MATHEMATICAL MODELING AND NUMERICAL OF THE ATMOSPHERIC POLLUTION AT THE LEVEL OF FREE SURFACES

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Abstract

The objective of the present work is numerical and theoretical modeling of the atmospheric pollution at the level of free surfaces (air and water), by studying tools for numerical simulation making it possible to very precisely determine the fields of concentration in terms to space and of time.

The fate of a pollutant depends primarily on the flow characteristics that transports. An extremely accurate representation of all the hydrodynamic phenomena in the receiving environment is therefore necessary. In particular, consideration of turbulence is essential. The progress of the pollution in the environment defined above is then modeled in terms of concentration through a convection-dispersion model.

These equations don't admit analytical solutions, so recourse to numerical methods proves mandatory. In our study, the equations are solved using the numerical method of finite differences, to determine the temperature, pressure, velocity components and concentrations of major pollutants that exist in the atmosphere.

This study, which is a model that allows understanding of the phenomena of pollution at the free surfaces can be adapted to other industrial applications.

Key word:*Turbulent flown, finite volume method, Newtonian fluid, atmospheric pollution, Process Emission-Dispersion-Transformation-Immission.*

1.Introduction:

The more and more frequent presence of punctual pollutions in the atmospheric layers encourages developing tools of numerical and theoretical modeling allowing determining very precisely the fields of concentration, velocity profile and the distribution of the temperature according to the space and of time. The level of modeling depends in general on the studied area. The future of a pollutant depends initially on the characteristics of the flow which transports it. An entirely precise presentation of all hydrodynamic phenomena present in receiving medium therefore proves to be necessary. Particularly, taking into account of the turbulence is essential. Thus, for a better understanding of the transport and the destiny of the existent pollutants in atmospheric layers, numerous numerical and theoretical models were developed. These numerical models allow today to treat a more and more broad range of problems met in nature, but certain phenomena remain taken into account in a very simplified or neglected way. Certain researchers, interested only in chemical reactions between the different pollutants, assume that the velocity of the wind and the tensor of conductivity are known. [1-4]. others, while trying to treat the three processes: flow, transport of the pollutant, and transport of energy, neglect some characteristics of flow; turbulence and compressibility of fluid [5].Equations describing such phenomena are solved, in general, numerically by using approximate methods such as finite difference, finite volumes, finite elements or spectral methods. The originality of the present study is the numerical and theoretical two-dimensional modeling of the phenomenon of atmospheric pollution by taking into account at the same time; equations of the transfer of energy, transport of pollutants, turbulent and non-stationary character of the flow, compressible character of the fluid and phenomena of diffusion, of advection and chemical reactions.

2. Mathematical Formulation

The requested relations to predict and describe the phenomenon of atmospheric pollution are based on three fundamental processes coupled between them. These equations are deduced from the principles of the conservation of the mass, the quantity of movement, the energy, and of the transport of aqueous solution. The variables which result from this in the most general case are the density (p), the velocity components (U, W), the pressure (P), the temperature (T) and the concentration of the pollutant (C). These variables are all functions of space and time Φ (x, z, t)).

2.1. Equations Setting

2.1.1. Equation of Fluid Flow

The turbulent flow of fluid is govemed by mass and quantity of motion conservation equations of Newtonian fluid in gravitational field :

$$\frac{\partial \rho *}{\partial t}+\frac{\partial(\rho * u *)}{\partial x}+\frac{\partial(\rho * w *)}{\partial z} \qquad (1)$$

$$\frac{\partial \rho * u *}{\partial t}+\frac{\partial(\rho * u * u *)}{\partial x}+\frac{\partial(\rho * u * w *)}{\partial z} = -\frac{\partial P *}{\partial x}+\frac{\partial \tau_{xx}}{\partial x}+\frac{\partial \tau_{xz}}{\partial z} \qquad (2)$$

$$\frac{\partial \rho * w *}{\partial t}+\frac{\partial(\rho * w * u *)}{\partial x}+\frac{\partial(\rho * w * w *)}{\partial z} = -\frac{\partial P *}{\partial z}+\frac{\partial \tau_{xz}}{\partial x}+\frac{\partial \tau_{zz}}{\partial z}+\rho * g \qquad (3)$$

In this study, we do not take into account the rotational forces of Coriolis and centrifugal which are negligible in front of the force of gravity owing to the fact that one is interested only in the process taking place in a space zone and a time scale limited. The tensor Components of viscous stress depend on the rate of strain of the fluid subjected to the field of speed and acceleration of gravity. From now, we work within the framework of the isotropic and Newtonian fluids knowing that all the gases (thus air) check this assumption . A fluid is isotropic when the relation between the components of the tensor of the viscous stress and those of the rate of strain is identical in all the directions. It is moreover Newtonian if this relation is linear:

$$\tau_{ij} = 2\mu\left[\frac{1}{2}\left(\frac{\partial u_i^*}{\partial x_j}+\frac{\partial u_j^*}{\partial x_i}\right)\right]+\mu'\frac{\partial u_k^*}{\partial x_k}\delta_{ij} \qquad (4)$$

Few things are known on this second dynamic viscosity as much as his effect is not very important in practice. It seems in spite of all, for a compressible fluid, a good approximation of g is given by relation :

$$\mu' = 2/3\mu.$$

For an incompressible fluid, it is not useful to define it since it does not intervene.

2.1.2. Equation of the Transfer of Energy

The transfer of energy in the atmosphere is governed

by following equation:

$$\frac{\partial \rho^* e}{\partial t}+div\left(\rho^* e\vec{u}^*\right) = -P^* div\vec{u}^* + div\left(\lambda \overrightarrow{grad} T^*\right)+\phi+S \qquad (5)$$

Φ is result of viscous dissipation and S generated by any source in fluid.

2.2. Simplifying Assumptions

In this study, we consider the flow of incompressible fluid but coupled with the fields of temperature and concentration by forces of floatability. In other words, it is supposed that the density ofthe fluid is independent of the pressure, assumption which is valid for gases proving the relation:

$$\frac{1}{2}M^2 \langle\langle 1 \text{ with } M = \frac{V}{c_l}.$$

Thus, as long as the speed of air does not reach 100 m/s, the density of the air can be regarded as independent of pressure

Moreover, it is considered that the variations of the density with the temperature and the concentration of the pollutant are negligible at the level of all terms ofequations except at the level of the term of gravity where they can produce important effects. These assumptions lead to the following equation of state:

$$\rho^* = \rho^*\left(P^*, T^*, c^{j*}\right) = \rho^*\left(T^*, c^{j*}\right) = \rho_0\left[1-\beta\left(T^* - T_0\right)+\alpha\left(c^* - c_0\right)\right] \qquad (6)$$

β, ρ_o, c^{j*} and T_o supposed to be constant.

This state equation appears only in the floatability term of the equations of the quantity of movement, it is at the origin of the coupling of the speed and the temperature. At the level of all other terms, the density is constant and equal to PO. It is about the approximation of Boussinesq [5].

In this study, the fluid is consideredcompressible but obeys to Boussinesq approximation. Therefore, internal energy is related to the temperature by relation:

$$de = c_v dT^* \qquad (7)$$

or:

$$e = c_v\left(T^* - T_{ref}\right) \qquad (8)$$

c_v is selected constant since the differences in temperatures are rather weak. Also, we consider molecular dynamic viscosity g and molecular thermal conductivity i constant. This approximation is valid since we will approach the flows of turbulent fluids in which molecular transport is negligible compared to turbulent transport. The variations of these molecular properties (with the temperature) will be therefore negligible faced with values taken by the turbulent properties.

III. Results

The temporal evolution of the profile of theconcentration in the plan z = H/2 and x =H/2 is plotted in Fig. 1. We notice on this figure that the concentration grows with time. This can explain by the fact that at this level pollutants settle in fur and as the time passes.

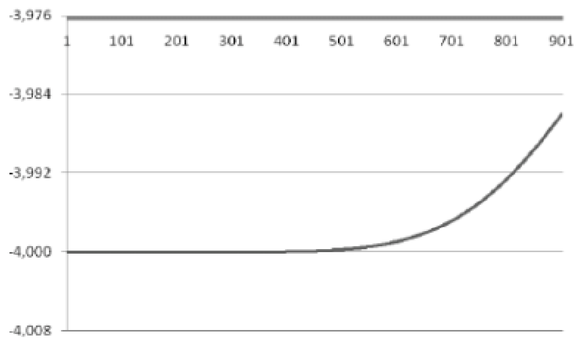

Fig. 1. Temporal evolution of the profile of the concentration (Lx=Lz=H/2)

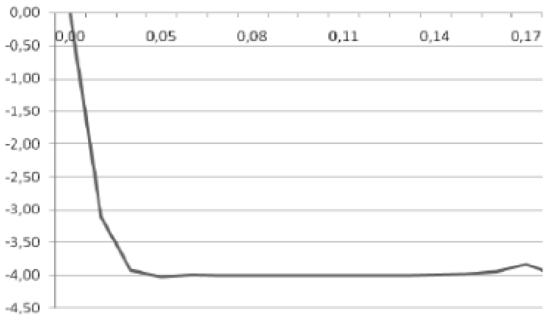

Fig. 2. Evolution of the profile of the concentration according to z (t=Tmax/2, Lx=H/2)

Fig. 2. illustrates the variation of the concentration of the pollutant according to altitude z in the half time of follow-up of the phenomenon

IV. Conclusion

The two-dimensional theoretical and numerical study of atmospheric pollution in the lowest layers was used to analyze the different stages of the process of propagation of pollutants. The obtained results are in concordance with results obtained by other authors and allow us to understand this problem and to be able to prevent it in the future.

V.References

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