0^\infty E_w(k,t,z)dk \tag{10}$$

and β_w is the ratio of the Lagrangian to the Eulerian time scales. Considering the equations (4), (5), (6), (10) and $\beta_w = \frac{0.55\bar{U}}{\sigma_w}$ ([7]) the eddy diffusivity (eq. 9) can rewrite as,

$$K_z(t,z) = 0.247\left(1-\exp\left(-4\frac{z}{z_i}\right) - 0.0003\exp\left(8\frac{z}{z_i}\right)\right) z_i \sigma_w(t,z) \tag{11}$$

2.2. The contaminant dispersion model

Atmospheric air pollution turbulent fluxes can be assumed to be proportional to the mean concentration gradient. This assumption, along with the equation of continuity, leads to the advection-diffusion equation. Considering a Cartesian coordinate system in which the *x* axis coincides with the direction of the average wind and *z* is the vertical axis, the crosswind time dependent advection-diffusion equation can be written as (neglecting the longitudinal diffusion) [8]:

$$\frac{\partial c(x,z,t)}{\partial t}+u\frac{\partial c(x,z,t)}{\partial x}+w\frac{\partial c(x,z,t)}{\partial z}=\frac{\partial}{\partial z}\left(K_z\frac{\partial c(x,z,t)}{\partial z}\right)-\lambda c(x,z,t) \tag{12}$$

for $0 < z < h$, t > 0 and $x > 0$; where h is the height of the ABL, u and w are, respectively, the longitudinal and vertical mean wind, K_z is the vertical eddy diffusivity, c is the crosswind integrated concentration and λ is the decay constant. The mathematical description of the dispersion problem represented by the Eq. (12) is well posed when it is provided by boundary and initial conditions. For this end, we introduce the usual boundary conditions of zero flux at the ground and ABL top and a source with emission rate Q at height H_s:

$$K_z\frac{\partial c(x,z,t)}{\partial z}=0 \qquad \text{at } z=0,\ z_i \tag{12a}$$

$$uc(0,z,t)=Q\delta(z-H_s) \qquad \text{at } x=0 \tag{12b}$$

where $\delta(z-H_s)$ is the Dirac delta function and H_s the source height. Indeed, it is assumed that at the beginning of the pollutant release the dispersion region is not polluted, this means:

$$c(x,z,0)=0 \qquad \text{at t} = 0 \tag{12c}$$

Using the Laplace transform technique, transforming t into r and c into C, applying the initial condition (12c), the eq. (12) becomes:

$$u\frac{\partial C(x,z,r)}{\partial x}+w\frac{\partial C(x,z,r)}{\partial z}=K_z\frac{\partial^2 C(x,z,r)}{\partial z^2}+K_z'\frac{\partial C(x,z,r)}{\partial z}-\lambda^* C(x,z,r) \tag{13}$$

where $\lambda^*=\lambda+r$. Taking advantage of the well-known solution of the stationary problem with advection in the x direction by the GILTT method ([9], [10], [11]), we pose that the solution of problem (12) has the form:

$$C(x,z,r)=\sum_{i=0}^{M}\bar{c}_i(x,r)\Psi_i(z) \tag{14}$$

where $\Psi_i(z)$ are the eigenfunctions of an associated Sturm-Liouville problem ($\Psi_i(z)=\cos(\lambda_i z)$ for i=0,1,2,3,... and $\lambda_i=i\pi/h$) and $\bar{c}_i(x,r)$ is the solution of the transformed problem which is given below.

Proceeding in a similar manner of the work of [10], we obtain the transformed problem that in matrix notation becomes:

$$Y'(x)+FY(x)=0 \tag{15}$$

where $Y(x)$ and $Y'(x)$ are, respectively, the column vector whose components are $\bar{c}_i(x)$ and $\bar{c}_i'(x)$ and $F=B^{-1}E$. The entries of the matrices B and E are written as:

$$b_{i,j} = -\int_0^h u \Psi_i \Psi_j dz$$

$$e_{i,j} = \int_0^h K_z' \Psi_i' \Psi_j dz - \lambda_i^2 \int_0^h K_z \Psi_i \Psi_j dz - \int_0^h w \Psi_i' \Psi_j dz - \lambda^* \int_0^h \Psi_i \Psi_j dz \ .$$

The transformed problem represented by the eq. (15) is solved analytically by the Laplace transform technique and diagonalization ([9]). Finally, the time dependent concentration is obtained by inverting numerically the transformed concentration $C(x,z,r)$ by a Gaussian quadrature scheme:

$$c(x,z,t) = \sum_{k=1}^{m} \frac{p_k}{t} a_k \sum_{i=0}^{M} \bar{c}_i(x, \frac{p_k}{t}) \Psi_i(z) \qquad (16)$$

where a_k and p_k are the weights and roots of the Gaussian quadrature scheme tabulated in [12], m is the number of the quadrature points and M is the truncation order. For more details about the GILTT method see the work [11].

In this work, we need to calculate three-dimensional concentration. This way, we assumed a Gaussian distribution in the lateral direction and we have taking into account the dispersion parameter σ_y. Therefore, the final equation to calculate the ground-level centerline concentration is:

$$C^*(x,0,0,t) = \frac{c(x,0,t)}{\sqrt{2\pi}\sigma_y} \qquad (17)$$

where the ground-level crosswind integrated concentration in the Eq. (16) is calculated employing the Eq. (11).

In the atmospheric diffusion problems, the choice of a turbulent parameterisation represents a fundamental decision for contaminant dispersion modeling ([13]). From a physical point of view, the turbulence parameterisation is an approximation in the sense that we are putting in the mathematical models an approximated relation that in principle can be used as a surrogate for the natural but unknown term. The reliability of each model strongly depends on the way the turbulent parameters are calculated and is related to the current understanding of the CBL. For the lateral dispersion parameter σ_y, we followed [14]:

$$\frac{\sigma_y^2}{z_i^2} = \frac{0.21}{\pi} \int_0^\infty \sin^2\left(2.26 \psi^{1/3} X n'\right) \frac{dn'}{(1+n')^{5/3} n'^2} \qquad (18)$$

where X is a nondimensional distance ($X = xw_* / uz_i$) and the dissipation function is given by $\psi^{1/3} = 0.97$ (w_* is the convective velocity and x is the source distance).

Thus, in this study, we introduce the vertical eddy diffusivity (Eq. (11)) in the GILTT model (Eq. (16)) and the lateral dispersion parameter (Eq. (18)) in the Eq. (17), to calculate the ground-level concentration of emissions released from an elevated continuous source point in an unstable/neutral atmospheric boundary layer. The wind speed profile is generated by the MesoNH model and the micrometeorological parameters by the LES model.

3. EXPERIMENTAL DATA AND NUMERICAL RESULTS

Bearing in mind that in this work our aim is to show the feasibility of the proposed models to simulate contaminant dispersion in atmosphere for more realistic problem, we are now in position to specialize the application of this methodology for a problem with the wind speeds evaluated by the MesoNH research model ([15], [16]).

The MesoNH has available different parameterisations and can be run in different modes, from mesoscale to LES. The model uses an anelastic system of equations written with a Gal-Chen and Sommerville vertical system of coordinates. The turbulence closures available are the eddy-diffusivity based on the TKE budget equation of [16] and the EDMF (Eddy-diffusivity/Mass-flux) scheme developed by [17]. The convection scheme is based on a bulk mass-flux convection parameterisation for deep and shallow convection ([18]). MesoNH has a statistical subgrid condensation scheme, based on the distributions of the grid scale values of θ_l and q_t, and their variances, which are supplied by the general turbulence scheme [19]. The radiative scheme implemented in MesoNH is the one of the ECMWF (European Center for Medium range Weather Forecasting) model.

This study is based in a simulation with 4 nested grids, the coarser two run in the regional mode and the inner two grids in LES mode, with two-way interaction between them. The outer grid is forced by re-analysis of the ECMWF model. The main properties of the 4 grids are the following: Grid 1 (Mesoscale, Horizontal resolution: 10 km, (nx,ny,nz) = 60x60x120 and Δt = 8s); Grid 2 (Mesoscale, Horizontal resolution: 2 km, (nx,ny,nz) = 60x60x120 and Δt = 4s); Grid 3 (LES, Horizontal resolution: 400 m, (nx,ny,nz) = 120x120x120 and Δt = 1s); Grid 4 (LES, Horizontal resolution: 100 m, (nx,ny,nz) = 96x96x120 and Δt = 0.5s).

The experiment consisted in the controlled releases of radioactive tritiated water vapour from the meteorological tower, 100 m height, close to the power plant in Itaorna Beach, from 28 November to 4 December 1984 [20]. The nuclear power plant is located at latitude -23.0079 and longitude -44.4612. The total time of emission was 90 minutes for each day, in all cases around midday LST. The collection of water vapour over cooled aluminium plates in the numbered location took place in three subsequent periods (1, 2 and 3) of 20 minutes each, 30 minutes after the beginning of the release, to allow the source and the plume transport to reach a supposed stationary condition on the measurement area. All relevant details, as well as the synoptic meteorological conditions during the dispersion campaign are also described in [20]. In this work, the simulations were accomplished on the first day (28 November). The emission rate utilized was Q = 20.5 MBq/s. The micrometeorological parameters generated by LES were: $w_* = 2m/s$, $z_i = 1500m$, heat flux = 0.24m/sK.

The Figure 1 show the eddy diffusivity calculated in $t_* = \frac{w_* t}{z_i}$ = 2.4, 14.4, 24, 48. Is considered $t_* = 0$ when the heat flux in the Earth's surface is zero. In $t_* = 48$ the CBL is stationary.

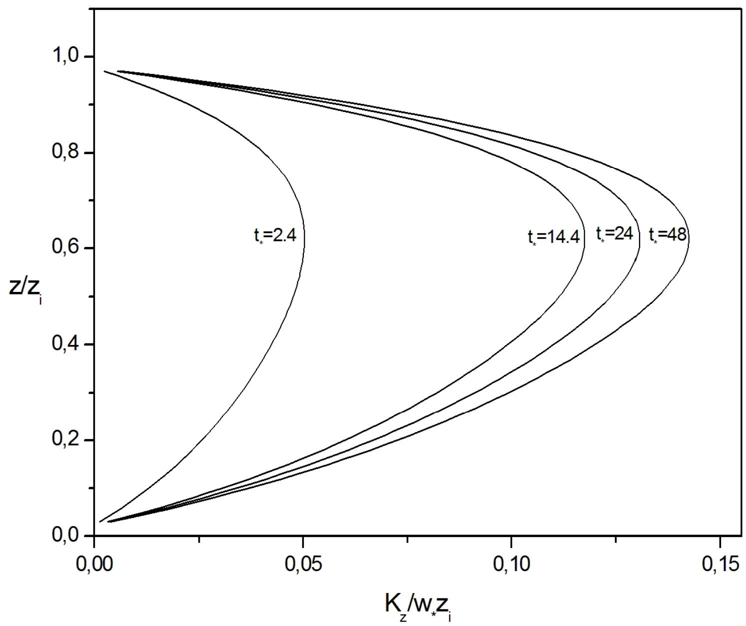

Figure (1) – Evolution in time of the eddy diffusivity.

Table 1 presents some statistical performances [21] using in the simulations for wind field and micrometeorological parameters from MesoNH (LES) and semi-empirical equations. The statistical index FB says if the predicted quantity underestimates or overestimates the observed ones. The statistical index NMSE represents the quadratic error of the predicted quantities related to the observed ones. The best results are expected to have values near to zero for the indices NMSE, FB and FS, and near to 1 in the indices COR, FA2 and FA5 (simulations in complex terrain is usual FA5). Promptly, we observed from Table 1 that the models satisfactorily reproduce the concentrations, particularly, the slightly better results with the GILTT method. GILTT* represent results simulations using semi-empirical equations to determine micrometeorological parameters and wind field. The best results were obtained with the use the micrometeorological parameters (LES) and wind field from MesoNH model. The analysis of the results shows a reasonably good agreement between the computed values against the experimental ones using data from MesoNH model and a new model for the CBL growth.

Table 1. Statistical evaluation for ground-level concentration. GILTT* represent results simulations using semi-empirical equations to determine micrometeorological parameters and wind field.

	GILTT	GILTT*
NMSE = $\overline{(C_o - C_p)^2} / \overline{C_o}\,\overline{C_p}$	0.35	2.05
COR = $\overline{(C_o - \overline{C_o})(C_p - \overline{C_p})} / \sigma_o \sigma_p$	0.47	0.36
FA2 = $C_p / C_o \in [0.5,2]$	0.73	0.25
FA5 = $C_p / C_o \in [0.2,5]$	1.00	0.37
FB = $\left(\overline{C_o} - \overline{C_p}\right) / \left(0.5\left(\overline{C_o} + \overline{C_p}\right)\right)$	0.05	0.88
FS = $(\sigma_o - \sigma_p) / 0.5(\sigma_o + \sigma_p)$	1.39	0.08

where the subscripts *o* and *p* refer to observed and predicted quantities, respectively, and the overbar indicates an averaged value. Observing these results is important to mention that the differences among the experimental data do not depend on the solution of the diffusion equation, but on the equation itself, which is only a model of reality. It must be borne in mind, when using models, that, while they are rather sophisticated instruments that ultimately reflect the current state of knowledge on turbulent transport in the atmosphere, the results they provide are subject to a considerable margin of error. This is due to various factors, including in particular the uncertainty of the intrinsic variability of the atmosphere and the CBL parameterization. Models, in fact, provide values expressed as an average, i.e. a mean value obtained by the repeated performance of many experiments, while the measured concentrations are a single value of the sample to which the ensemble average provided by models refer. This is a general characteristic of the theory of atmospheric turbulence and is a consequence of the statistical approach used in attempting to parameterize the chaotic character of the measured data.

4. CONCLUSIONS

Focusing the main objective of this work consisting, for the first time, in the use of a new model to calculate the CBL growth (with micrometeorological and wind profile generated by LES and MesoNH models) (the MesoNH model has the ability to run both Large-Eddy and Mesoscale Simulations), we must emphasize the improvement of the results attained when compared with semi-empirical results. The improvement is expected because, besides micrometeorological parameters considered, we use a LES version code that allow us to perform calculations with a refined grid (~100 m). Therefore, we would like to point out that we hit our goal in this work showing the aptness of the discussed methods to solve contaminant dispersion problem in the atmosphere considering more realistic micrometeorological parameters and wind field. Furthermore, we also show the coupling of the analytical solutions with the micrometeorological parameters (LES) and wind profile generated by MesoNH model. Finally, we will focus our future attention to the task of solve this sort of problem by the three-dimensional GILTT solution considering the new model to estimate CBL growth with micrometeorological parameters and wind field generated by LES and MesoNH for all Angra dos Reis experiments.

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