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SMR/760-58

"College on Atmospheric Boundary Layer
and Air Pollution Modelling"
16 May - 3 June 1994

"Long-Range Air Pollutants Transport and Diffusion Model with Atmospheric Chemistry"

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LONG-RANGE AIR POLLUTANTS TRANSPORT AND DIFFUSION MODEL WITH ATMOSPHERIC CHEMISTRY

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1. INTRODUCTION

Air pollution may be defined as any atmospheric condition in which substances are present at concentrations high enough above their normal ambient levels to produce a measurable effect on man, animals, vegetation, or materials. By "substance" we mean any natural or man-made chemical elements or compound capable of being airborne. These substances may exist in the atmosphere as gases, liquid drops, or solid particles. Our definition includes any substance, whether noxious or benign; however, in using the term "measurable effect" we will generally restrict our attention to those substances that cause undesirable effects.

The problem of long-range pollutant transport is a challenge. Experimental data show that background air quality in various regions is affected by the long-range of pollutants. This is considered as a major reason for the observed increase of acidic rains over Scandinavia during the last few years.

Nature has given a comprehensive example of this phenomenon. The smoke cloud from a big forest fire in Alberta, Canada which had burned from the 17 to the 24 of September 1950 was observed on the 25 of September over the East coast of the U.S.A.(see Munn and Bolin, 1971). On the 26 of September it was seen over the British islands and on the 28 over Europe - from Scandinavia to Gibraltar. The consecutive change of the cloud's thickness were 2.5-4.5 km over U.S.A., 5-6km over the Atlantic Ocean, 9-10 km over England and more than 11km over Europe. Similar pictures have been observed during volcanic eruptions, nuclear explosions, dust storms, and other phenomena.

These examples indicate that the long range transport of air pollutants caused by the general atmospheric circulation is essentially a three-dimensional process. Its modelling is rather hampered by inadequate knowledge of the atmosphere diffusivity in the cross flow direction, the strength of pollutant sources, pollutant transformations as well as the influence of planetary boundary layer (PBL) dynamics and vertical motions at distances exceeding 1000km.

The air pollution problem can be simply depicted as a system consisting of the following basic components exhibited in Fig.1:

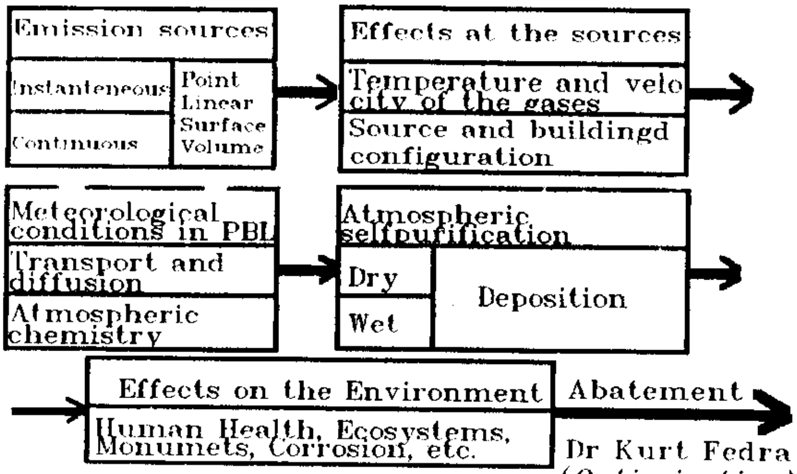


Fig.8.1 System diagram of air pollution phenomenon

2. Atmospheric Diffusion Theories

A major goal of our study of the atmospheric aspects of air pollution is to be able to describe mathematically the spatial and temporal distribution of contaminants released into the atmosphere. It is common to refer to the behavior of gases and particles in turbulent flow as turbulent "diffusion" or, in this case, as atmospheric "diffusion", although the processes responsible for the observed spreading or dispersion in turbulence are not the same as those acting in ordinary molecular diffusion. A more precise term would perhaps be atmospheric dispersion, but to conform to common terminology we will use atmospheric diffusion. This paragraph is devoted primarily to developing the two basic ways of describing turbulent diffusion. The first is the *Eulerian* approach in which the behavior of species is described relative to a fixed coordinate system. The Eulerian description is the common way of treating heat and mass transfer phenomenon. The second approach is the *Lagrangian* in which concentration changes are described relative to the moving fluid.

2.1 Eulerian Approach

Let us consider N species in a fluid. The concentration of each must, at each instant, satisfy a material balance taken over a volume element. Thus, any accumulation of material over time, when added to the net amount of material convected into the volume element, must be balanced by an equivalent amount of material that is produced by chemical reaction in the element, that is emitted into it by the source, and that enters by molecular diffusion. Expressed mathematically, the concentration of each species, c_i, must satisfy the continuity equation

$$\frac{\partial c_i}{\partial t} + \frac{\partial}{\partial x_j} u_j c_i = D_i \frac{\partial^2 c_i}{\partial x_j \partial x_j} + R_i(c_1, \ldots\ldots c_N, T) + S_i(\vec{x}, t) \qquad (1)$$

where u_j is the jth component of the fluid velocity, D_i is the molecular diffusivity of species i in the carrier fluid, R_i is the rate of generation of species i by chemical reaction (which depends in general on the fluid temperature T), and S_i is the rate of addition of species i at the location $\vec{x}=(x_1,x_2,x_3)$ and time t.

In addition to the requirement that the c_i satisfy Eq.1 , the fluid velocities u_j and the temperature T, must satisfy the Navier-Stokes and energy equations, which themselves are coupled through the u_j, c_i and T with the total continuity equation and the ideal gas law. In general, it is necessary to carry out a simultaneous solution of the coupled equations of mass, momentum, and energy conservation to account properly for the changes in u_j, T, and c_i and the effects of the changes of each of these on each other. In dealing with atmospheric pollutants, however, since species occur at parts-per-million concentrations, it is quite justifiable to assume that the presence of pollutants does not affect the meteorology to any detectable extent, thus, the equation of continuity can be solved independently of the coupled momentum and energy equations. Consequently, the fluid velocities u_j and the temperature T can be considered independent of the c_i. From this point on we will not explicitly indicate the dependence of R_i on T.

The advantage of the Eulerian approach is that the turbulent diffusion equation is integrated in a fixed geographical mesh in which the necessary meteorological fields: wind velocity, temperature , precipitations, as well as roughness and emissions are naturally determined by the meteorological network. Thus the concentration fields are also determined in the same system. In the framework of the Eulerian approach it is easy to determine the vertical wind velocity gradients, the interaction of pollutants with the underlying surface, linear and nonlinear chemical reactions and other processes. Still there are not fully solved the problems of securing proper initial conditions, the approximation of the advective terms, the appearance of fictitious waves at the boundary of the integration region and lack of physically sound theories for modelling the horizontal turbulence for distances larger than hundreds of kilometers.

2.2 Lagrangian Approach

The Lagrangian approach to turbulent diffusion is concerned with the behavior of representative fluid particles. We therefore begin by considering a single particle which is located at $\vec{x}'$ at time t' in a turbulent fluid. The subsequent motion of the particle can be described by its trajectory, $\vec{X}[\vec{x}',t',t]$, that is, its position at any later time t. Let $\psi(x_1,x_2,x_3,t)dx_1dx_2dx_3=\psi(\vec{x},t)d\vec{x}$= probability that the particle at time t will be in volume element x_1 to x_1+dx_1, x_2 to dx_2, and x_3 to dx_3, that is that $x_1 \le X_1 < x_1+dx_1$, and so on. Thus $\psi(\vec{x},t)$ is the probability density function (pdf) for the particle's location at time t. By the definition of a probability density function

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \psi(\vec{x},t)dx = 1$$

The probability density of finding the particle at $\vec{x}$ at t can be expressed as the product of two other probability densities:

1. The probability density that if the particle is at $\vec{x}'$ at t' it will undergo a displacement to $\vec{x}$ at t. Denote this probability density $Q(\vec{x},t|\vec{x}',t')$ and call it the *transition probability density* for the particle.
2. The probability density that the particle was at $\vec{x}'$ at t', $(\vec{x}',t')$, integrated over all possible starting points $\vec{x}'$. Thus,

$$\psi(x,t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} Q(\vec{x},t\,|\,\vec{x}',t')\;\psi(\vec{x}',t')d\vec{x}' \qquad (2)$$

The density function $\psi(\vec{x},t)$ has been defined with respect to a single particle. If, however, an arbitrary number m of particles are initially present and the position of the ith particle is given by the density function $\psi_i(\vec{x},t)$, it can be shown that the ensemble mean concentration at the point $\vec{x}$ is given by

$$<c(\vec{x},t)> = \sum_{i=1}^{m} \psi_i(\vec{x},t) \qquad (3)$$

By expressing the pdf $\psi_i(\vec{x},t)$ in Eq.2 in terms of the initial particle distribution and the spatial temporal distribution of particle sources $S(\vec{x},t)$, say in units of particles per volume per time, and then substituting the resulting expression into Eq.3, we obtain the following general formula for the mean concentration:

$$<c(x,t)>=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} Q(\vec{x},t\,|\,\vec{x}'_0,t'_0)<c(\vec{x}_0,t_0)d\vec{x}_0 + \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{t_0}^{t} Q(\vec{x},t\,|\,\vec{x}',t')S(\vec{x}',t')dt'd\vec{x}' \qquad (4)$$

The first term on the right-hand side represents those particles present at t_0, and the second term on the right-hand side accounts for particles added from sources between t' and t.

Equation 4 is the fundamental Lagrangian relation for the mean concentration of species in turbulent fluid. The determination of $<c(\vec{x},t)>$, given $<c(\vec{x}_0,t)>$ and $S(\vec{x}',t)$, rests with the evaluation of the transition probability $Q(\vec{x}_0,t\,|\,\vec{x}',t')$. If Q were known for $\vec{x}$, $\vec{x}'$, t, and t', the mean concentration $<c(\vec{x},t)>$ could be computed by simply evaluating Eq.4 . However, there are two substantial problems with using Eq.4. . First, it holds only when the particles are not undergoing chemical reactions. Second, such complete knowledge of the turbulence properties as would be needed to know Q is generally unavailable except in the simplest of circumstances. The major advantage of the Lagrangian method is the easy integration along the particles trajectory thus avoiding the difficulties with the numerical modelling of the advective terms in the turbulent diffusion equation.

3. A Combined Eulerian-Lagrangian Description of the Turbulent Diffusion

The analysis of the two basic fluid dynamics approaches for the description of flow properties clearly reveals there advantages and shortcomings. There is , however, hope that some appropriate unification of the Eulerian and Lagrangian approaches may enhance our ability to tackle the problem. The basis for this idea stems from the experimental facts that the turbulence in vertical direction is small scale and it would be appropriate to use the diffusion equation while in horizontal direction the turbulence is large scale, the turbulent eddies are not limited by the earth surface and the diffusion process requires a statistical description in this direction. The theoretical investigations confirmed that in a direction perpendicular to the wind velocity the concentration distribution is Gaussian while in vertical direction there is no appropriate statistical description of the process.

In this lecture we dwell on the possibility to describe the diffusion process independently in vertical and horizontal direction thus making it possible to combine and utilize the advantages of the Eulerian and Lagrangian approaches and to minimize their shortcomings. Therefore the following formula is postulated

$$c^k(x,y,z,t) = \sum^{M} \sum^{N_i} Q_{ij}(t_{ij}) q_h(x, x^c_{ij}, y, y^c_{ij}, t_{ij}) q_z(z, z^c_{ij}, t_{ij}) q_w(t_{ij}) \quad (5)$$

where $Q_{ij}(0)$ is the quantity of the k^{th} pollutant in the j^{th} volume (puff) of pollutants emitted by the i^{th} source at the moment $t_{ij} = 0$, M is the number of sources, N_i is the number of puffs, q_z and q_h are the vertical and horizontal pollutant distribution functions, q_w is wet deposition function and t_{ij} is the life time of existence of the individual puffs.

This formula clearly indicates the application of the idea of separate description of the diffusion process in vertical and horizontal direction.

Now, using the Equation (5) one should be able to construct a model for the diffusion process in the APBL.

4. Long-Range Air pollutants Transport and Diffusion Model with Atmospheric Chemistryy

The major structural element of the model will be the puff i.e. volume of pollutants with given dimensions which will be transported by the atmospheric motions of different scales. The wind field, therefore, is external to the model or in another words the pollutants do not influence the atmospheric dynamics in appreciable way. The volume sources-puffs will be of ellipsoidal shape. It is further assumed that they change there size only by the diffusion process which condition is justified in the case of long-range transport and diffusion . If the diffusion phenomenon is of a smaller scale the dynamic deformation of the puff, say because of the wind shear, should be taken into account.

The continuous pollution field is formed by periodically created puffs in the different cells; these puffs are transported by the flow and diffused by the turbulence. The location of the puff is determined by the position of its center, and the displacement velocity is equal to the wind speed at that point. In this case, the coordinates of the puff center change according to:

$$\begin{aligned} x_c(t) &= x_c(t-\Delta t) + u(x_c, y_c, z_c)\Delta t \\ y_c(t) &= y_c(t-\Delta t) + v(x_c, y_c, z_c)\Delta t \qquad (6) \\ z_c(t) &= z_c(t-\Delta t) + w(x_c, y_c, z_c)\Delta t \end{aligned}$$

where Δt is a properly chosen time interval. The wind components $u(x,y,z)$, $v(x,y,z)$, $w(x,y,z)$ are obtained from the standard aerological observations or numerical weather forecasting models. They are assumed to be constant during time interval T_c between two consecutive observations, usually 12 hr apart.

New puffs are emitted at times equal to T_c, a simplification which is not a principal cause of uncertainty in the model. In order to achieve satisfactorily smooth trajectories, the time interval Δt is taken small in comparison with T_c.

Equation (6) clearly demonstrates the elegancy of using the Lagrangian approach in describing the advection process.

4.1 HORIZONTAL DIFFUSION

For the determination of the analytical expression for the horizontal diffusion we choose a cartesian coordinate system which origin of coincide with the puff center. In the model, it is assumed that the horizontal diffusionprocess is defined by the equation:

$$\frac{\partial q}{\partial t} = \frac{\partial}{\partial \zeta_1} K_1 \frac{\partial q}{\partial \zeta_1} + \frac{\partial}{\partial \zeta_2} K_2 \frac{\partial q}{\partial \zeta_2} + \frac{\partial}{\partial \zeta_3} K_3 \frac{\partial q}{\partial \zeta_3} \tag{7}$$

where $q(\zeta_1,\zeta_2,\zeta_3)$ is the pollutant concentration at a point $(\zeta_1,\zeta_2,\zeta_3)$ and K_1,K_2,K_3 are the turbulent diffusion coefficients.

The turbulent diffusion process in the horizontal direction, in accordance to the experimental evidence, is considered isotropic. If during a time interval Δt, $K_1 = K_2 = K$ and K_3 do not significantly change in time and space, Equation (7) describes a Fickian type diffusion, which is nonisotropic in vertical direction.

The the initial condition is:

$$q(r,\zeta_3,0) = \begin{cases} A \exp\left(-\dfrac{r^2}{a^2} - \dfrac{\zeta_3^2}{a_3^2}\right) & |r| \le r_0 , \quad \zeta_3 \le \zeta_3^0 \\ 0 & |r| > r_0 \quad\ \ \zeta_3 > \zeta_3^0 \end{cases} \tag{8}$$

where $r^2 = \zeta_1^2+\zeta_2^2$; r^0 and ζ_3^0 are the radius and semi-thickness of the volume source; and A is a constant which should be determined from the mass conservation condition.

The solution of Equation (2) subject to the initial condition Equation (8) and zero boundary condition at infinity can be found in the paper by Djolov and Syrakov (1971). In this paper it is shown that the solution can be rather simplified if the puff is considered infinite. The puff boundary condition is then taken as the surface where the concentration is p% (usually (p = 0.01) of the puff center concentration. This rather accurate approximation is admissible because of the fast decrease of the concentration with the distance from the center. This allows the constant A in the Equation (8) to be determined as:

$$A = \frac{Q_0}{\pi^{3/2} a^2 a_3} \tag{8}$$

where Q_0 is the total pollutant mass of the source and a, a_3 are dispersions given by

$$a = \frac{r_0}{\sqrt{-\ln p}} \qquad a_3 = \frac{\zeta_3^0}{\sqrt{-\ln p}} \tag{9}$$

The solution of Equation (7) has the form

$$q(r,\zeta_3,t) = \frac{Q_0}{\pi^{3\backslash 2}} \frac{\exp\left[-\dfrac{r^2}{a^2+4Kt}-\dfrac{\zeta_3^2}{a_3^2+4K_3t}\right]}{(a^2+4Kt)\sqrt{a^2+4K_3t}} \tag{10}$$

Formula (10) gives the opportunity to consider a puff at any moment t as an infinite volume source with time dependent dispersions. Transforming the results to a fixed coordinate system and assuming that the pollutants are reflected by the earth's surface, the concentration at a given point x,y,z, and time t is given by:

$$q(x,y,z,t)=\frac{Q_0}{\pi^{3/2}}\cdot\frac{\exp\left[-\dfrac{(x-x_c(t))^2+(y-y_c(t))^2}{a^2(t)}\right]\left[\exp\left[-\dfrac{(z-z_c(t))^2}{a_z^2(t)}\right]+\exp\left[-\dfrac{(z+z_c(t))^2}{a_z^2(t)}\right]\right]}{a^2(t)a_z(t)} \tag{11}$$

where

$$\begin{aligned} a^2(t) &= a^2(t-\Delta t) + 4K\Delta t \\ a_z^2(t) &= a_z^2(t-\Delta t) + 4K_z\Delta t \end{aligned} \tag{12}$$

In equations (7) and (8), $K_z=K_3$ and $a_z=a_3$. The concentration at the earth surface (z=0) is

$$q(x,y,0,t)=\frac{2Q_0}{\pi^{3/2}}\cdot\frac{\exp\left[-\dfrac{(x-x_c(t))^2+(y-y_c(t))^2}{a^2(t)}-\dfrac{z_c^2(t)}{a_z^2(t)}\right]}{a^2(t)a_z(t)} \tag{12}$$

4.2 Vertical Diffusion

The function q_z which describes the vertical pollutants' distribution is determined again in the framework of Eulerian approach in the moving coordinate system with origin at the the respective puff center. The diffusion process, which is caused by microscale turbulence in vertical direction, is described by the semiempirical turbulent diffusion equation:

$$\frac{\partial q_z}{\partial t} = K_z \frac{d^2 q_z}{dz^2}, \qquad K_z = \text{const} \tag{14}$$

which is solved subject to the following boundary conditions

$$\begin{aligned} q_z(z) &= \delta(z-z_c) && t = 0 \\ K_z\frac{\partial q_z}{\partial z} &= \beta z && z = 0 \\ K_z\frac{\partial q_z}{\partial z} &= 0 && z = z_i. \end{aligned} \tag{15}$$

where β is the constant of interaction between the pollutants and the underlying surface and z_i is the mixing height.

The system of Equations (14)-(15) describes the different cases of possible vertical diffusion in APBL. In the cases when the puffs have not reached the ground the obvious solution $q_z=0$. The most frequent condition is when the puff diffuses between the partially absorbing earth surface and reflecting inversion height. The asymptotic solution of uniform concentration distribution with altitude will be realized at large times.

The solutions of Equation (14) after appropriate integration to obtain the solutions for volume source at ground level are:

Zone 1 (the volumes have not reached the surface)

$$q_z = 0 \tag{16}$$

Zone 2 (the volumes have reached the earth surface but not the mixing height)

$$q_z = 2\exp(-z_c^2/a_z^2)(1 - \sqrt{\pi}\,\frac{b}{a_z}\,\mathrm{erfc}(\eta)/\sqrt{\pi}\,a_z) \tag{17}$$

where

$$\mathrm{erfc} = \frac{2}{\pi}\int_0^\infty e^{-\xi^2} d\xi$$

Zone 3 (the volumes have reached both ground and z_i)

$$q_z = \frac{1}{z_i}\sum_{n=0} \frac{2\cos\alpha_n(1-z_c/z_i)\cos\alpha_n}{1+\sin 2\alpha_n/2\alpha_n}\exp^{-\left(\frac{b^2}{a_z^2 tg^2\alpha_n}\right)} \tag{18}$$

where α_n is determined from the equation

$$\alpha\ tg\ \alpha = \beta z_i/K_z$$

Zone 4 (uniform vertical mixing)

$$q_z = \frac{1}{z_i}\exp(-b/2z_i). \tag{19}$$

In the above formulae the following quantities are used:

$$a_z^2(t+\Delta t) = a_z^2(t) + 4K_z\Delta t, \qquad a_z(0) = 0$$

$$b(t+\Delta t) = b(t) + 2\beta\Delta t \qquad b(0) = 0 \tag{20}$$

$$\eta = (z_c+b)/a_z$$

Equations (20) allow to take into account the horizontal inhomogeneity of the vertical turbulent exchange coefficient. The function q_z depends on K_z and time trough a_z and the change in the position of the volume in regions with different K_z is reflected by the rate of change of a_z.

4.3 TRANSFORMATION OF POLLUTANTS

A simple and widely spread way of treating the transformation process is to assume a constant rate of changeλ. The most effective mechanism of pollutants transformation in APBL is their washout by the precipitations. The constant λ apparently depend on the life time of every puff. The equation describing this process is:

$$\frac{\partial q_w}{\partial t} = -\lambda_w t \qquad q_w(0\ ) = \cdot \qquad (21)$$

Its solution is

$$q_w(t) = \delta_w \exp(-\lambda_w t) \qquad (22)$$

where $\delta_w = 1$ in the case of precipitations and $\delta_w = 0$ during dry events.

4.4 ATMOSPHERIC CHEMISTRY

The major atmospheric pollutants at present are the sulphur, nitrogen and carbon compounds. The quantity and the life of the sulphur and nitrogen compounds are the basic source for the formation of acid precipitations.

The most important mechanism for the formation of acid rains is the direct transformation:

$$SO_2 \xrightarrow{k_1} SO_4^= \qquad (23)$$

where $k_1(r,t)$ is the transformation constant which is a function of the time and space.

The chemical reactions amongst the two major nitrogen pollutants NO and NO_2 are more complicated. Investigations in a gas chamber reveal that 90% of the chemistry of these compound can described by the system of equations:

$$\begin{aligned}
\frac{d}{dt}\left[NO_2 \right] &= -k_2 \left[NO_2 \right] + k_4 \left[PAN \right] \\
\frac{d}{dt}\left[PAN \right. &= 0.5k_2 \left[NO_2 \right] - (0.5k_3 + k_4) \left[PAN \right] \qquad (24) \\
\frac{d}{dt}\left[NO_3^- \right. &= 0.1k_2 \left[\left[NO_2 \right] + k_3 \left[PAN \right] \right] \\
\frac{d}{dt}\left[HNO_3^- \right] &= 0.4k_2 \left[\left[NO_2 \right] + k_3 \left[PAN \right] \right] \\
0 &= \left[NO_2 \right] + k_5 \left[NO \right]
\end{aligned}$$

The system of equations is linear. The transformation constants can be function of time and space.

The chemical reactions (Formula (24)) are calculated for every puff at every of their transport and diffusion.

Basic and desirable quantity which should be calculated by the long-range pollutants models is the pH (acidity) of the precipitations. The calculations of the major sulphur and nitrogen compounds allows this task to be realized. The model for calculation of the pH value is developed using experimental data for the acidity of precipitation and the mechanism of the interaction between the pollutants and precipitations.

Without going into details the following formula with empirically determined coefficients, which are however different for the different seasons (i.e. they are dependent on the particular cloud microphysics), is utilized:

$$pH = a \left[-\log \left(10^{-6} W \left[\frac{2}{96} [SO_4^{=}] + \frac{1}{62} [NO_3^{-}] + [\text{background}] \right) \right] + b \qquad (25)$$

where a and b are coefficients, W is the washout coefficient, which is defined as the ratio between the concentration of pollutants in the air and in the precipitation. The numerical coefficient in Equation (25) come from the valences of the different chemical compounds and the coefficient 10^{-6} results from the conversion of mole/l to mg/m^3.

The success of the application of formula (25) depends on the appropriate determination of the wash out coefficient which varies seasonally. This requires a proper parameterization of the time and space climatic peculiarities of the precipitations taking place in different seasons.

The results of two simple experiments show the possibility the chemistry model to be successfully utilized. In Fig.2 the influence of the pollutants flux in the clouds is demonstrated. The dashed line presents the pH values in the case that there is precipitation over the entire region under investigation,. The solid line connects the pH values for a precipitations events which are taking place at different distances from the pollution source.

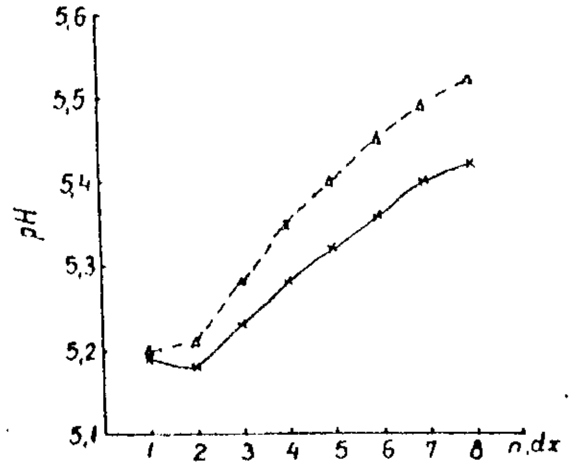


FIG.2 Influence of the pollutants flux (Δx=150 km)

Fig.3 exhibits the monthly variation of pH at the axis of a plume for precipitation events at different distances.

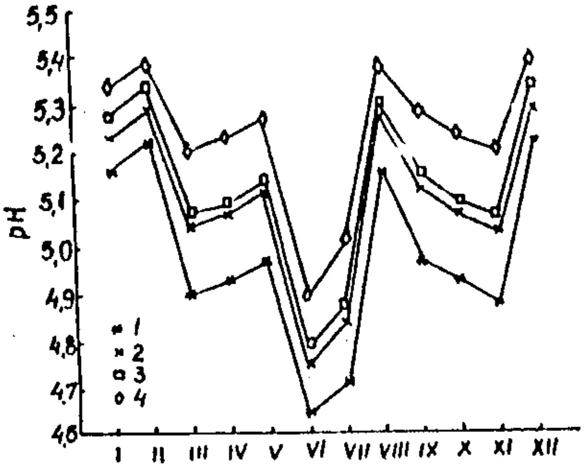


FIG.3 Variation of the monthly pH values for different distances from the source (1-150 km, 2-300 km, 3-1050 km, 4-1200 km)

3. NUMERICAL MODEL

The development of a numerical model for long-range transport and diffusion model of air pollutants requires the satisfaction of two, to a certain degree conflicting conditions : an accurate and realistic description of the phenomenon and minimal requirement on the computer memory and run time.

The input information consists of the time intervals Δt, Δt_c, Δt_l: the time step, the period during which the meteorological conditions are assumed steady, the integration period, the horizontal turbulent exchange coefficient K, the decrease of the concentration p% at the cloud boundary, the minimum observable concentration q_{min}; and the source parameters: Q_0, the total pollutant emitted in a given grid cell $\Delta x \Delta y$ for time Δt_c; x_c, y_c, z_c, the initial coordinates of the puff center; and ζ_3^0, the vertical semitickness of the ellipsoid.

The initial dispersions of the volume source are calculated in accordance with Equation (9), where $r^0 = (\Delta x \Delta y/\pi)^{1/2}$. The consecutive location of every puff is determined by Equation (6) and the surface concentration field by Equation (13). The concentrations are calculated and summed for the points which satisfy the following conditions.

(a) they are located within the puff, i.e., their distances to the point (x_c, y_c) is less or equal to

$$r_\varphi^2 = -a^2(t)\ \ln \frac{p(1+\exp(-4z_c^2(t)/a_z^2(t))}{2\exp(-z_z^2(t)/a_z^2(t))}; \qquad (26)$$

(b) the concentration is greater or equal to q_{min}. These are the points for

$$r_c^2 = -a^2(t)\ \ln \frac{q_{min}\pi^{3/2}}{2Q_0}\ \frac{a^2(t)a_z(t)}{\exp(-z_c^2(t)/a_z^2(t))} \tag{27}$$

The combination of Equations (10) and (11) gives the criterion:

$$(x - x_c(t))^2 + (y - y_c(t))^2 \le \min\ (r_\varphi^2, r_c^2) \tag{28}$$

The workshop participants may gain more insight on the long-range transport and diffusion of pollutants as well as the acidity of precipitation, the dry and wet deposition by running different scenarios relevant to situation which they are familiar with.

The numerical model is realized for the region of Europe as shown on the Fig.4 below.

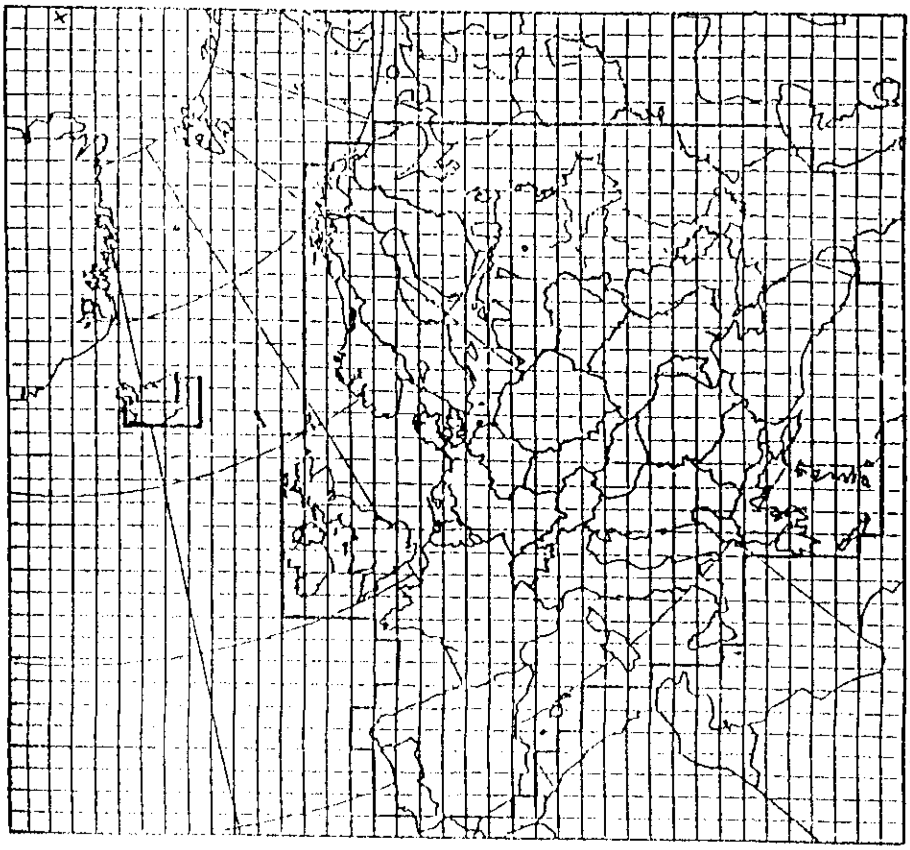


FIG.4 European mesh for studying long-range pollution.
Figura za mregata.

The model calculates the concentration, dry and wet deposition fields for all compounds listed in the chemistry equation (24) as well as the value of pH for the regions where there is a precipitation event. Some results with model for the region of South East Europe are shown to demonstrate some of the possible outputs from the model.

In Fig.5 the concentration field for vanadium is shown and in the next Fig.6

its deposition. It can be pointed out that one can run the model for every country with its emission sources and thus to produce the emitter-receive matrix which can be used to develop the optimum abatement strategy.

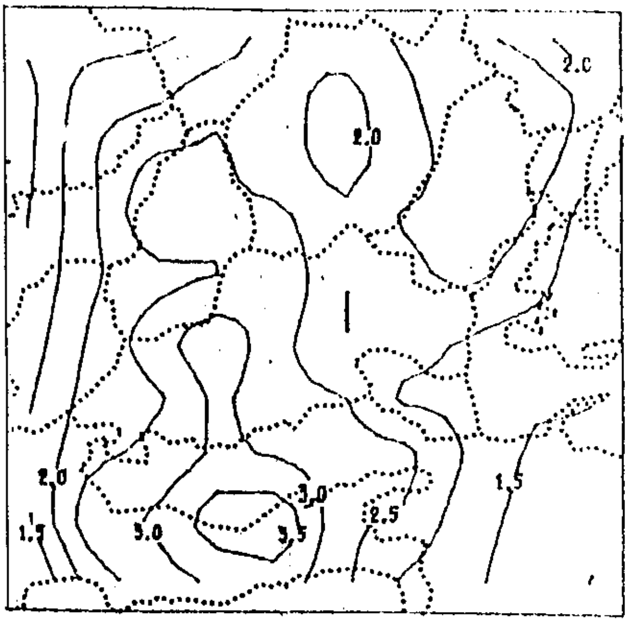


FIG.5 Concentration of vanadium in ng/m^3 for all sources in the region.

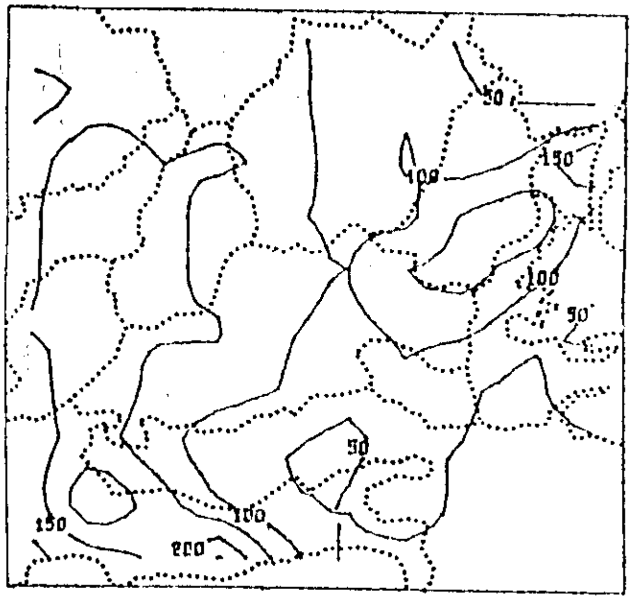
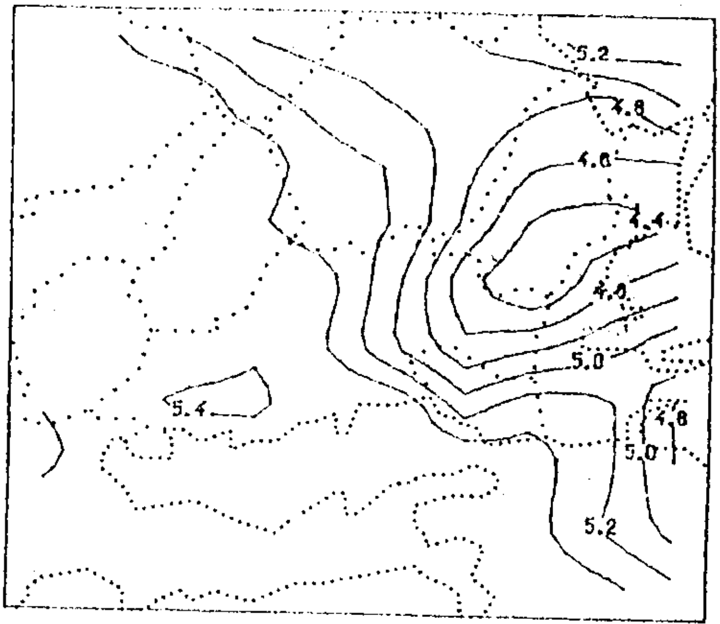


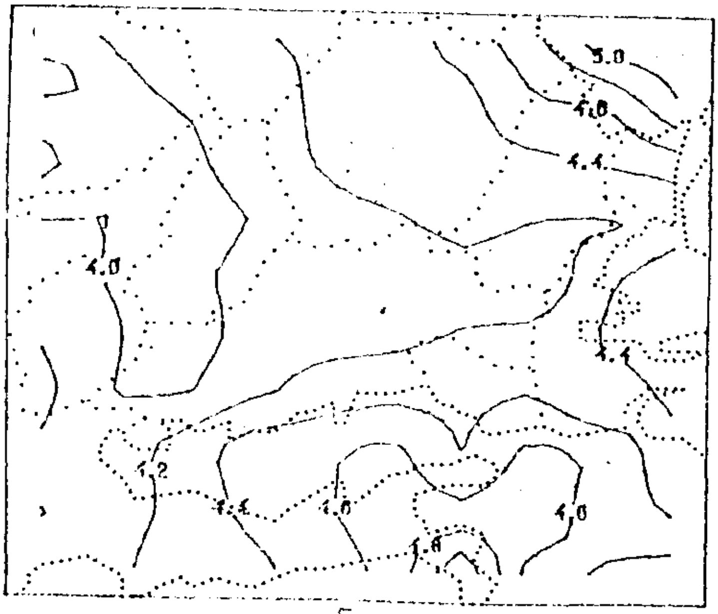
FIG.6 Deposition field for vanadium for all sources in the region.

Fig.7 exhibits the pH field for the same region when only the bulgarian region are taken into account. One can asses the role of the local (country) sources for a given typical unfavorable situation or long term consequences of the continuous action of the sources in the region.



a)

FIG.7 Monthly values ofpH from the bulgarian sources.



δ)

FIG.8 Monthly values of pH from all sources in the region.