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Mathematical Modeling and Numerical Simulation of Atmospheric Pollutant Dispersion

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Abstract. This work presents a mathematical modeling and numerical solution of dispersion of pollutants in the atmosphere. The equations of conservation of mass, amount of movement, energy and a chemical species are solved by the Finite Volume Method in Cartesian coordinates and the turbulence closure is based on the Reynolds averages (RANS models), using the model k-ε for the determination of the fields of velocity, temperature and, in a specific case, concentration of pollutant. The numerical results are compared with data from the classic Prairie Grass experiment, showing excellent agreement.

Introduction

The calculation of the concentration distribution of pollutants in the atmosphere is fundamental for the elaboration of emission control legislation, environmental impact assessment, implementation of industrial complexes, etc. Mathematical models are essential tools for calculating the concentration in the atmosphere. Many numerical models developed to estimate the concentration in the atmosphere are presented in the literature. Hanna, Hansen and Dharmavaram [1,2], evaluated the performance of the FLACS CFD model in the study of dispersion of pollutants in the atmosphere, in situations with and without obstacles, comparing their data with observations from three field experiments (Kit Fox, MUST and Prairie Grass) and a wind tunnel (EMU). In their simulations they obtained results with about 86% of the predictions within a factor of two, geometric mean of 1.32, geometric variance of 1.28, normalized mean square error of 0.29 and slope fraction of 0.18, Attesting the good performance of the model. Tsai and Chen [3] developed an experiment and performed numerical simulations of the dispersion of CO, NOx and SO2 emitted by motor vehicles in an urban canyon using the RNG k-ε turbulence model. Their simulations were developed with Ansys CFX commercial software and the observed differences between experimental and numerical results were 5% to 50%. Demael and Carissimo [4] compared the performance of the Mercure_Saturne CFD model using the standard k-ε model and two Gaussian plume models in the case-neutral simulation of the Prairie Grass experiment. Although they achieved results with good levels of precision, the simulations showed the difficulty that the turbulence models based on the Boussinesq hypothesis have in describing the rapid dispersion that occurs near the source. Another limitation of the closures based on the k-ε model was pointed out by Mazzoldi, Hill and Colls [5] who performed simulations of the Prairie Grass and Kit Fox experiments under stable, neutral and unstable atmosphere conditions. This limitation refers to the overestimation of distant source concentrations under unstable conditions which, as suggested by the authors themselves, may be due to the underestimation of the turbulent dissipation by the turbulence model. Pontiggia et al [6] presented a technique for importing complex three-dimensional geometries from topographic databases to use them in CFD simulations and conducted a case study that considers the dispersion of ammonia in an urban perimeter. Their simulations were developed using the standard k-ε model, plus a source term to take into account the effects of thermal stratification (considered neutral and stable atmospheres). The results indicated that in neutral case simulations, when shear stress plays a dominant role in turbulent production, the k-ε model achieves a good level of precision, but in stable cases, when the thrust plays an important

role in the Reduction of atmospheric turbulence, the same does not occur. In this case the model tends to overestimate the turbulence and, consequently, to underestimate the concentrations. Tauseef, Rashtchian and Abbasi [7], employing the k-ε Realizable model, simulated the dispersion of a dense gas over a cubic obstacle on a flat terrain. Their results were compared with experimental data. Although the two models reached considerable levels of accuracy, the k-ε Realizable model was shown to be slightly higher, mainly in the representation of the concentration fluctuations in the solution of the transient problem. The standard k-ε model was also used by Liu et al. [8] in the simulation of the dispersion of carbon dioxide on complex terrains. Two cases were analyzed: one in which the ground was flat, with the presence of a parabolic mountain; and another in which the environment was an idealized urban area, where the constructions were defined as hexahedral blocks. The influence of topography, wind speed and source intensity on dispersion of contaminants were evaluated in the work and the results were compared with experimental data.

In this work, the dispersion of pollutants in the atmosphere is modeled considering the equations of conservation of mass, conservation of momentum, conservation of energy and conservation of a chemical species (transport of pollutant), by the Finite Volumes Method, in Cartesian coordinates. Turbulence is modeled using the k-ε model. The problem considered involves the dispersion of sulfur dioxide, released by a low source (almost at ground level), under conditions of great instability (when there is strong convection caused by the incidence of solar radiation on the earth's surface), on flat ground with low aerodynamic roughness. The equations are two-dimensional and in steady state. For the validation of the results we use data from the classic Prairie Grass experiment, originally described by Barad [9, 10], Record and Cramer [11] and Haugen [12].

The Mathematical Model

To describe and forecast the state of the Boundary Layer, we turn to the equations of fluid mechanics that describe the dynamics and thermodynamics of the gases in our atmosphere [13],

$$\frac{\partial(\rho\bar{u})}{\partial x} + \frac{\partial(\rho\bar{w})}{\partial z} = 0 \tag{1}$$

$$\frac{\partial(\rho\overline{uu})}{\partial x} + \frac{\partial(\rho\overline{uw})}{\partial z} = - \frac{\partial\bar{P}}{\partial x} + \frac{\partial}{\partial x}\left[(\mu + \mu_t)2\frac{\partial\bar{u}}{\partial x}\right] + \frac{\partial}{\partial z}\left[(\mu + \mu_t)\left(\frac{\partial\bar{u}}{\partial z} + \frac{\partial\bar{w}}{\partial x}\right)\right] \tag{2}$$

$$\frac{\partial(\rho\overline{wu})}{\partial x} + \frac{\partial(\rho\overline{ww})}{\partial z} = - \frac{\partial\bar{P}}{\partial z} + \frac{\partial}{\partial x}\left[(\mu + \mu_t)\left(\frac{\partial\bar{u}}{\partial z} + \frac{\partial\bar{w}}{\partial x}\right)\right] + \frac{\partial}{\partial z}\left[(\mu + \mu_t)2\frac{\partial\bar{w}}{\partial z}\right] + \rho g\beta(T - T_\infty) \tag{3}$$

$$\frac{\partial(\rho\overline{uT})}{\partial x} + \frac{\partial(\rho\overline{wT})}{\partial z} = \frac{\partial}{\partial x}\left[\left(\frac{\mu}{Pr} + \frac{\mu_t}{\sigma_T}\right)\frac{\partial\bar{T}}{\partial x}\right] + \frac{\partial}{\partial z}\left[\left(\frac{\mu}{Pr} + \frac{\mu_t}{\sigma_T}\right)\frac{\partial\bar{T}}{\partial z}\right] \tag{4}$$

where (1) is the continuity equation, (2) is the conservation of momentum equation in longitudinal direction, (3) is the conservation of momentum equation in vertical direction and (4) is the energy equation. In equation (4) Pr and σ_T are the numbers of Prandtl and turbulent Prandtl, respectively. The concentration equation is given by,

$$\frac{\partial(\rho\overline{uC})}{\partial x} + \frac{\partial(\rho\overline{wC})}{\partial z} = \frac{\partial}{\partial x}\left[\left(\frac{\mu}{Sc} + \frac{\mu_t}{Sc_t}\right)\frac{\partial\bar{C}}{\partial x}\right] + \frac{\partial}{\partial z}\left[\left(\frac{\mu}{Sc} + \frac{\mu_t}{Sc_t}\right)\frac{\partial\bar{C}}{\partial z}\right] + S^C \tag{5}$$

where Sc is Schmidt number and S^C is the source term.

The turbulence is described by the $k - \varepsilon$ model.

$$\frac{\partial(\rho\overline{uk})}{\partial x} + \frac{\partial(\rho\overline{vk})}{\partial z} = \frac{\partial}{\partial x}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial\bar{k}}{\partial x}\right] + \frac{\partial}{\partial z}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial\bar{k}}{\partial z}\right] + P_k + G_k - \rho\bar{\varepsilon} \tag{6}$$

$$\frac{\partial(\rho\bar{u}\bar{\varepsilon})}{\partial x} + \frac{\partial(\rho\bar{v}\bar{\varepsilon})}{\partial z} = \frac{\partial}{\partial x}\left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial\bar{\varepsilon}}{\partial x}\right] + \frac{\partial}{\partial z}\left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial\bar{\varepsilon}}{\partial z}\right] + \left[C_{\varepsilon 1}P_k - \rho\, C_{\varepsilon 2}\bar{\varepsilon}\right]\frac{\bar{\varepsilon}}{\bar{k}} \quad (7)$$

where,

$$P_k = \mu_t\left[2\left(\frac{\partial\bar{u}}{\partial x}\right)^2 + 2\left(\frac{\partial\bar{w}}{\partial z}\right)^2 + \left(\frac{\partial\bar{u}}{\partial z} + \frac{\partial\bar{w}}{\partial x}\right)^2\right] \quad (8)$$

$$G_k = \frac{\mu_t}{\sigma_T} g\beta\frac{\partial T}{\partial z} \quad (9)$$

The constants of the model are $C_{\varepsilon 1} = 1.21$, $C_{\varepsilon 2} = 1.92$, $C_\mu = 0.03$, $\sigma_k = 1$, $\sigma_\varepsilon = 1$.

The turbulent viscosity coefficient, μ_t, is calculated by

$$\mu_t = \rho C_\mu \frac{\bar{k}^2}{\bar{\varepsilon}} \quad (10)$$

Boundary Conditions

The Table 3 shows the boundary conditions used in the simulation.

Table 3. Boundary conditions used in the simulation.

	for (u)	for (w)	for (C)
Inlet		$\bar{w} = 0$	$\bar{C} = 0$
Top		$\bar{w} = 0$	$\frac{\partial\bar{C}}{\partial x} = 0$
Surface	$\bar{u} = 0$	$\bar{w} = 0$	$\frac{\partial\bar{C}}{\partial x} = 0$
Outlet	$\frac{\partial\bar{u}}{\partial x} = 0$	$\bar{w} = 0$	$\frac{\partial\bar{C}}{\partial x} = 0$

Law of the Wall

To begin the iterative process, the scalar fields of $k - \varepsilon$ are started with the quantities

$$k(z) = \frac{u_*^2}{C_\mu^{1/2}} \qquad \varepsilon(z) = \frac{u_*^3}{\kappa z} \quad (11)$$

where κ is the von Karman constant.

However, for variables k-ε, periodic boundary conditions are applied, which implies that their values do not remain fixed, but are corrected in the course of the iterative process, according to the partial differential equation employed. Thus, the k-ε profile in the input is a result of the numerical simulation itself and depends on the characteristics of the flow.

At the upper boundary, the null flux boundary condition is applied,

$$\frac{\partial\bar{k}}{\partial z} = \frac{\partial\bar{\varepsilon}}{\partial z} = 0 \quad (12)$$

At the lower boundary, k and ε are defined as the wall function, based on the evaluation of the dimensionless distance z^+, from the surface to the first internal point of the mesh, defined by

$$z^+ = \frac{\rho\, u_* z}{\mu} \tag{13}$$

where u* is the friction velocity at the surface, defined as

$$u_* = \sqrt{\frac{\tau}{\rho}} \tag{14}$$

where τ is the shear stress, calculated by,

$$\tau = \mu\left(\frac{\partial u}{\partial z}\right) \tag{15}$$

The values of k and ε in the wall can be written as

$$k = \frac{{u_*}^2}{C_\mu^{1/2}} \qquad \varepsilon = \frac{k u_* C_\mu^{1/2}}{\kappa(z_g + z_0)} \tag{16}$$

The construction of the mesh is done iteratively, ensuring that $11.6 < z^+ < 30$.

The Numerical Model

The set of partial differential equations that describe the problem studied in this work has no analytical solution, so numerical resolution techniques are necessary. To solve the system of equations (1, 2, 3, 4, 5, 6 and 7) the Finite Volume Method (FVM) was used. The code was written in FORTRAN. For the mesh independence test, the Prairie-Grass experiments 7 were selected, and the longitudinal profile of the pollutant concentration at height z = 1.5m was evaluated. It was established as accuracy that the difference between two successive meshes had a maximum relative error of 5%. The application of the boundary condition for the k-ε model is not trivial. In general, the correct k-ε values are not known for a specific situation and experimental values are rare and valid only for that particular case. It is for this reason that in this work we opted to adopt the strategy of using periodic boundary conditions for k-ε. Thus, it is possible to eliminate the difficulty in relation to the ignorance of the value of the boundary condition that should be applied and to obtain a more precise numerical solution, since the imposition of erroneous boundary conditions compromises the validity of the numerical solution.

The simulations are performed in 2D, so that the computational domain (shown in Fig. 1) consists of a rectangle with the following measures: 850m on the x-axis and $0.1z_i$ on the z-axis, where z_i is the height of the Convective Boundary Layer and varies in each experiment. The pollutant source is located 0.05m from the input, and 0.5m from the earth's surface. The fixed longitudinal length of 850m was established due to the locations of the samplers in the Prairie Grass experiment (which are arranged from 50m to 800m in x, at the fixed height of z = 1.5m).

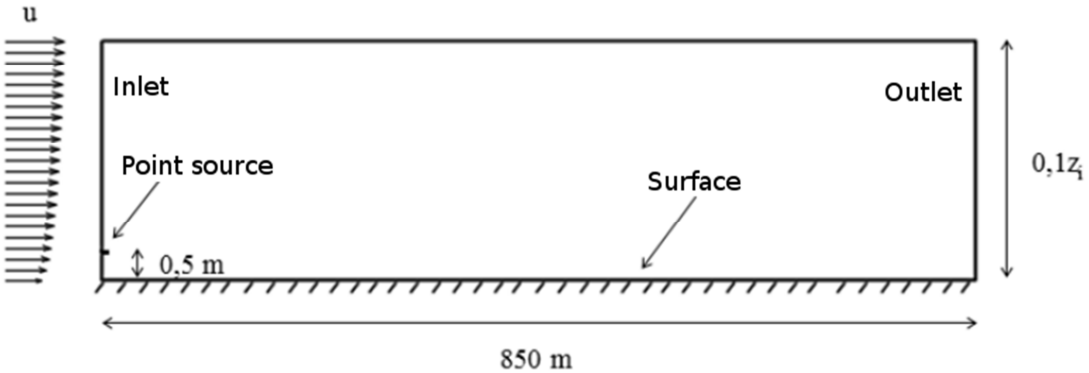

Figure 1. Domain of solution and location of the point source of pollutant release.

Performance of the model

The performance of model presented in this paper (Eqs. 1, 2, 3, 4, 5, 6 and 7) was evaluated against experimental ground-level concentration using the Prairie Grass dispersion experiment [1]. In the Prairie Grass experiment the tracer SO2 was released without buoyancy at a height of 0.46 m, and collected at a height of 1.5 m at five downwind distances (50, 100, 200, 400 and 800 m) at O'Neill, Nebraska in 1956 (see Fig. 2). The Prairie Grass site was quite flat and much smooth with a roughness length of 0.6 cm.

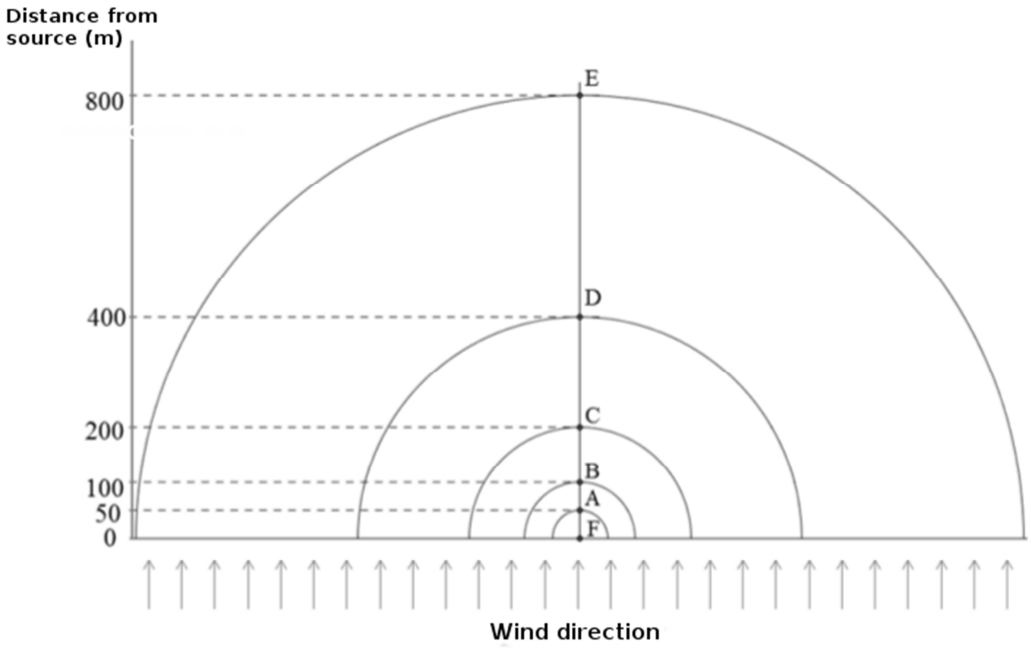

Figure 2. Prairie Grass Experiment (top view).

The meteorological conditions of the Prairie Grass experiment are shown in Table 1, where L is the Monin-Obukhov length, w_* is the convective velocity scale, U_m is the mean wind speed and Q is the emission rate of the source.

Table 1. Meteorological conditions during the Prairie Grass experiment.

Experiment	L (m)	z_i(m)	w_*(m s^{-1})	U_m(m s^{-1})	Q(10^{-4} kg s^{-1})
1	- 9	260	0.84	3.2	820
5	- 28	780	1.64	7.0	780
7	- 10	1340	2.27	5.1	900
8	- 18	1380	1.87	5.4	910
9	- 31	550	1.70	8.4	920
10	- 11	950	2.01	5.4	920
16	- 5	1060	2.03	3.6	930

19	- 28	650	1.58	7.2	1020
20	- 62	710	1.92	11.3	1020
25	- 6	650	1.35	3.2	1040
26	- 32	900	1.86	7.8	980
27	- 30	1280	2.08	7.6	990
30	- 39	1560	2.23	8.5	980
43	- 16	600	1.66	6.1	990
44	- 25	1450	2.20	7.2	1010
49	- 28	550	1.73	8.0	1020
50	- 26	750	1.91	8.0	1030
51	- 40	1880	2.30	8.0	1020
61	- 38	450	1.65	9.3	1020

Usually, the performance of dispersion models is evaluated from a well know set of statistical described by

$$\text{NMSE (normalized mean square error)} = \frac{\overline{(C_o - C_p)^2}}{\overline{C_o}\,\overline{C_p}}$$

$$\text{Cor (correlation coefficient)} = \frac{\overline{(C_o - \overline{C_o})(C_p - \overline{C_p})}}{\sigma_o \sigma_p}$$

$$\text{FB (fractional bias)} = \frac{\overline{C_o} - \overline{C_p}}{0.5(\overline{C_o} + \overline{C_p})}$$

$$\text{FA2 (factor of two)} \rightarrow 0.5 \leq \frac{C_p}{C_o} \leq 2$$

where C_p is the computed concentration, C_o is the observed concentration, σ_p is the computed standard deviation, σ_o is the observed standard deviation and the overbar indicates an averaged value. The best results are indicated by values nearest to 0 in NMSE, FS and FB, and nearest to 1 in Cor and FA2.

Table 2 shows the good performance of the model presented in this work when compared with results of other models in the literature.

Table 2. Comparison of the model proposed in this work with other results of the literature.

Model	NMSE	FB	FA2	Cor
Model proposed	0.08	- 0.02	0.78	0.93
Hanna et al. [1]	0.43	0.18	0.90	-
Carvalho, et al. [14]	0.41	-0.004	0.67	0.80
Kumar and Sharan [15]	0.22	0.13	0.81	0.95
Moreira et al. [16]	0.17	0.04	0.74	0.97

Conclusion

In this work, we studied the dispersion of pollutants continuously released by point sources located at ground level, under conditions of strong instability. The objective was to develop a numerical methodology capable of modeling and simulating transport in the atmospheric surface boundary layer. The mathematical model is composed of equations of conservation of mass, amount of movement, energy and chemical species (transport of pollutant), associated to the equations of the k-ε model of turbulence. To solve the system of equations, the Finite Volume Method (FVM), written in the FORTRAN language, was used. For the mesh independence test, the Prairie-Grass experiments 7 were selected, and the longitudinal profile of the pollutant concentration at height z = 1.5m was evaluated. The obtained results were compatible with those in the literature. The main contribution of the present study is the proposal of an efficient numerical methodology to simulate the dispersion of pollutants in the atmosphere, with low computational effort (from the RANS model).

Acknowledgments

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