

MATHEMATICAL MODEL FOR AIR POLLUTANTS DISPERSION EMITTED BY FUEL COMBUSTION

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This paper deals with the study of atmospheric pollution to mathematically describe the spatial and temporal distribution of pollutants emitted into the atmosphere. The mathematical dispersion modeling of pollutants from power plants is performed in the software package FlexPDE. Thus, an estimation of severity of air pollution can be achieved, using the pollutants concentration and atmospheric conditions. The monitored pollutants are SO₂, NO_x, and PM.

Keywords: air quality, mathematical modeling, numerical simulation, pollutant dispersion.

1. Introduction

In general, the atmospheric diffusion refers to the behavior of gases and particles in turbulent flow. In the scientific literature, there are two fundamental models for describing atmospheric diffusion. The first one is the Eulerian approach, in which the behavior of species is described relative to a fixed coordinate system. The Eulerian description is the common model of treating heat and mass transfer phenomena. The second model is the Lagrangian approach, in which the concentration variations are described as a function of moving fluid. The two approaches yield different types of mathematical relationships for the species concentrations that can, ultimately, be related. Each of the two models of expression is a valid description of turbulent diffusion [1], [2].

There are different software packages that can simulate various transformation processes occurring in presence of pollution and based on experimental data. The main difficulty with these programs is their calibration, such that the displayed results will be as close as possible to the real environmental case [3]. AERMOD is the most used software to mathematically model air pollutants dispersion. This software uses an atmospheric dispersion model based on the structure of turbulent atmospheric layers and on the scaling concept, including the treatment of multiple point sources at ground level or at height. This software uses the Gaussian dispersion model for the stable

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atmospheric conditions and non-Gaussian model for unstable atmospheric conditions [4].

2. Atmospheric dispersion models

The atmospheric dispersion characterizes the time and space evolution of a set of particles (aerosols, gases, dust) emitted into the atmosphere. The atmospheric dispersion phenomenon is influenced by the atmospheric conditions, the terrain parameters and emission values. The mathematical simulation of pollutants' dispersion into the atmosphere is used for estimating the concentration of pollutants emitted from the industrial activity or automobile traffic downwind [5].

The inputs for the atmospheric dispersion models are:

- the meteorological conditions (wind speed and direction, atmospheric turbulence, air temperature);
- the emission parameters (source location and height, chimney diameter, mass flow rate and velocity, and exhaust temperature);
- the geographic data of the source and receiver;
- the location and sizes of obstructed objects (buildings or other structures).

The main atmospheric dispersion models are: Gaussian model, Eulerian model, Lagrangian model, the model of rising smoke cloud, semi-empirical model, chemical model, receptor model, and stochastic model [6].

2.1. The dispersion coefficients

The standard deviation σ values, also called dispersion coefficients, appearing in the equations describing the concentration, are based on experimental data obtained from the study of pollutants evolution. The most used dispersion coefficients are;

- Pasquill-Gifford coefficients, also called rural Pasquill coefficients;
- McElroy-Pooler coefficients, also called urban Briggs coefficients.

The standard deviations depend on the terrain configuration (rural area with open level ground, or urban area with tall buildings) and the atmospheric stability (the tendency of the mixture on the vertical direction due the natural currents convection) [7]. Pasquill has divided the atmospheric stability into six classes to represent the progressive increase of the atmospheric stability that influence the lateral and vertical dispersion. Table 1 reports the Pasquill stability classes, as a function of solar radiation influence and time of day when the atmospheric dispersion model is considered [8].

The characteristics of the stability classes are:

- A: extremely unstable, the temperature gradient $< -1.5^{\circ}\text{C}/100\text{ m}$, and the plume is strongly oscillating describing the loops;

- B: moderately unstable, the temperature gradient in the range $-1.5 - -1$ °C/100 m, the plume is strongly oscillating with turbulences;
- C: slightly unstable, the temperature gradient in the range $-1 - -0.5$ °C/100 m, the plume is slightly oscillating, strongly conical;
- D: neutral (adiabatic), the gradient temperature in the range $-0.5 - 0.5$ °C/100 m, the plume is conical without convective turbulence;
- E: isothermal, the temperature gradient in the range $0.5 - 1.5$ °C/100 m, the plume is conical without convective turbulence;
- F: inversion, the temperature gradient > 1.5 °C/100 m, the plume has the flag form with lowering tendency [Error! Bookmark not defined.].

Table 1

Estimation of Pasquill Stability Classes*

Surface (10m) Windspeed (m/s)	Daytime			Nighttime	
	Incoming solar radiation**			Cloud cover fraction	
	High	Moderate	Low	$\geq 4/8$	$\leq 3/8$
<2	A	A-B	B	-	-
2-3	A-B	B	C	E	F
3-5	B	B-C	C	D	D
5-6	C	C	D	D	D
>6	D	D	D	D	D

*A-extremely unstable, B-moderately unstable, C-slight unstable, D-neutral, E-slight stable, F-moderately stable. **Solar radiation: high (> 700 W/m²), moderate (350-700 W/m²), low (< 300 W/m²).

3. Air pollutants dispersion

3.1. The pollutant concentration

The general Gauss dispersion equation, for a continuous point source of pollutants as a cloud of smoke resulting from the chimney of evacuated pollutants in the atmosphere, is calculated with [9]:

$$C(x, y, z) = \frac{Q}{u\sigma_z\sqrt{2\pi}} e^{-\frac{y^2}{2\sigma_y^2}} \cdot \left[e^{-\frac{(H_r-H_e)^2}{2\sigma_z^2}} + e^{-\frac{(H_r+H_e)^2}{2\sigma_z^2}} \right] \quad (1)$$

where, as shown in Fig. 1, C is the emission concentration [g/m³], Q – emission source rate [g/s], u – horizontal wind velocity, y – lateral distance from the plume center, H_e – the effective plume height above the ground [m], H_r – receiver height [m], σ_z – standard deviation of the vertical distribution emission [m], σ_y – standard deviation of the horizontal distribution emission [m].

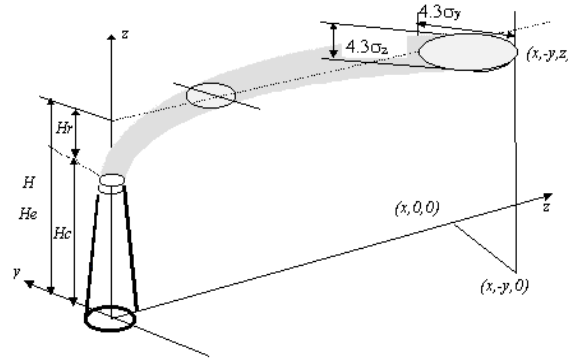


Fig. 1. Gaussian coordinates system for horizontal and vertical dispersion [Error! Bookmark not defined.].

The two sets of dispersion coefficients are illustrated in Fig. 2 (a), for the horizontal direction, respectively Fig. 2 (b) for the vertical direction.

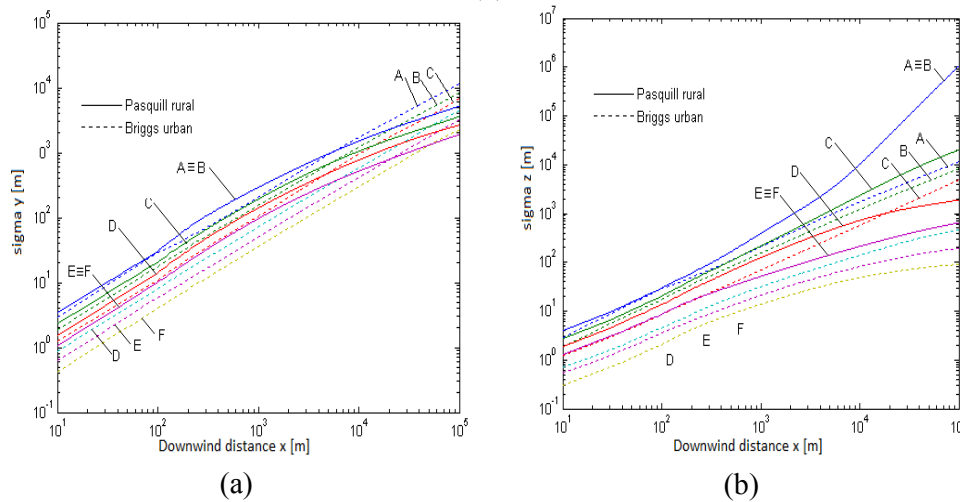


Fig. 2. Dispersion coefficients: (a) horizontal direction, and (b) vertical direction [Error! Bookmark not defined.].

While the Gaussian equations have been widely used for atmospheric diffusion calculations, the lack of ability to include changes in wind velocity with height and nonlinear chemical reactions limits the situations in which they may be used. The atmospheric diffusion equation provides a more general approach to atmospheric diffusion calculations than do the Gaussian models. The Gaussian models have been shown to be special cases of that equation when the wind velocity is uniform and the eddy diffusivities are constant. Expression (2) is the atmospheric diffusion equation in the absence of chemical reaction [10]:

$$\frac{\partial c}{\partial t} + \bar{u} \frac{\partial c}{\partial x} + \bar{v} \frac{\partial c}{\partial y} + \bar{w} \frac{\partial c}{\partial z} = \frac{\partial}{\partial x} \left(K_{xx} \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_{yy} \frac{\partial c}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_{zz} \frac{\partial c}{\partial z} \right) \quad (2)$$

where u , v , w are the functional forms of wind velocity, and K_{xx} , K_{yy} , K_{zz} are the eddy diffusivities.

The expressions available for K_{zz} are based on the Monin - Obukhov similarity theory, coupled with observational or computationally generated data, [11]. These expressions can be organized according to the type of stability.

3.2. The lifting height of the smoke plume

To calculate the pollutant concentration, the height from which the dispersion is starting must to be known. Because of the potential of easy computation, Briggs, [12] is the preferred method. This method accounts for the rise of plume function of downwind distance, the plume carry capacity, and wind velocity [7, 12]. The calculation algorithm is:

- Calculating the ascending F

$$F = \frac{g}{4} \pi w_{e,c} D_{i,c}^2 \frac{T_{e,c} - T_a}{T_{e,a}} = g V_{e,c} \frac{T_{e,c} - T_{e,c}}{T_a} = \frac{g Q_{e,c}}{c_{p,a} \rho T_a} \quad (3)$$

where F is the ascending flow; $g = 9.80665$ [m/s²], the gravitational acceleration; $w_{e,c}$ the exhaust gas velocity from chimney [m/s]; $D_{i,c}$ the inner diameter of chimney [m]; $T_{e,c}$ the absolute temperature of the gas to exit from chimney [K]; T_a the absolute air temperature on top [K]; $V_{e,c}$ the volumetric flow of the exhaust gases [m³/s]; $Q_{e,c}$ thermal flow emitted by chimney [kJ/s]; $c_{p,a}$ the air specific heat at constant pressure [kJ/kgK]; ρ_a air density [kg/m³].

- Calculating the downwind distance x_f where the plume height is maximum

$$x_f = \begin{cases} 49 \cdot F^{5/8}, & \text{for } F < 55 \\ 119 \cdot F^{2/5}, & \text{for } F \geq 55 \end{cases} \quad (\text{for stability classes A, B, C, D}) \quad (4)$$

$$x_f = 3.14 \frac{u}{S^{0.5}} \quad (\text{for stability classes E, F}) \quad (5)$$

where u is wind velocity to chimney height [m/s]; $S = 0.02 \cdot g/T_a$ for E stability class and $S = 0.035 \cdot \frac{g}{T_a}$ for F stability class [s⁻²], the atmospheric stability parameter.

- Calculating the lifting height of the plume Hr

$$Hr = \begin{cases} 1.6 \cdot F^{1/3} \frac{x_f^{3/2}}{u}, & \text{for } x < x_f \\ 1.6 \cdot F^{1/3} 5 \frac{x_f^{2/3}}{u}, & \text{for } x \geq x_f \end{cases} \quad (\text{for A, B, C, D stability classes}) \quad (6)$$

$$Hr = \{\min(Hr_1, Hr_2)\} \quad (\text{for stability classes E, F})$$

where $Hr_1 = 2.4 \frac{F^{1/3}}{uS}$ [m], $Hr_2 = 5 \frac{F^{1/4}}{S^{3/8}}$ [m].

4. Mathematical modeling

4.1. Software description

The software package FlexPDE was used for the mathematical modeling of air pollution dispersion. This finite element model builder and numerical solver implements the mathematical model and presents the graphical output of the results. FlexPDE is also a problem solving environment, performing the entire range of functions necessary to solve partial differential equation system: an editor for preparing scripts, a mesh generator for building finite element meshes, a finite element solver to find solutions, and a graphics system to plot results. The scripting language allows the user to describe the mathematics of his partial differential equations system and the geometry of his problem domain [13].

4.2. 2D air pollutants dispersion modeling

Using the equations and the coefficients of the atmospheric dispersion, different representations of the pollutants concentration function of surface and contour can be obtained.

For the mathematical modeling of pollutants (SO_x, NO_x, PM 10) from a point source of pollution, i.e. the exhaust chimney of the fuel gasses, the following inputs are required:

- the dimensions of the modeling domain;
- wind velocity (u);
- the pollutant flow (Q);
- the chimney stack (H);
- stability class (A-F);
- the terrain type (rural or urban).

For the mathematical modeling, the following inputs were used $u = 6$ m/s, $Q = 200$ g/s, $c = 20$ g/m³, $H = 50$ m, stability class A, rural terrain, the domain dimension 500×200 m.

Two models were implemented, for different time periods like $t = 50$ s and $t = 100$ s. Fig. 3 illustrates the pollutant concentration profile in the simulation domain for the two time periods. As shown, the pollutant evolution increases with the growth of computation time. In order to accomplish a pollutant dispersion modeling on a wider field, a higher computation time is recommended, but leading to a longer response time.

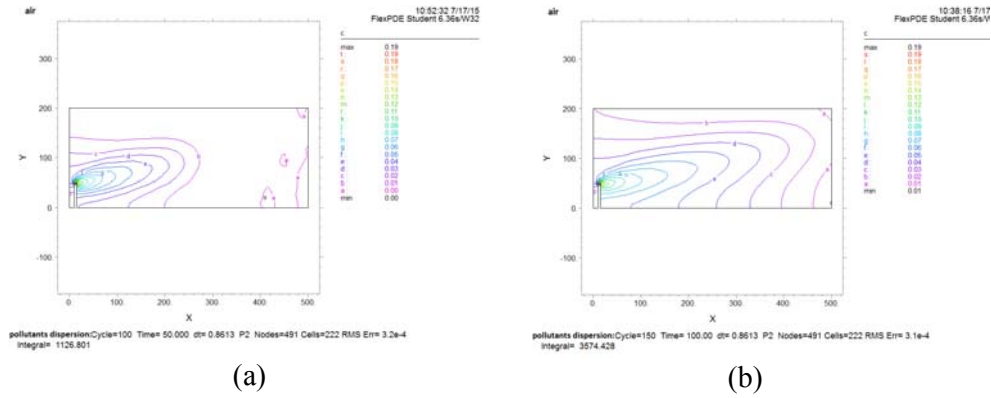


Fig. 3. The pollutant concentration profile in the simulation domain (a) s, (b) s
 Fig. 4 shows the evolution of pollutant's concentration for the two time periods. Fig. 5 shows a zoom image of the results obtained in Fig. 4.

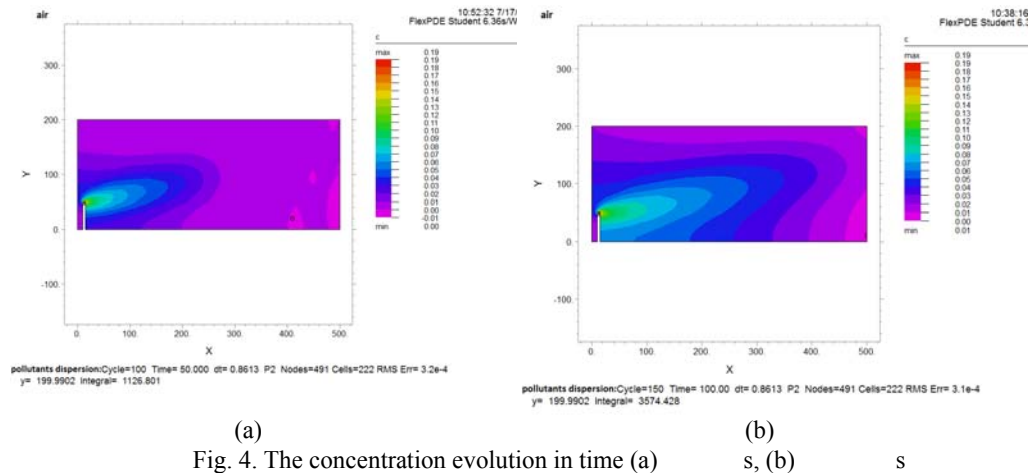


Fig. 4. The concentration evolution in time (a) s, (b) s

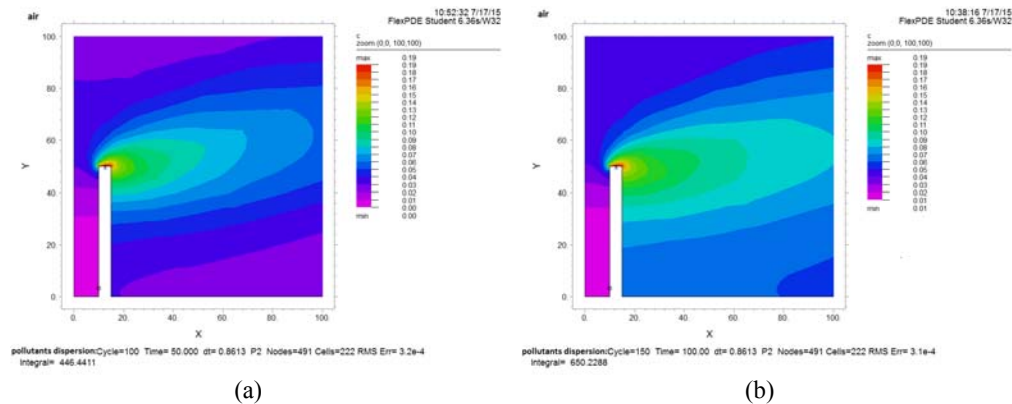


Fig. 5. Zoom on the concentration evolution in time (a) s, (b) s

The considered pollutant is the mixture composed of SO_x , NO_x and PM_{10} with a total concentration $c = 0.19 \text{ g/m}^3$.

5. Conclusions

Due to the atmospheric dispersion process, the pollutant concentration may vary in each point of the domain. Based on the conducted analysis, the errors vary inverse proportionally with the computing time.

The inputs data must comply, as accurately as possible, with the meteorological conditions, geographic location, and the pollution emissions source parameters. The wind velocity is very important within the mathematical model for describing the evolution of the plume as close to the reality. The results of the numerical simulation using the FlexPDE software shows the dispersion of pollutant's concentration.

The results confirm the theoretical studies as the variation of emission's concentration remains constant with the modification of height. However, the concentration of emission (the soil deposition) is modifying in space with the height. This mathematical model can be a useful tool in evaluating air pollution from the industrial areas.

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REFERENCES

- [1] J. H. Seinfeld, S. N. Pandis, Atmospheric chemistry and physics from air pollution climate change, California Institute of Technology, University of Patras and Carnegie Mellon University, John & Sons Inc., Hoboken, New Jersey, 2006.
- [2] G. T. Csanady, D. Reidel, Turbulent Diffusion in the Environment, Dordrecht, Holland 1973.
- [3] L. C. Andrei, Dispersia poluantilor in cursurile naturale (Pollutants dispersion in natural courses), National Institute of Hydrology and Water Management, 2011.
- [4] V. Busini, L. Capelli, S. Sironi, G. Nano, A. N. Rossi, S. Bonati, Comparison of CALPUFF and AERMOD Models for Odour Dispersion Simulation, Chemical Engineering Transactions, 2012.
- [5] M. C. Tita, Craiova University, Modelarea dispersiei atmosferice a poluantilor (Atmospheric dispersion modeling of the pollutants), AGIR 2012.
- [6] N. Moussiopoulos, E. Berge, T. Böhler, K. Grönskei, S. Mylona, M. Tombrou, Ambient air quality pollutant dispersion and transport models, European Environment Agency, January 1996
- [7] G. Lazaroiu, Impactul CTE asupra mediului (Impact of power plant on the environment), Politehnica Press, 2005.
- [8] S. Ivanov, Modelare și simulare—sisteme electromecanice, procese de mediu (Modeling and simulation—electromechanical systems, environmental processes), Editura Universitaria, Craiova, 2007, ISBN 978-973 742-626-0.
- [9] M. Beychok, Fundamentals of stack gas dispersion, 2005, ISBN 0-9644588-0-2.
- [10] R. G. Lamb, and D. R. Duran, (1977) Eddy diffusivities derived from a numerical model of the convective boundary layer, *NuovoCimento*1C, 1-17.
- [11] M. Pahlow, M. B. Parlange, F. Porte-Agel, On Monin-Obukhov similarity in the stable atmospheric boundary layer, Department of Geography and Environmental Engineering, Kluwer Academic Publishers, 2001.
- [12] J. G. Lazaroiu, Dispersia particulelor poluante (Pollutant Particles Dispersion), Editura AGIR 2006.
- [13] FlexPDE, User Guide, 2000