PARAMETRIZATION OF POLLUTING SUBSTANCES TRANSPORT IN THE ATMOSPHERE OF A BIG CITY

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Received November 15, 1993

Turbulent exchange and admixture transport by vertical ordered fluxes (a convective inflow) play an important role in spatial distribution of atmospheric admixtures and time variation of their concentration. Parametrization of a turbulent coefficient has been made and a model of vertical distribution of admixture concentration, wind velocity, and air temperature in the ground layer of the atmosphere has been constructed based on representations of the theory of similarity and dimensionality. The model is in good agreement with the experimental results and allows one to determine the effect of different factors on the admixture concentration profile.

The problem of polluting the atmosphere of a big city (with population larger than 0.5–1.0 million) by trafic emissions and other industrial processes is the most urgent in ecology. Although a vast literature material can be found on this problem (e.g. Refs. 1, 2, 5–9, 14) there exist many problems that call for further development and investigation.

According to the equation of the inflow of polluting substances (admixtures) into the atmosphere

$$\frac{\partial q}{\partial t} = -\left(u\frac{\partial q}{\partial x} + v\frac{\partial q}{\partial y} \right) - w\frac{\partial q}{\partial z} + k_s\left(\frac{\partial^2 q}{\partial x^2} + \frac{\partial^2 q}{\partial y^2}\right) + \frac{\partial}{\partial z} k_z \frac{\partial q}{\partial z} - \frac{q}{\tau} \quad (1)$$

the rate of temporal variation of concentration q at a fixed point in space is determined by: a) an advective flux (the first term in the right–hand side, where u and v are projections of wind velocity onto the horizontal axes x and y); b) a convective flux (the second term, where w is the component of vertical along z axis speed of substance transport); c) a flux of the admixture under the effect of horizontal and vertical turbulent exchange (k_s and k_z are the coefficients of turbulence); and d) decrease of polluting substance due to its sink (capture) on droplets and crystals of clouds, fogs, and precipitation or due to radioactive decay (τ is the time of relaxation or the time of substance half-decay).

An advective inflow of admixture is estimated from the data on distribution of q and wind velocity (u, v) over a horizontal plane. An admixture inflow under the effect of horizontal exchange is usually estimated assuming normal (Gaussian) distribution along a horizontal direction.[4]

In general, the solution of Eq. (1) which should be combined with the equations of motion (to determine u and v), the equation of continuity (for w) as well as some additional relations (to calculate k_z, k_s, and τ) can be constructed only by numerical methods on big computers under certain boundary and initial conditions. The principle problems on constructing models of propagation of admixtures coming into the atmosphere from different sources were discussed elsewhere.[1,9,13]

In this paper we dwell on parametrization of the convective and turbulent (in vertical direction) inflows of an admixture, which play a decisive role in vertical transport of the admixture and therefore in formation of pollution levels near the earth's surface.

Vertical Turbulent Exchange. It is known[4,11] that in the ground layer of thickness h between 50–100 and 250–300 m distribution of wind velocity, temperature, and admixture concentration is described by equations with an error not exceeding 10%:

$$l\, dc/dz = u_*; \quad (2)$$

$$l\, d\theta/dz = \theta_*; \quad (3)$$

$$l\, dq/dz = q_*, \quad (4)$$

where $c = \sqrt{u^2 + v^2}$ is the absolute value of wind velocity; θ is the potential temperature; u_* is the dynamic speed (speed scale); $\theta_* = -Q_h(0)/(c_p \rho u_*)$, $q_* = -Q_q(0)/(\rho u_*)$ are the scales of θ and q (more accurate, scales of variations of θ and q within the ground layer); $Q_h(0)$ and $Q_q(0)$ are turbulent fluxes of heat and admixture near the earth's surface; ρ is the air density; and c_p is the specific heat of air.

The parameter l in Eqs. (1)–(3) is the path of mixing of turbulent moles related to the coefficient k_z through the relation

$$k_z = l\, u_*. \quad (5)$$

According to the similarity theory developed by Prandtl and Karman for incompressible liquid (as applied to the atmosphere, of neutral or equilibrium stratification) and generalized in Ref. 10 for nonequilibrium stratification, the path of the mixing can be represented as

$$l = -\kappa \frac{dc/dz}{d^2c/dz^2} f(\mathrm{Ri}) \quad (6)$$

where $f(\mathrm{Ri})$ is the unknown function of the Richardson number

$$\mathrm{Ri} = \frac{g}{T}\frac{\mathrm{d}\theta / \mathrm{d}z}{(\mathrm{d}c / \mathrm{d}z)^2}; \qquad (7)$$

$\kappa = 0.38$ is the Karman constant; g is the acceleration due to gravity; and T is the air temperature.

With the account of Eqs. (2) and (3) the expression for Ri takes the form

$$\mathrm{Ri} = (g/T)\ l\ \theta_*/u_*^2 \qquad (8)$$

If now Eq. (2) is differentiated with respect to z:

$$\frac{\mathrm{d}l}{\mathrm{d}z}\frac{\mathrm{d}c}{\mathrm{d}z} + l\frac{\mathrm{d}^2c}{\mathrm{d}z^2} = 0,$$

and the obtained expression for d^2c / dz^2 is put into Eq. (6), then, taking into account Eq. (8), we obtain

$$\mathrm{d}l/\mathrm{d}z = \kappa\ f\ (l/\kappa\ Z_*), \qquad (9)$$

where the Monin-Obukhov scale Z_* is introduced, which, as follows from Eq.(8), has the form

$$Z_* = \frac{u_*^2}{\mathrm{k}\ (g/T)\ \theta_*} = \frac{c_p\ \rho\ u_*^3}{\mathrm{k}\ (g/T)\ \mathrm{q}_\theta\ (0)}\ . \qquad (10)$$

In the case of equilibrium (neutral) stratification, where the flux $Q_\theta(0)$ and the number Ri are equal to zero (Ri = 0), the function $f(\mathrm{Ri})$ should be taken to be the unit: $f(0) = 1$, since formula (6) must coincide here with the known Prandthl–Karman formula.

Let us now present the function f as a series expansion truncated at small values of the first order

$$f\ (l/\kappa\ Z_*) = 1 - l/\kappa\ Z_*\ . \qquad (11)$$

When Ri approaches to zero, Z* approaches to ±$ and $f(\mathrm{Ri})$ approaches to unit.

Equation (9) takes the form

$$\mathrm{d}l/\mathrm{d}z = \kappa\ (1 - l/\kappa\ Z_*)\ . \qquad (12)$$

By integrating this equation from $z = 0$, to arbitrary z and l values, and assuming $l = l_\mathrm{m}$, we obtain

$$l(z) = \kappa\ Z_*\ [1 - (1 - l_\mathrm{m}/\kappa\ Z_*)\ \exp\ (-\ z/Z_*)]\ . \qquad (13)$$

Here, l_m is the path of mixing (molecular) in the immediate vicinity to the earth's surface (in a viscous sublayer) which are several orders of magnitude smaller than Z_*. Therefore the ratio $l_\mathrm{m} / \kappa\ L*$ can be neglected in comparison with unit.

The height dependence of the turbulence coefficient k_z, according to Eqs. (5) and (13), is described by the formula

$$k_z = \kappa\ u_*\ Z_*\ [1 - \exp\ (-\ z/Z_*)]\ . \qquad (14)$$

To derive formulae describing the vertical distribution of c, θ, and q we introduce a new variable instead of z:

$$\eta(z) = \exp\ (-\ z/Z_*) - 1\ . \qquad (15)$$

In new variables the Eqs. (1)–(3), with l determined from the relation (13), take the form

$$\mathrm{d}c = (u_*/\kappa)\ (\mathrm{d}\eta/\eta)\ ; \qquad (16)$$

$$\mathrm{d}\theta = (\theta_*/\kappa)\ (\mathrm{d}\eta/\eta)\ ; \qquad (17)$$

$$\mathrm{d}q = (q_*/\kappa)\ (\mathrm{d}\eta/\eta)\ ; \qquad (18)$$

Integrating these equations within the limits from the level of roughness z_0 to an arbitrary height z we obtain

$$c(z) = (u_*/\kappa)\ \ln(\eta/\eta_0)\ , \qquad (19)$$

$$\theta(z) = \theta_0 + (\theta_*/\kappa)\ \ln(\eta/\eta_0)\ , \qquad (20)$$

$$q(z) = q_0 + (q_*/\kappa)\ \ln(\eta/\eta_0)\ , \qquad (21)$$

where θ_0 and q_0 are the values of θ and q at the level of roughness z_0 (the wind velocity at this level, according to its definition, vanishes), $\eta_0 = \exp(z_0/Z_*) - 1$.

The formulae (13)–(14) and (19)–(21) are in good agreement with the experimental results as well as with those regularities of the layer structure well established, by now, in numerous investigations. Using these formulae, as a particular case, it is easy to derive some known expressions that approximate universal functions of the similarity theory (in particular, a logarithmic law and "logarithmic plus linear" one).

The formulae (19)–(21) describe distribution of meteorological parameters in the ground layer both under unstable ($\mathrm{Ri} < 0$, $Z_* < 0$) and stable ($\mathrm{Ri} > 0$, $Z_* > 0$) (in particular, inversion) stratifications. However in fog or without it, in big cities there often occur formations of the so-called elevated temperature inversions. Thus in Moscow, on the average, 44% observations show the presence of elevated inversions and only 13% observations show the presence of near ground inversions (in a small town Obninsk this ratio is quite different: 15% – elevated and 38% – near ground inversions).

The frequency of ocurrence of the temperature inversions that create particularly high levels of pollution is sufficiently high: it is, as a rule, more than 50%, and in some cases it is 70%–80%. In this connection the formulas describing distribution of c, θ, and q during the formation of elevated temperature inversions should be refined.

Our measurements showed that in the layer from the earth's surface to the bottom z^* of the elevated temperature inversion the temperature profile is close to the adiabatic one, and most frequently to the moist–adiabatic ($\gamma \approx \gamma_{\mathrm{m\ ad}}$), since in this layer water vapor is close to the state of saturation. As a consequence, in the layer between z_0 and z^* the distribution of c and q are described using the logarithmic formulae

$$c(z) = (u_*/\kappa)\ \ln(z/z_0)\ ; \qquad (22)$$

$$q(z) = q_0 + (q_*/\kappa)\ \ln(z/z_0)\ ; \qquad (23)$$

In the inversion layer (between z^* and h) vertical distributions of c, θ, and q are described by Eqs. (19)–(21).

Above the ground layer whose depth h can be assumed to be an absolute value of scale Z_* (according to its definition) the coefficient k_z does not, in fact, change with height. Thus for $z > h$, as follows from Eq. (14), we have

$$k_z \approx k_z(h) = \kappa\, u_*\, Z_*\, (1 - e^{-1}) \approx \kappa\, u_*\, Z_*\,; \text{ at Ri} > 0\ (Z_* > 0)\ ,$$
$$k_z = k_z(h) = \kappa\, u_*\, Z_*\, (1 - e)\ ; \quad \text{at} \quad \text{Ri} < 0\ (Z_* < 0)\ , \qquad (24)$$

where $e = 2.72...$ is the base of natural logarithms.

Convective Inflow of an Admixture. This inflow is formed due to ordered vertical motions that, in turn, are caused by convergence of air currents in a horizontal plane (wind velocity divergence). The integration of the continuity equation over height yields the relation for vertical velocity w:

$$w = -\int_0^z (\partial u/\partial x + \partial v/\partial y)\, \mathrm{d}z\ . \qquad (25)$$

In the regions of lower pressure (cyclones and troughs) under the frictional force (in combination with pressure gradient and Coriolis force) there exists convergence of air flows (divergence of wind velocity is less than zero) and, hence, ascending vertical motions ($w > 0$). In the regions of higher pressure (anticyclones and crests) there occurs the horizontal convergence of flows ($\partial u / \partial x + \partial v / \partial y > 0$) and descending vertical motions ($w < 0$).

In big cities, the ascending motions appear, in addition, under the effect of a heat region (island) (the effect of the force of buoyancy).

In the general case, in order to determine w from Eq. (25) one should use the motion equation. In this case, we obtain very cumbersome relations. To derive simpler expressions for w, providing the required accuracy, we make use of an obvious fact (supported also with quantitative estimates) that the largest absolute values of wind velocity divergence are observed near the earth's surface (where the frictional force is also maximum) and the divergence decreases with the height increase. Since the exact law of this decrease is not known, we use the simplest and most reasonable assumption that the wind velocity divergence is a linearly decreasing function of height:

$$\partial u/\partial x + \partial v/\partial y = a - b\, z\ . \qquad (26)$$

Analysis of the aforementioned cumbersome relations for w derived first in Ref. 3 shows that the vertical velocity equals zero on a plane earth's surface (outside the mountains) increases in the lower troposphere with the height z increase, reaches its maximum w_m at some height z_m (in the middle troposphere), then it decreases and vanishes for the second time in the upper troposphere.

The relation (25) with the change of divergence determined by Eq. (26) takes the form

$$w = -\, z\, (a - b\, z/2)\ . \qquad (27)$$

According to this condition w reaches its maximum equal to w_m when $z = z_m$, therefore $\partial w/\partial z = -(a - bz_m) = 0$ and $w_m = -z_m(a - bz_m/2)$; hence, $b = -2w_m/z_m^2$ and $a = -2w_m/z_m$, and the relation (27) takes the form

$$w(z) = 2\, w_m\, (z/z_m)\, (1 - (z/z_m))\ . \qquad (28)$$

Vertical velocity vanishes when $z = 0$, and when $z = 2\, z_m$. Most frequently, $z_m = H_t/2$ is used where H_t is the tropopause height.

The maximum absolute value of the vertical velocity is reached at the upper boundary of the layer within which the velocity divergence keeps the same sign. In particular, with ascending motion ($w_m > 0$) in the layer between the earth's surface and the level z_m we observe the negative divergence (convergence) and with descending motion the divergence is positive. Since the velocity divergence keeps, as a rule, its sign within the atmospheric boundary layer, it follows that w_m coincides with the vertical velocity w_{H} formed at the upper boundary H of the boundary layer under the effect of divergence (convergence) of an air flow in this layer.

Using the motion equation in the boundary layer and the relation (25) it is easy to notice that the formula for w_{H} has the form

$$w_{\mathrm{H}} = \frac{1}{2\, \omega_z\, \rho_H} \left[\frac{\partial \tau_y(0)}{\partial x} - \frac{\partial \tau_x(0)}{\partial y} \right], \qquad (29)$$

where $\tau_x(0) = (\rho k_z \partial u/\partial z)_0$ and $\tau_y = (\rho k_z \partial v/\partial z\,)_0$ are the components of the turbulent friction stress near the earth's surface; $2\omega_z$ is the Coriolis parameter.

The method of calculating these components as well as some other characteristics of the ground and boundary layers is described elsewhere.[11,12] Here we give only the Dyubyuk formula obtained assuming the height independence of k_z within the entire boundary layer:

$$w_{\mathrm{H}} = D\, \nabla^2\, p_0\ , \qquad (30)$$

where $\nabla^2 p_0 = \partial^2 p_0/\partial x^2 + \partial^2 p_0/\partial y^2$ is the air pressure Laplacian at the level of the earth's surface ($z = 0$), $D = (k_z/2)^{1/2}/(2\omega_z)^{3/2}\rho_{\mathrm{H}}$.

In conclusion, let us give the solution of Eq. (1) for one of the simplest case. This solution allows one to elucidate qualitatively the role of meteorological parameters in formation of the pollution levels of the atmosphere over a city.

Since the left–hand side ($\partial q/\partial t$) and the advective inflow in the right–hand side of Eq. (1) has, as a rule, the same sign and the same order of magnitude, we can neglect them as the first approximation. Such an assumption is all the more justifiable, if the admixture concentration averaged over the city and over certain time interval is considered. In this averaging, the inflow due to horizontal mixing is also excluded. Thus, Eq. (1) takes the form

$$\frac{\mathrm{d}}{\mathrm{d}z}\, k_z\, \frac{\mathrm{d}q}{\mathrm{d}z} - w\, \frac{\mathrm{d}q}{\mathrm{d}z} - \frac{q}{\tau} = 0\ . \qquad (31)$$

In the general case the solution to this equation can be sought only numerically.

Above the ground layer k_z is practically constant with height $k_z = k_z(h) = \text{const}$. The assumption of height independence of w and τ is less justified. Nevertheless, the dependence of admixture vertical distribution on meteorological conditions that has been stated based on this assumption is in a good agreement with the experimental results and qualitative-physical representations.

By introducing a new function

$$q^*(z) = q(z)\, \exp[(-\, \overline{w}/2\, k_z(h))\, (z - h)]\ , \qquad (32)$$

equation (31), after the replacement of $q(z)$ for $q^*(z)$ in it, is reduced to

$$d^2q^*(z) / dz^2 - b^2q^*(z) = 0 , \quad (33)$$

where

$$b^2 = (\overline{w}/2\, k_z(h))^2 + 1/\tau\, k_z(h) , \quad (34)$$

$\overline{w}$ is the mean value of w over the height in the layer between h and H; $k_z(h)$ is the coefficient k_z at the upper boundary of the ground layer determined from Eq. (24).

The solution of Eq. (33) has a well–known form

$$q^*(z) = A \exp [b (z - h)] + B \exp [- b (z - h)] .$$

Taking into account the relations (32) the expression for $q(z)$ is written as follows

$$q(z)=\exp\left[\left(\frac{\overline{w}}{2\,k_z(h)}+b\right)(z-h)\right]\{A+B\exp[-2b(z-h)]\}. \quad (35)$$

The integration constants A and B are determined from the following conditions:

$$q(h) = q_h \text{ and } q(H) = q_H , \quad (36)$$

where q_h is the value of q at the upper boundary of the ground layer $h = \pm Z_*$ determined by the formula (21); q_H is the value of q at the level H that is taken as the upper boundary of the boundary layer, where the admixture concentration is small compared to q_h (which is, e.g., $0.01q_h$). It can be assumed, without a large error that H is equal $z_m = H_t/2$ or to the doubled height of the Ekman boundary layer $H = 2\pi\sqrt{k_z(h)/\omega_z}$.

Determining the constants A and B from the conditions (36) we reduce the solution of Eq. (35) to the form

$$q(z) = \exp\left[\left(\frac{w}{2\,k_z(h)}+b\right)(z-h)\right]\times$$

$$\times\left\{q_h+\frac{q_h-q_H\,r_1}{1-r_2}\left[\exp\left(-2\,b\,(z-h)\right)-1\right]\right\}, \quad (37)$$

where

$$r_1=\exp\left[-\left(\frac{\overline{w}}{2\,k_z(h)}+b\right)(H-h)\right];\quad r_2=\exp[-2\,b\,(H-h)] .$$

In a particular case, when there is no washing-out of admixtures with clouds and precipitation ($\tau\to\infty$) and radioactive decay formula (37) takes the form

$$q(z)=q_h+\frac{q_h-q_H}{r-1}\left\{1-\exp\left[\frac{\overline{w}}{2\,k_z(h)}(z-h)\right]\right\}, \quad (38)$$

where

$$r = \exp [\overline{w}\,(H - h)/k_z(h)] .$$

It should be noted that the solution of Eq. (37) can take into account the effect of both nonstationarity and an advective admixture inflow. It is sufficient to assume that $\partial q/\partial t + u\partial q/\partial x + v\partial q/\partial y = q/\tau'$, where τ' is the relaxation time taking into account these factors (nonstationarity and advection).

The last parameter in Eq. (1), the relaxation time τ, is a complicated function of size of admixture particles and cloud, fog, and precipitation droplets. This is the most important problem in aerosol mechanics. Let us consider here the data on the values of τ determined for clouds and precipitation assuming that the distribution density of cloud droplets and admixture particles is described by the following expressions:

$$f(R) = 4(R/R_m)^2\exp(-2R/R_m);\ f(r)=4\,(r/r_m)^2\exp(-2r/r_m);$$

where R and r are the radii of droplets and particles, respectively; R_m and r_m are the radii of droplets and particles at which the function f reaches its maximum.

For some mean values R_m and r_m and moderate intensity of precipitation the following values of relaxation time τ were obtained[11] (in hours):

	Rain:		
drizzle	shower	moderate	heavy
0.6	0.8	0.9	1.5
	Clouds:		
stratus	nimbostratus	stratocumulus	fog
1.2	0.8	0.6	0.5

The above described parametrization of the principal mechanisms of propagation of polluting substances has been used in developing numerical models for forecasting ecological situations in big cities.

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