THE ELEMENTS OF THE DISPERSION THEORY APPLIED TO THE MATHEMATICAL SHAPING OF THE ATMOSPHERE POLLUTION BY HIGH BURNING INSTALLATION – I.M.A.

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Abstract:
The focus of this article will be centered on the establishing of the impact made by pollutant sources represented by high burning installations as they are defined by EC Direction 2001/80/EC regarding the limitation of emissions in the air of some pollutants coming from high burning installations – H.B.I., at a distance of 10 – 20 km from the emission source.

Key words: *atmosphere pollution, pollutant, dispersion models*

***JEL classification**:* Q53- Environmental Economics - Air Pollution

The development of the theories (models) about the way of the dispersion of the air's pollution represents a complex science. The main variables used to describe "the power" of pollution are mass and volume concentration. The concentration's mass is usually defined as the content's mass on the unit volume of the liquid, the most often unit measure of the concentration in the atmosphere is the $\mu g / m^3$. The volume of the concentration is usually defined in terms like: parts per million – p.p.m. or parts per billion – ppb and also zone terms.

The various roles given by the models of air pollution that covered a great part of fields applied local or globally, lead no doubt to the distinguishing of the modeling's request.

A model should incorporate the essential elements regarding the physics of the dispersion processes and also to supplier rezonable and repeatable appreciations regarding the concentration's level of the pollutant emissions on the direction of the wind. A model of dispersion represents, essentially, a procedure of prediction of the concentration of the pollutant source on the wind direction, based on the analyzing of the next notes:

- the characteristics of the emissions (the exit speed from the stack, the temperature of cloud's burnt gazes, the diameter of the stack);
- the characteristics of the land (rigidity of the surface, the place topography, the nearby buildings);
- the state of the atmosphere (the speed of the wind stability, the mixing height).

The modeling of the dispersion of the pollutants is completed by the usage of the mathematical algorithms. There are more models that utilize mathematical algorithms bared on the analysis of dispersion, the most important being [1]: the primary model of Hanna [7], the Box model, the Gaussian model, Eulerian model and Langrangian model.

(a) The Hanna model is based on the following formula for the situation's estimation of the highest concentrations of pollutant emitted by a pointly source on the wind direction:

$$C_{WC} = \frac{10^9 Q}{U H_{WC} W_{WC}} \quad , \quad \text{where:} \qquad (1)$$

Q – the rate of gas emission or of the particle / powder, in kg /s;
C_{WC} –the biggest concentration, in $\mu g / m^3$;

U – the most dangerous speed of the wind at the height z = 10 m, normally 1 m / s;
W_{WC} – the biggest breadth of the pollutant cloud, in meters, usually given by W = 0,1 x, where x is the distance from source;
H_{WC} – the biggest depth of the pollutant cloud, in meters, considered useful at 50 m

The equation generally represents the preservation of the pollutant, mass but depends on many base parameters connected by the modeling of the dispersion this way:

1. The medium concentration is proportionally reverse with the medium wind speed;
2. The medium concentration is proportionally direct with the evacuation rate;
3. The medium concentration is proportionally reverse with the transversal section of the pollutant cloud.

(b) The Box model's algorithm is the most simple of the models' algorithms. It considers the air deposit has a box shape. The air from inside the box is considered to have a homogenous concentration.

The algorithm of the Box-models is represented by the next equation:

$$\frac{dCV}{dt} = QA + uC_{in}WH - uCWH \text{, where:} \qquad (2)$$

Q – the rapport of the emission of the pollutant on the surface unit;
C – the concentration of the homogenous types from inside the deposit
V – volume described by box;
C_{in} – concentration of the type of pollutant that enter the deposit;
A – horizontal surface of the box (L x W);
L – length of the box;
W – width of the box;
u – the wind speed witch acts perpendicularly on the box
H – mixing height

Although it is often used, this model has limitations. It is considered that the pollutant is homogenous in front of the deposit and it is used to estimate the medium concentration of pollutant above a very large surface but it doesn't offer clues regarding the spatial dispersion.

(c) The algorithm of the Gaussian model is the most common in the modeling of the analyzing of the air dispersion. It is based on the supposition that the pollutant will disperse according to the normal statistics distribution.

The Gaussian equation used, generally for the emission in comparison with the point source is written starting from:

$$\frac{dC}{dt} + U\frac{dC}{dx} = \frac{d}{dy}\left(K_y \frac{dC}{dy}\right) + \left(K_z \frac{dC}{dz}\right) + S \text{ , where:} \qquad (3)$$

x – the measured coordinate from the source along the wind direction;
y – the measured coordinate from the source perpendicularly to the wind direction;
z – the vertical coordinate measured from soil;
C(x,y,z) – the medium concentration of the dispersed substance at the (x,y,z) point, in kg / m^3;
K_y, K_z – diffusions of the turbulence on the direction of the axes y and z, in m^2/ s;
U – the medium speed of the wind along the axis x, in m / s;
S – Source / definition of the evacuation, in (kg / m^3) / s.

The analytical solutions of the equation for the passive pollution dispersion's case in a turbulent system were obtained for the first time by Roberts [2] and Richardson.

The relative diffusions to the turbulent fluxes of material are calculated after medium grades of the concentration from the equations:

$$\overline{\upsilon' c'} = -K_y \frac{\partial C}{\partial y}; \quad \overline{w' c'} = -K_z \frac{\partial C}{\partial z} \qquad (4)$$

Noting the coordinates referring to the terms of the turbulent fluctuations with: c(t) = C + c', u(t) = U + u' and considering: $K_y > K_z$, to explain the elliptical configuration of the cloud in the transversal section can be analyzed term by term the first equation, this way:

$\frac{dC}{dt} + U\frac{dC}{dx}$, as being the medium time rate of the adjustment of the pollutant cloud at the medium speed;

$\frac{d}{dy}\left(K_y \frac{dC}{dy}\right)$, as being the material's turbulence diffusion relatively to the centre of the pollutant cloud (the cloud will expand in time due to these terms).

S, as being the source term that represents the net production (or the destruction) of the pollutant due to the sources or the moving / changing mechanisms.

Terms σ_y and σ_z represent the standard deviation on horizontally and vertically distribution.

By simplifying, some approximations have to be solved:

- the pollutant concentrations doesn't effect the evacuated flow (passive dispersion);
- molecular diffusion and longitudinal diffusion (along wind direction) are negligible;
- the wind's speeds and concentrations can be divided into medium component and a fluctuant one with a stockpots value (fluctuant) that points to zero;
- the turbulent fluxes are linear;
- the lateral medium speed, V and the wind vertical speed W are zero, the ideal case of the flat ground.

Based on these hypothesis, changes can be operated into the initial equation that lead to the following formula:

$$C(x,y,z) = \frac{Q}{4\pi x\sqrt{K_y K_z}} \exp\left(\frac{-y^2}{4K_y\left(x/U\right)}\right) \exp\left(\frac{-z^2}{4K_z\left(x/U\right)}\right) \qquad (7)$$

Noting: $\sigma_y = \sqrt{2K_y \frac{x}{U}}$ and $\sigma_z = \sqrt{2K_z \frac{x}{U}}$ (8)

and introducing the original expression, we obtain:

$$C(x,y,z) = \frac{Q}{4\pi U_p \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right)\left[\exp\left(-\frac{(z-H_p)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z+H_p)^2}{2\sigma_z^2}\right)\right] \qquad (9)$$

in witch considering that the pollutant can't diffuse descendant to the ground, z = 0 and that the source is always above the ground, so $z = -H_p$, we reach to an equation given by Turner [3] according to which the cloud's height represents the sum of actual height of the evacuation stack and "the plume rise" or rising height: $H_p = H_s + \Delta H$ for witch it is admitted that the medium wind speed must be considered at the level of the evacuation stack's height.

With z = 0 we get to the following equation:

$$C(x, y, z = o) = \frac{Q}{\pi U_p \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \exp\left(-\frac{H_p^2}{2\sigma_z^2}\right) \qquad (10)$$

and even more we consider $H_p = 0$ (the vertical distribution case at the ground level) then we can write:

$$C(x,y,z) = \frac{Q}{\pi U \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \exp\left(-\frac{z^2}{2\sigma_z^2}\right) \quad (11)$$

where, if we think that the model is not very precise, in the vertical profile it varies after $\exp(-z^{1,5})$ or more likely under the Gaussian formula $\exp(-z^2)$, diffusivity K_z varies in large limits tile almost to the ground [5] and results:

$$C(x,y,z) = \frac{Q}{\sqrt{2\pi} U_p \sigma_y} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \quad (12)$$

$$\iint_{y,z} CU dy dz = Q \quad (13)$$

in which the integration takes place in the plan of y – z perpendicular to the cloud axis.

The Gaussian algorithm will be taken for the mould Gaussian dispersion of the pollutant emitted by IMA that uses solid fuels as the type of coal and refined derivates from oil and/or natural gases used to represent the pollutant cloud.

These coefficients are based on atmospherical stability coefficients established by Pasquill and Gifford and they generally became larger at long measured distances on the wind direction in comparison with the source.

The greatest deviation appears when the Gaussian curve or cloud have a low point and a large distribution; the smallest deviation occurs when the Gaussian curve and cloud, have a high point and a limited/narrow distribution (fig.1)

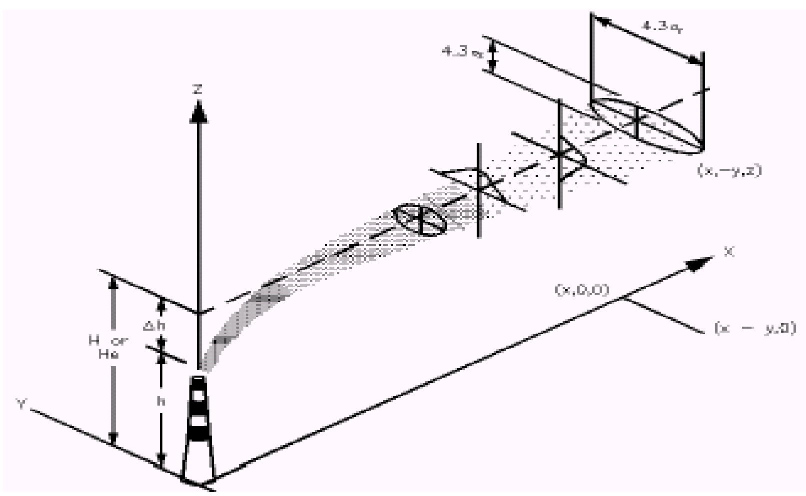

Fig. 1 Gaussian distribution graph of dispersion [9]

When we use this equation to calculate the pollutant's dispersion there are a few assumptions to be done in order to this equation to be valid:

- the emission should be constant and uniform;
- the wind direction and dispersion are constant;
- the diffusion on the wind direction is negligible in comparison with the vertical diffusion and the normal direction at the wind direction;
- the ground is relatively flat, doesn't have normal limits on the wind direction;
- there aren't no deposit or pollutant absorption;
- the diffusion on the vertical direction or on the normal direction at the wind's direction follows a Gaussian distribution;
- the shape of the cloud may be considered expanded;
- use of the standard deviation σ_y and σ_z imposes that the turbulence of the cloud must be homogeneous on the whole cloud [6].

The exactness of this model in prediction of the pollutant concentration by directly introducing the data should be in the field of 20 % for emission at the ground level, 1 km away.

For high emission, punctuality is found in the field of 40 %. For larger distances more then 1 km, the equation is estimated to be exact by multiplying with the factor 2 [7].

The Gaussian model has also limited use and can't be used for subtime intervals of the concentration [8].

The pro and against theories of the Gaussian dispersion model sustain the following:

- The Gaussian dispersion models are computer models used to control the impact of air's pollution sources already existing and for the proposed ones at the urban and local air quality, especially for adjustment application;
- The theoretical bases of these models limit to the uniform fluxes with homogenous idealized turbulences;
- For continuous points and linear sources the constant wind speed should be greater then the standard deviation of the fluctuation's turbulent speed so that the superior stream or longitudinal spreading to be neglected;
- The constant wind and the turbulences met in the atmosphere, especially in the transition layer (PBL), rarely are like these simplify suppositions. Frequently, in reality, there are strong winds, turbulences and weak winds that make theoretical bases of the Gaussian dispersion models, surely insufficient, but not entirely invalid;
- The main reason for that these models are used is the evaluation and validation against the experimental dispersion data. Many data that are used for this purpose, are still limited when approaching the land or maximum concentration level at the ground level and of the metheorological parameters and of the source, wich are used as an entrance is the Gaussian models.

Other reasons for to use these models are:

- they are on outlook approach able and analytical;
- compatible with random nature of the turbulences;
- low costs of use;
- they have obtained an official status of accreditation in the official settlements.

Limits of Gaussian dispersion models appear also by the simplification of the suppositions and physical models. More sophisticated numerical models should be used to simulate and predict the dispersion in complex flux conditions.

(d) The algorithm of Eulerian model. Eulerian models solve the preservation of the mass equation for a given pollutant. General equation must be written like this:

$$\frac{\partial(c_i)}{\partial t} = -\overline{U}\cdot\forall(c_i) - \forall\cdot(c_i^{'}) + D\forall^2\langle c_i\rangle + \langle S_i\rangle \qquad (14)$$

where: $U = \overline{U} + U'$

U – the wind main vector U(x,y,z);

$\overline{U}$ – medium domain vector of the wind;

U' – the vector of the wind's domain's fluctuations;

c = $\langle c\rangle$+c';

c – pollutant's concentration;

$\langle c\rangle$ – pollutant's medium concentration;

c' – pollutant's concentration's fluctuation;

D – molecular diffusivity;

S_i – source term.

The wind's domain vector, which is frequently used, is considered turbulent and results in $\overline{U}$ and U', which are part of the domain of the turbulent wind from the algorithm equation.

The vector of the turbulent wind's domain is also affected by the pollutant's concentration, c, and in the some measure by the terms $\langle c \rangle$ and c'.

The term is molecular diffusivity and is neglected if its measure is rather small.

When the diffusion rate is considered constant, the term of the turbulent diffusion: $\forall \cdot \langle c_i^{,} U^{,} \rangle$ is mould as the $\langle c_i^{,} U^{,} \rangle = -K \forall \langle c_i \rangle$ where K is the tensor of the turbulent diffusivity.

This tensor is simplified if the transport diffusivity is along the turbionary vector, this way showing the diffusivity on the tensor's diagonal, and the normal diffusivity on the vector's direction being neglected.

$$K = \begin{bmatrix} K_{xx} & 0 & 0 \\ 0 & K_{yy} & 0 \\ 0 & 0 & K_{zz} \end{bmatrix}, \text{ where} \qquad (15)$$

$K_{xx} = K_{yy} = K_H$, K_H – horizontal diffusivity

Eulerian algorithm equation is very hard to solve out because the first term has hyperbolical structure and the turbulent diffusion term is parabolic, so a set of differential equation is necessary, but even though the solutions can be found by computer, the problem can be diminished to one or too dimensions, a side of using the three-dimensional system.

(e) Lagrangian model algorithm predicts the pollutant's dispersion knowing the change of the base grill. This change of the base grill generally depends on the fact that the wind direction or the wind field vector gets on the direction of the pollutant cloud.

Lagrangian model has the following formula:

$$\langle c(r,t) \rangle = \int_{-\infty} \int p(r,t | r^{,},t^{,}) S(r^{,},t^{,}) dr^{,} dt^{,} \text{ , where} \qquad (16)$$

$\langle c(r,t) \rangle$ – is the medium concentration of the pollutant at location r and time t;

$S(r^{,},t^{,})$ – defines the emission source;

$p(r,t | r^{,},t^{,})$ – probability's function for the air parcel to move from the location $r^{,}$ and time $t^{,}$, to location r and time t.

The probability function should be defined as a function full of meteorological data being close to the gas sources. If the emission source includes mechanical dust, particles, then it must be added as a distribution of measure and density of particles. Mathematical model called LASAT (Lagrangian Simulation of Aerosol Transport – fig. 2) has limits because its results must be compared to the measurements, due to the model dynamic nature.

The measurement are generally made in stationary point, most of the time based on given models depending on the pollutant concentration.
Still this is the model that makes the connection between theoretical calculations and effective measurements.

These four mathematical models are a main approach for to mould of the air dispersion, having more solutions that uses the described equations.

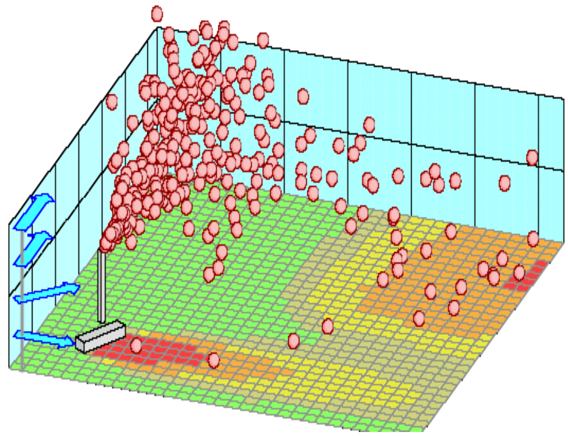

Fig. 2 LASAT model scheme [9]

These variant add the static functions that represent the random character of the wind's direction, speed and turbulence; other parts are based on specific emission source terms.

Due to the increased computers capacity, these models become more complex and diverse, in the end getting to a close appreciation of mathematical model of the air dispersion towards the reality.

(f) Molding based on fluid's dynamic calculations (Computational Fluid Dynamics – CFD) appeared as a result of determination of the dispersion of pollutant emissions in small areas, along the access ways, rivers' valleys, gorge or pass through high geographical profiles (hills, mountains, etc.).

The models have appeared as a result of stability for main directions of dispersion of the mines or quarries, but also for prominent made by ash deposits of IMA that uses coals as fuel.

Propagation errors into air from dispersion models can be describe as:

- ❖ Models of air dispersion have developed before 1930, in the last 15 – 25 years; strict rules regarding the environment and the availability of the computers have provided a huge increase in the use of mathematical models to predict the dispersion of the smoke clouds that pollute the air. The paper [10] details the evolution of the Gaussian's models of dispersion in air of pollutant clouds, spread on large scale together with assumptions and limits. Unfortunately, a lot of user of these models doesn't recognize the ideas and constrictions and believe in a wrong way that the equations solved by computers are very precise.
- ❖ The propagation of, apparently, slight errors in Gaussian model parameters can cause large variation in model predictions.
- ❖ For most of the dispersion models, the determination of the concentration at the ground level through receivers from behind ascendant clouds of pollutant smoke, floating, that spreads, is made in 2 main steps:
  a) first step: calculation of the height that raises the cloud to a given distance in the wind direction from the source of the cloud. The calculated (increase) raise of the cloud of smoke is added to the height of the source point of the pollutant cloud to get so called "the height effect of the smoke stack" or "emission height".
  b) second step: the concentration of the pollutant at the ground level from behind the smoke cloud, at a certain distance on a wind given direction, is predictable using dispersion Gaussian equation.

Table 1 presents a comparison between the models of dispersion of pollutant emissions and used in existing practice.

Table 1

Shows a comparison between the main models of dispersion of existing and used pollutant emissions

Model property	ISC 3	RAM	CTDMPLUS	INPUFF used in Romania [26]	CALPUFF	DEGADIS
Source type	Point form, Area, Volume	Point form, Area	Point form	Point form, Area	Point form, Area, Volume, Linear	Point form, Area
Ground type	Simple, Complex	Simple	Complex	Simple	Simple, Complex	Even, except obstruction
Release model	Continuous	Continuous	Continuous	Continuous, Instantly	Continuous, Instantly, Variably	Continuous, Instantly, Variably
Medium time	1h...annually	1h...annually	1h...annually	Minute...few hours	1h...annually	1 h or less
Location	Rural or Urban	Urban	Rural or Urban	Rural or Urban	Rural or Urban	Rural or Urban
Pollutant type	Gas, dust	Gas, dust	Gas, dust	Gas, dust	Gas, dust	Gas, aerosols
Available field	≤ 50 km	≤ 50 km	≤ 50 km	10 s to km	100 s la km	Calculated by model
Weather data nature	Real	Real	Real	Real	Real, limited	Real, limited
Model of chemical reactions	No	No	No	No	Yes, common reactions	No
Calculation of dry deposits	Yes	No	No	Yes	Yes	No
Calculation of wet deposits	Yes	No	No	No	Yes	No
Molding of the transport capacity	No	No	No	No	No	Yes
Simulation through singular multiple sources	Multiple	Multiple	Multiple	Multiple	Multiple	Singular

Conclusions

With al these disadvantages, many models of atmospherically dispersion are available to the evaluation of the emergency potential in different given situations.

These four mathematical models are a main approach for to mould the air dispersion, having more solutions that use the equations.

Due to the computers capacity increase, these models become more complex, in the end getting to a close appreciation of mathematical model of the air dispersion towards the reality.

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