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Modeling Of The Dispersion Of Polluting Particles In A Room.

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ABSTRACT

The air inside the buildings is a mixture of physical, chemical and biological pollutants which originate from the surrounding air, materials, the devices of combustion and the human activities. For materials, we can distinguish the emission from volatile organic compounds, paintings with lead and fibers. The attendance time of the townsmen inside the buildings can be more important for certain fragile or critical populations like younger children, the elderly people or patients, or also of the particularly sensitive people. Interior air quality becomes an increasing concern of our fellow-citizens, partly due to the presence of symptoms or diseases related to the buildings. In this paper, we are presenting some numerical models which have been to simulate the dispersion of pollutants in the atmospheric boundary layer in different stability, and During our work, we are going to study the dispersion of the fine particles inside a room, with the Discretization in 3 dimensions by the finite volume method of the flow of the incompressible air polluting occupying this room, modeled by the Navier-Stokes equations . We chose to couple them with the equation of the heat in the case where the viscosity depends on the temperature with conditions in the limits concerning the speed and the temperature.

CCS Concepts: Sciences and technology of the engineer

Keywords: Pollution, Particles, Dispersion, Discretization, Emission, Algorithms, The volume Finite Method, Navier-Stokes.

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INTRODUCTION

Previously, atmospheric pollution has been mainly of industrial origin, therefore, often specific, related in particular to the car, is more diffuse and affects especially urban environment. Moreover, pollution with trend moves on very long distances, several hundreds, and even of the thousands of kilometers. Today, atmospheric pollution is less visible and its effects on the environment and health are less perceptible. One tends also to be worried more interior pollution in the public buildings and the residences. Various studies show that the majority of the population passes most of its time inside. From this point of view, often wrongly, atmospheric pollution is perceived like having a secondary impact. Indeed, the micro-environments external and interior are regarded to the pollutants of the surface. Certain metropolises or certain areas are still nowadays affected by atmospheric pollution. The description of effects on health with concentrations lower than what was known previously [1].

External pollution (atmospheric) has its fact, but its implication in the constitution of the disease is very difficult to show. Its effects on the respiratory function have been really studied only for about twenty years, thanks to studies of troops, long and tiresome, which explains the controversies concerning their conclusions and the difficulties of highlighting results statistically significances. These difficulties are all the more large as pollution is made of a set of molecules (gas, particles…).

In spite of the improvement of the situation in most developed countries, atmospheric pollution remains a concern of important public health. Indeed, at several places, a broad part of the population is still exposed to high concentrations of traditional pollutants. In several cases, the population is exposed to relatively high concentrations of toxic pollutants or to the photochemical smog [2]. New knowledge which was developed recently on the effects of the particles indicates that important effects could occur with current concentrations. The analysis of risks which were made in Europe and in the United States indicate that impact on the public health is very important [3], especially with regard to the respiratory diseases.

PROPERTY OF THE FINE PARTICLES

"Dust" is a generic term indicating all the suspended matter particles in the ambient air. They are also called "aerosols" or "Particulate Mater (PM)". They are a complex mixture into small solid particles and liquid droplets. It is the only an atmospheric pollutant for which no chemical definition is used because of the vast range of phytochemical composition of these last. According to the temperature and hygroscope, certain suspended particles can contain a significant amount and variety of moisture and volatile compounds. Other particles, like ammonium salts, dissociate when the temperature increases and the air becomes drier. Considering the great variation of size and physic-chemical composition, the impacts on the health are very varied.

Emission of particles

The emission [4], expressed in a unit of mass per unit of time (for example, kilo thunders a year, kt/year) represents the quantity of particles emitted directly or indirectly by road transport, the residential sector, the tertiary sector or the industrial sector. These emissions are quantified by using the data of consumption of the principal transmitting sources and by using the emission factor (expressed by g/J) which evaluate the quantity of pollutant emitted for a certain quantity of power consumption. The emissions make it possible to determine the contributions of various sources of the pollutants and to target the sectors towards which it is necessary to act. Once emitted, the particles are dispersed more or less effective in the air, according to the weather conditions (wind, height of the layer of mixture, temperature inversion). The values of the emissions correspond to the concentrations measured in the ambient air, they are expressed in a unit of mass per volume of air (for example in µg/m3 for the PM). The evaluation of air quality is based on the emissions and not on the emissions.

Classification of the particles

Considers various sizes of particles [5] which are given according to the aerodynamic diameter, called here after "Diameter":

Total particles (PM): the whole particles in the air

Fine particles (PM10): particles of diameter lower than 10 µm

Very fine particles (PM2,5): particles of diameter lower than 2,5 µm

Ultra-fine particles (PM1): particles of diameter lower than 1 µm

Nano-particles (PM0,1): particles of diameter lower than 0,1 µm which are regarded as the most harmful particles for health.

It should be noted that PM10 enter the PM2,5, PM1 and PM0,1, just like those of the PM2,5 include the PM1 and PM0,1, and PM1 the PM0,1.

THE ROLE OF MODELING

The role of the modeling of atmospheric dispersion can appear secondary compared to the legislative measures of reduction of the emissions. However, this latter is an important component of the management of pollution for the public authorities, but also for the owners of industrial sites. Modeling makes it possible to better understand the concerned physical phenomena and constitutes essential tools to conceive the means of fight against pollution. Thus the place of modeling in the problems of industrial pollution is at several levels.

Room Monitoring

Modeling intervenes first in all the industrial monitoring sites. It can come to supplement and specify the measurements carried out by the fixed sensors of pollution disseminated on the site. The numerical models then make it possible to exploit the data resulting from these sensors by making cartographies of concentration and to visualize thus the zones with strong concentrations of pollutant while evaluating the real exposure of the population to the neighborhoods of the industrial sites, but also that of the employees in the vicinity of the installations. Besides its capacity of studying last episodes of strong pollution, it allows for operators to improve their reactivity in front of similar scenarios, but also to choose in an optimal way the site of future sensors which will allow an increasingly precise monitoring. The monitoring of the sites also passes by a control in real time estimated of pollution. Modeling allows the creation of tools, then ensuring the follow-up in real time of the concentrations of the accesses as of sites, but also, according to weather forecasting and of the activities of the site, these estimated tools can ensure the piloting of the production by limiting this latter in the event of position risk on the cities bordering.

Decision-making aid

One of the principal interest of modeling for the owners of industrial sites is to be able to study the modifications generated by a change of the conditions of a problem. Thus, it is possible with the current tools to predict the impact of the addition of geometry or a source term on the industrial sites. Several scenarios can be tested and simulated in order to help the policies and the owners to choose the best compromise between profitability and protection of the populations in the neighborhoods. Thus modeling takes a very important place in the studies of the dangers which are carried out party by models of calculation, which during particular installations (establishment of factory reorganization of town planning in the neighborhoods of a site; etc.) bring information generated pollution and evaluate the effectiveness of the various policies put in work. Finally, the contribution of atmospheric modeling at the level of the decision-making aid is very important and makes it possible to facilitate to coexistence between the profitability and the production of the industrial world and the security of the surrounding populations [6].

PROBLEMATIC AND HYPOTHESIS

Problematic

Our study falls under the set themes of the dispersion of the polluting particles inside the buildings and more particularly on the development of a digital tool of prediction of the behavior of particles by using modeling based on the Discretization of Navier-Stokes equations [7] with the methods of finite volumes. The problem of the prediction of the movement of the particles is introduced by the study of the elementary forces which are exerted on the particles. This study is devoted to develop one digit code of calculation of the particle concentrations inside. We regard in this code the air polluted as a single entity, and treat the exchanges with the outside and on the walls of the building in their globalities.

Hypothesis

In order to simplify the formulation of the mathematical model, we will consider the following approximations, which are often used in the study of natural convention:

- The fluid is Newtonian and incompressible;
- The physical properties of the fluid are constant;
- The flow is stationary and three-dimensional;
- The flow is laminar;
- The transfer of heat per radiation is negligible;
- The dissipated density power density is negligible;

SIMULATION NUMÉRIQUE

Various steps to model a complex system:

- Search for a mathematical model representing physics. Setting in the equation.
- Development of a grid. Discretization of the equations of physics.
- Resolution of the discrete equation (often linear systems to solve).
- Data-processing, transcription and programming of the discrete relations.
- Digital simulation and analysis of the results.

The engineer can have to intervene on one or several of these various stages

BASIC EQUATIONS

We need to point out certain equations which control the dynamics of CLA and on this occasion, to define certain parameters of this dynamic. The various phenomena which occur in the atmosphere are closely related to flows of energy and matter within this latter. These flows are described by the equations of mechanics of the fluids or of Navier-Stokes [7] which translate the conservation of the three following physical quantities:

- Mass, expressed through the density
- Momentum
- Energy to the conservation of these three physical sizes, the equation of state of the perfect gas and the conservation of scalar sizes are added.

Conservation equation

Conservation of mass [8]

The weight breakdown of the fluid on an element of volume is written as:

Conservation of momentum [8]

$$\frac{\partial \rho}{\partial t} + \nabla.(\rho u) = 0$$

The conservation of momentum is provided by the relation:

$$\frac{\partial \vec{u}}{\partial t} + \nabla.(\vec{u} * \vec{u}) = -\frac{1}{\rho}\nabla p + \nabla\overline{\overline{\sigma}} + F$$

F corresponds to the sum of voluminal forces, and $\bar{\bar{\sigma}}$ represents the tensor of the viscous constraints which, for a Newtonian fluid, is given by the law:

$$\bar{\bar{\sigma}} = \nu(\nabla\vec{u} + \nabla^t\vec{u})$$

Conservation of energy [8]

The total conservation of energy of the fluid E is written:

$$\frac{\partial(\rho E)}{\partial t} + \nabla.(\rho E u) = -\nabla.(P u) - \nabla.q + \nabla.(\bar{\bar{\sigma}}.u) + \rho F.u + \rho H$$

The first term of the second member represents the power of the compressive forces. The second term corresponds to the transfers of heat by conduction, q represent the heat flow connected to the temperature by the Fourier analysis:

$$q = -\lambda\nabla T$$

While λ is the thermal conductivity of the fluid.

The third term is the mechanical dissipation of energy by viscous friction, being the tensor of the viscous constraints; the fourth term corresponds to the power of the voluminal forces. Lastly, H represents the sources of heat in the fluid. In the continuation, this equation will be reformulated to reveal the temperature T instead of energy.

Equation of continuity [8]

It translates the conservation of the matter in the system considered:

$$\mathrm{div}(\vec{u}) = 0$$

FINITE VOLUME METHOD

The method of volumes of control integrates, on ground volumes of simple form, the equations written in the form of the law of conservation. It provides thus in a natural way of the conservative discrete approximations and thus is particularly well adapted to the equations of the mechanics of the fluids. Its implementation is simple, if ground volumes are rectangles (or parallelepipeds in 3D). However, the method of volumes of control makes it possible to use ground volumes of an unspecified form, therefore, to treat complex geometries, which is an advantage of the finished differences.

Monodimensional study

Permanent mode

The problem of the propagation of the heat in a permanent mode:

$$\frac{d}{dx}\left(k\frac{dT}{dx}\right) + S = 0$$

T: Temperture
K: Thermal conductivity
S: Heat source

Distribution of volumes of control (Discretization of the zone of calculates):

The method of volumes of control consists in subdividing the zone of integration in a finished number of volumes of control. The points of the grid are all in the center of gravity of these volumes of control.

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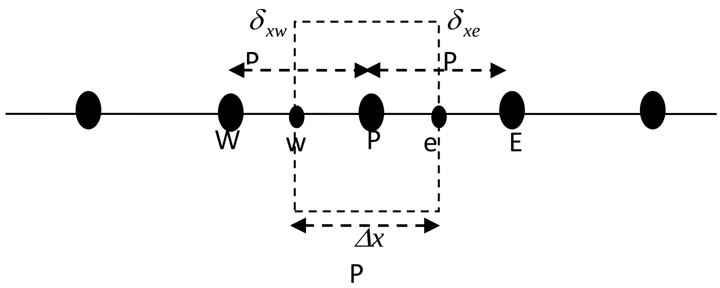

P: centers of the volume control
E: easter node of the VC
W: western node of the VC
e and w are the faces east and west of the VC

In this mono-dimensional case, volumes of control are segments [w,e] the integration of the equation of heat [8] on the VC gives:

$$\int_{w}^{e} \frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) dx + \int_{w}^{e} S\, dx = 0$$

$$k\frac{\partial T}{\partial x}\bigg|_{w}^{e} + \bar{S}\,\Delta x = 0$$

, or

$$\left(k\frac{\partial T}{\partial x}\right)_{e} - \left(k\frac{\partial T}{\partial x}\right)_{w} + \bar{S}\,\Delta x = 0$$

$\bar{S}$ is the median value of S on the V.C

One approaching the derivative by the formula of Taylor, one finds:

$$k_e\frac{T_E - T_P}{\delta_{xe}} - k_w\frac{T_P - T_W}{\delta_{xw}} + \bar{S}\,\Delta x = 0$$

We got

$$a_P T_P = a_E T_E + a_W T_W + b$$

With

$$a_E = \frac{k_e}{\delta_{xe}}\ ;\ a_W = \frac{k_w}{\delta_{xw}}\ ;\ a_P = \frac{k_e}{\delta_{xe}} + \frac{k_w}{\delta_{xw}} = a_E + a_W\ ;\ b = \bar{S}\,\Delta x$$

For the resolution of this system of equation it is necessary for us:

- The boundary conditions
- The thermal conductivity
- The term source S

Boundary conditions

For the treatment of the boundary conditions, one integrates the equation on the volume of control surrounding the nodes being neighboring the borders.

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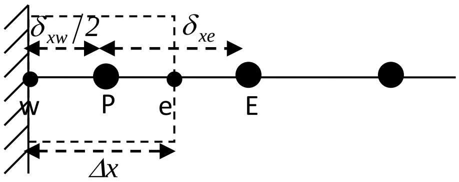
Borders



Let us suppose we have the heat flow q_n'' in the borders

$$\int_w^e \frac{d}{dx}\left(k\frac{dT}{dx}\right)dx + \int_w^e S\,dx = 0$$

$$\left(k\frac{dT}{dx}\right)_e - \left(k\frac{dT}{dx}\right)_w + \bar{S}\Delta x$$

$$\frac{k_e(T_E - T_P)}{\delta_{xe}} + q_w'' + \bar{S}\,\Delta x = 0$$

The treatment of this case depends on q_n''

- If q_n'' is constant, the problem is very simple to solve.
- If q_n'' is a function of T_P, one needs a linearization of this term.

For example, $q_w'' = h(T_\infty - T_P)$ when a fluid with T_∞ heat the border.

In this case we can write q_n'' as: $q_w'' = f_c + f_P T_P$

$$\begin{cases} f_c = hT_\infty \\ f_P = -h \end{cases}$$

And the linear equation becomes in the following form:

$$a_P T_P = a_E T_E + b$$

Nonlinear equations

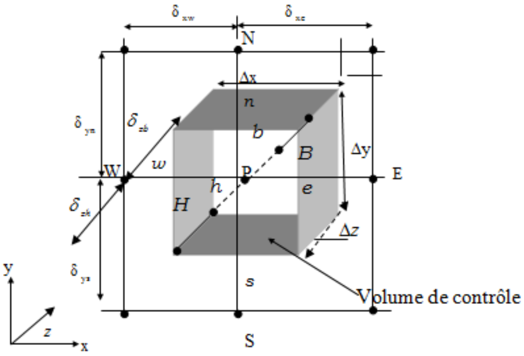
When thermal conductivity or the source term is a function of the temperature $\left(k = f(T_p), Sf(T_p)\right)$, there will be nonlinear equations discretized in the following form:

$$k_e(T_P)\frac{T_E - T_P}{\delta_{xe}} - k_w\frac{T_P - T_W}{\delta_{xw}} + \bar{S}(T_P)\,\Delta x = 0$$

To cure this problem, we calculate (K) according to the temperature of the previous iteration. $\left(k = f(T_p^*)\right)$ and we propose a linearisation of the source term in the following form:

$$\bar{S} = S_c + S_P T_P$$

Three-dimensional study



$$\int_s^n\int_w^e\int_h^b\int_t^{t+dt}\rho c\frac{\partial T}{\partial x}\,dtdxdydz=\int_t^{t+dt}\int_h^b\int_s^n\int_w^e k\frac{\partial T}{\partial x}dxdydz+\int_t^{t+dt}\int_h^b\int_w^e\int_s^n k\frac{\partial T}{\partial y}dydxdz+\int_t^{t+dt}\int_s^n\int_w^e\int_h^b k\frac{\partial T}{\partial z}dzdxdy$$

Using the implicit method, we find:

$$\rho c\left(T_p-T_p^0\right)\Delta x\Delta y\Delta z=\left(\frac{k_e(T_E-T_P)}{\delta_{xe}}\right)\Delta y\Delta z\Delta t-\left(\frac{k_w(T_P-T_W)}{\delta_{xw}}\right)\Delta y\Delta z\Delta t+\left(\frac{k_n(T_N-T_P)}{\delta_{yn}}\right)\Delta x\Delta z\Delta t$$
$$-\left(\frac{k_s(T_P-T_S)}{\delta_{ys}}\right)\Delta y\Delta z\Delta t+\left(\frac{k_b(T_B-T_P)}{\delta_{zb}}\right)\Delta x\Delta y\Delta t-\left(\frac{k_h(T_P-T_H)}{\delta_{zh}}\right)\Delta x\Delta y\Delta t+\left(S_C+S_PT_p\right)\Delta x\Delta y\Delta z\Delta t$$

We got

$$a_PT_P=a_ET_E+a_WT_W+a_NT_N+a_ST_S+a_BT_B+a_HT_H+b$$

With

$$a_E=\frac{k_e\Delta y\Delta z}{\delta_{xe}};\,a_W=\frac{k_w\Delta y\Delta z}{\delta_{xw}};\;a_N=\frac{k_n\Delta x\Delta z}{\delta_{yn}};\;a_S=\frac{k_s\Delta x\Delta z}{\delta_{ys}};\,a_B=\frac{k_b\Delta x\Delta y}{\delta_{zb}};\;a_H=\frac{k_h\Delta x\Delta y}{\delta_{zh}}$$
$$a_P^0=\rho c\Delta x\Delta y\Delta z/\Delta t\,;\,b=S_C\Delta x\Delta y\Delta z+a_P^0T_P^0$$
$$a_P=a_E+a_W+a_N+a_S+a_B+a_H-S_P\Delta x\Delta y\Delta z$$

DISCRETIZATION OF THE EQUATION IN 3 DIMENSIONS

We have the following general equation:

$$\frac{\partial}{\partial t}(\rho\phi)+\frac{\partial}{\partial x}\left(\rho u\phi-\Gamma\frac{\partial\phi}{\partial x}\right)+\frac{\partial}{\partial y}\left(\rho v\phi-\Gamma\frac{\partial\phi}{\partial y}\right)+\frac{\partial}{\partial z}\left(\rho w\phi-\Gamma\frac{\partial\phi}{\partial z}\right)=S$$

The equation of continuity is:

$$\frac{\partial\rho}{\partial t}+\frac{\partial}{\partial x}(\rho u)+\frac{\partial}{\partial y}(\rho v)+\frac{\partial}{\partial z}(\rho w)=0$$

After integrate these equations we get:

$$\int_h^b\int_s^n\int_w^e\int_t^{t+dt}\frac{\partial}{\partial t}(\rho\phi)\,dtdxdydz=\int_t^{t+dt}\int_h^b\int_s^n\int_w^e\frac{\partial}{\partial x}\left(\rho u\phi-\Gamma\frac{\partial\phi}{\partial x}\right)dxdydzdt+\int_t^{t+dt}\int_h^b\int_w^e\int_s^n\frac{\partial}{\partial y}\left(\rho v\phi-\Gamma\frac{\partial\phi}{\partial y}\right)dydxdzdt$$
$$+\int_t^{t+dt}\int_s^n\int_w^e\int_h^b\frac{\partial}{\partial z}\left(\rho w\phi-\Gamma\frac{\partial\phi}{\partial z}\right)dzdxdydt=\int_t^{t+dt}\int_h^b\int_s^n\int_w^e(S_c+S_P\phi_P)dxdydzdt$$

Or,

$$[(\rho\phi)_P-(\rho\phi)_P^0]\frac{\Delta x\Delta y\Delta z}{\Delta t}+\left[\frac{F_e}{2}(\phi_E+\phi_P)-D_e(\phi_P-\phi_E)\right]-\left[\frac{F_w}{2}(\phi_W+\phi_P)-D_w(\phi_P-\phi_W)\right]$$
$$+\left[\frac{F_n}{2}(\phi_N+\phi_P)-D_n(\phi_P-\phi_N)\right]-\left[\frac{F_s}{2}(\phi_S+\phi_P)-D_s(\phi_P-\phi_S)\right]+\left[\frac{F_b}{2}(\phi_B+\phi_P)-D_b(\phi_P-\phi_B)\right]$$

$$-\left[\frac{F_h}{2}(\phi_H + \phi_P) - D_h(\phi_P - \phi_H)\right] = (S_c + S_P\phi_P)\Delta x\Delta y\Delta z$$

Where

$$F_e = (\rho u)_e \Delta y\Delta z \, ; D_e = \frac{\Gamma_e \Delta y \Delta z}{\delta_{xe}}; F_w = (\rho u)_w \Delta y\Delta z \, ; D_w = \frac{\Gamma_w \Delta y \Delta z}{\delta_{xw}}$$

$$F_n = (\rho v)_n \Delta x\Delta z \, ; D_n = \frac{\Gamma_n \Delta x \Delta z}{\delta_{yn}}; F_s = (\rho v)_s \Delta x\Delta z \, ; D_s = \frac{\Gamma_s \Delta x \Delta z}{\delta_{ys}}$$

$$F_b = (\rho w)_b \Delta x\Delta y \, ; D_b = \frac{\Gamma_b \Delta x \Delta y}{\delta_{zb}}; F_h = (\rho w)_h \Delta x\Delta y \, ; D_h = \frac{\Gamma_h \Delta x \Delta y}{\delta_{zh}}$$

The final expression which corresponds to the Discretization of the transport equation is written in the following general form:

$$a_P T_P = a_E T_E + a_W T_W + a_N T_N + a_S T_S + a_B T_B + a_H T_H + b$$

Where

$$a_E = D_e - \frac{F_e}{2} \quad ; \quad a_W = D_w + \frac{F_w}{2}$$

$$a_N = D_n - \frac{F_n}{2} \quad ; \quad a_S = D_s + \frac{F_s}{2}$$

$$a_B = D_b - \frac{F_b}{2} \quad ; \quad a_H = D_h + \frac{F_h}{2}$$

$$a_P^0 = \rho_P^0 \Delta x \Delta y \Delta z / \Delta t$$

$$b = a_P^0 \phi_P^0 + S_c \Delta x \Delta y \Delta z$$

$$a_P = \left[\frac{F_e}{2} + D_e\right] - \left[\frac{F_w}{2} - D_w\right] + \left[\frac{F_n}{2} + D_n\right] - \left[\frac{F_s}{2} - D_s\right] + \left[\frac{F_b}{2} + D_b\right] - \left[\frac{F_h}{2} - D_h\right] + \rho_P \frac{\Delta x \Delta y \Delta z}{\Delta t} - S_P \Delta x \Delta y \Delta z$$

Notice

To solve the transport equations, we need the rates of the flow at the points e, w, n, s, b, h, for that and to solve several problems which give unrealistic results, we choose to use a grid shifted for the calculation of the components speeds (u, v and w). It is a question of estimating speeds U, V and W with the three faces of the volume control while the other variables (pressure, temperature ...) are calculated in the center of volumes of control.

ALGORITHM OF CALCULATES

The whole of steps calculation intervening in the resolution of the Navier-Stokes equations using the algorithm below:

- Read the definition of the grid, the conditions at the borders and to build the grid shifted for the components speed;
- Define a field of pressure estimated P^*;
- Calculate the intermediate components speed U^*, V^* and W^* with the nodes of their grids shifted from solving the conservation equations of the momentum;
- Calculate the correction P', pressure necessary to correct the field of speed in order to satisfy the equation with continuity;
- Calculate the field of pressure P by associating P' with P^*;

- Calculate the components of speed U, V and W;
- Solve the equations discretized for K, ε, C and T;
- Pose $P^* \leftarrow P'$ and take again the execution of the third step by repeating all the procedure until the condition of convergence is met;

CONCLUSIONS

Concerning the study of the particulate deposit inside the building, we defined an experimental protocol allowing the evaluating of the deposit rate of the particles according to its density. We noted that this deposit rate relatively invariant according to the rate of flow of air. Once we know the concentration of the pollutant particle which really penetrates inside a part, it remains us to determine the influence of ventilation in the buildings on the particulate pollution, and will show that the movement of the particles of the interior air depends not only on the ventilation rate, but also on the way borrowed by the flow of air in the environment.

An experimental study at the University of Rochelle in France showed that the influence of the positions of the entry and the exit of air was stronger for the fine particles (lower than 5 µm of diameter) than for the more important particles of size, and then an increase in the ventilation rate necessarily a higher deposit of the suspended particles did not imply.

In order to highlight this phenomenon, we chose to use either a comprehensive approach of the phenomenon, but a fine modeling. In other words, we are going to use a computer code which will make it possible to simulate the flows of air of the cell, for the same type of coating.

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