Numerical investigation of the urban heat island: verification of the Eulerian atmospheric diffusion models

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The Eulerian models of the dispersal of a passive air pollutant are formulated. Those are the high-order closure model of the dispersal, in which the concentration fluxes $<u_i c>$ are calculated by the transport equations (DC-model), and the algebraic model of turbulent fluxes $<u_i c>$ (AC-model) obtained by simplification of the DC-model to the algebraic expressions in the approximation of weak-equilibrium turbulence. Both of the models use the mean wind and turbulence values from the second-order closure model of the atmospheric boundary layer (the three-parameter E–ε–$<\theta^2>$ turbulence model). The basic characteristics of the thermohydrodynamic fields of a turbulent thermal plume above an urban heat island are reproduced by the E–ε–$<\theta^2>$ model in quite a good agreement with the experimental data and *in situ* measurements of the turbulence intensity. Calculated results on the dispersal of a passive pollutant from the surface source obtained by use of the DC and AC models show that the maximum difference in the concentration near the source does not exceed ten percent. Besides, it is shown that diffusion terms of the DC-models, excluded while obtaining the AC-model, act to smooth out flux gradients. The verification performed demonstrated the validity of using the algebraic AC-model in practice of simulating the atmospheric pollutants dispersal.

Introduction

The growing interest in protection of the urban environment and climate, as well as monitoring of the urban air quality demands from calculations proper accuracy in the concentrations of pollutants in the urban atmospheric boundary layer (UABL). The meteorological UABL parameters needed for calculation of pollutant dispersal should also be known with high accuracy. The accuracy needed can be achieved with the use of a three-parameter E–ε–$<\theta^2>$ mesoscale model of the UABL turbulence.[1]

Calculations of the dispersal are being made using different models for different applications. The Gaussian model of the turbulent thermal plume modified to take into account the surface orography is mostly investigated and applied in the papers by foreign authors.[2,3] Significant deviations from the idealized conditions introduce restrictions on the validity of Gaussian models, because uncertainties in the Gaussian model of plume may be too large. The assumed conditions may be, for example, meteorological situations with gentle wind and stable atmospheric stratification, convective conditions, and very irregular and rough surface. All these situations may occur in a real UABL during a day.

Another one approximation is based on the Lagrangian model of the dispersal of a great amount of liquid particles transported by the mean wind in turbulent fields calculated with one or another atmospheric model.[4,5] There are some examples of using the Large Eddy Simulation (LES) techniques to simulate the behavior of passive and buoyant plumes in the convective atmospheric boundary layer.[6–8]

The third approximation uses the Eulerian diffusion model, whose first principle is the equation of conservation of mass. This model closed at the level of the second-order moments for the concentration field was used, for example, in Ref. 9 in solving the well known problem of diffusion of a passive pollutant from a point sources in the convective boundary layer.

In this paper, we formulate two approximations for simulating the atmospheric pollutant diffusion. The first approximation is the differential Eulerian model of atmospheric diffusion (DC-model). This model includes prognostic equations for the mean concentration $C(x_i,t)$ and the second-order moments, i.e., the fluxes $<u_i c>$ and $<c\theta>$. The second approximation is the algebraic Eulerian model of the atmospheric diffusion; it includes anisotropic equations for the vector of turbulent flux of a passive pollutant $<u_i c>$, which exactly account for the effect of buoyancy on the turbulent transport of a pollutant. The model is derived from the differential transport equation for the fluxes $<u_i c>$ in the approximation of weak-equilibrium turbulence in the same way as in Refs. 1 and 10 where analogous equations were derived for the vector of turbulent flux of active scalar (heat) $<u_i\theta>$.

The basic meteorological parameters (mean wind, turbulence parameters) needed for realization of both

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models of the atmospheric diffusion are calculated using earlier developed three-parameter E–ε–$<\theta^2>$ mesoscale model of the UABL. Note that the effects of thermal stratification during formation of large-scale circulation over the urban heat island are reproduced using the three-parameter UABL model in a good agreement with the data of instrumental laboratory and *in situ* measurements.[11]

The aim of this work was to verify both atmospheric diffusion models in a real meteorological situation of the nighttime UABL (gentle wind, stable thermal stratification of the atmosphere) based on numerical simulation of the dispersal of a passive pollutant from a surface source, whose extent coincides with the extent of the surface heat source.[1,10,11] This verification will allow us to judge on the possibility of using the algebraic AC model of atmospheric diffusion, in contrast to the DC-model, as a simpler and easier realizable model. In addition, it should be noted that the three-parameter theory of turbulent transport developed enables one to use realistic boundary conditions on the surface accounting for the morphology of the urban surface (buildings, etc.). However, the detailed measurements in laboratory experiment[11] were conducted for the large-scale circulation over the urban heat island of the short relative length ($z_i/D \ll 1$, where z_i is the height of the mixing layer; D is the diameter of the heat island), that is, without resolution of the current details near the aerodynamically smooth surface of the prototype of a real urban heat island. Therefore, in this study we used the boundary conditions, which are usually applied to the aerodynamically smooth surface.

1. Eulerian model of transport equations for turbulent mass fluxes

To describe atmospheric dispersal of a passive pollutant, the basic three-parameter E–ε–$<\theta^2>$-model of turbulence[1,10] (where $E = 1/2<u_iu_i>$ is the kinetic energy of turbulence; ε is its dissipation rate; $<\theta^2>$ is the variance of the turbulent temperature fluctuations) should be complemented by the equations for the averaged concentration $C(x_i,t)$, the vector of the turbulent flux of pollutant $<u_ic>$, and the correlation between the concentration and temperature fluctuations $<c\theta>$.

In the tensor designations, the equation of conservation of mass has the form

$$\frac{DC}{Dt} = -\frac{\partial <u_jc>}{\partial x_j} + S_c, \qquad (1)$$

where S_c is a source.

The transport equation for turbulent fluxes of the concentration is written neglecting the terms of molecular transport and the effect of the Coriolis force on the covariance:

$$\frac{D<u_ic>}{Dt} = P_{ic} + G_{ic} + D_{ic} + \Phi_{ic} - \varepsilon_{ic}, \qquad (2)$$

where

$$P_{ic} = -<u_iu_j>\frac{\partial C}{\partial x_j} - <u_jc>\frac{\partial U_i}{\partial x_j}$$

is the generation of turbulent fluxes of the scalar;

$$G_{ic} = -\beta g_i < c\theta >$$

is the generation by buoyancy;

$$D_{ic} = -\frac{\partial}{\partial x_j}(<u_iu_jc> + <c\frac{p}{\rho}>\delta_{ij}) = $$

$$= \frac{\partial}{\partial x_k}\left\{\alpha_{1s}\frac{E}{\varepsilon}<u_ku_l>\frac{\partial <u_ic>}{\partial x_l}\right\}$$

is the turbulent diffusion;

$$\Phi_{ic} = <\frac{p}{\rho}\frac{\partial c}{\partial x_i}>$$

is the "pressure–concentration gradient" correlation; ε_{ic} is the dissipative vector.

For the two last balance accounts of Eq. (2), the model, which yielded good test results,[12] is used:

$$\Phi_{ic} - \varepsilon_{ic} = -\alpha_{1c}\frac{\varepsilon}{E}<u_ic> +$$

$$+\alpha_{2c}<u_jc>\frac{\partial U_i}{\partial x_j} + \alpha_{3c}g_i\beta <c\theta>.$$

The equation for the vector of the turbulent flux of concentration can be written in a more compact form

$$\frac{D<u_ic>}{Dt} = -<u_iu_j>\frac{\partial C}{\partial x_j} - <u_jc>\frac{\partial U_i}{\partial x_j} +$$

$$+\frac{\partial}{\partial x_k}\left\{\alpha_{1s}\frac{E}{\varepsilon}<u_ku_l>\frac{\partial <u_ic>}{\partial x_l}\right\} -$$

$$-\alpha_{1c}\sqrt{\frac{\varepsilon}{E}\frac{\varepsilon_c}{<c^2>}}<u_ic> + \alpha_{2c}<u_jc>\frac{\partial U_i}{\partial x_j} +$$

$$+\alpha_{3c}g_i\beta <c\theta> - g_i\beta <c\theta>, \qquad (3)$$

where ε_c is the destruction of the scalar field, and the value of the ratio of the time scales $R = (<c^2>/2\varepsilon_c)/(E/\varepsilon)$ is taken in the calculations to be equal to 0.6.

The equation for the covariance $<c\theta>$ has the form

$$\frac{D<c\theta>}{Dt} = -<u_j\theta>\frac{\partial C}{\partial x_j} - <u_jc>\frac{\partial \Theta}{\partial x_j} +$$

$$+\frac{\partial}{\partial x_k}\left\{\alpha_{2s}\frac{E}{\varepsilon}<u_ku_l>\frac{\partial <c\theta>}{\partial x_l}\right\} - \epsilon_{c\theta}, \qquad (4)$$

where the molecular destruction term $\epsilon_{c\theta}$ is parameterized, following Ref. 13, as $\epsilon_{c\theta} = \alpha_{3c}\frac{\varepsilon}{E} < c\theta >$. In Eqs. (1)–(4)

$$\frac{D}{Dt} \equiv \frac{\partial}{\partial t} + U_j \frac{\partial}{\partial x_j}$$

is the material derivative; g_i is the vector of acceleration due to gravity;

$$\beta = -(1/<\rho>)(\partial<\rho>/\partial\Theta)_p$$

is the coefficient of thermal expansion; p is the pressure; ρ is the density. The model constants α_{1c}, α_{2c}, α_{3c}, α_{1s}, and α_{2s} are equal to 4.0, 0.4, 0.4, 0.22, and 0.22, respectively. The mean temperature Θ and the vector of turbulent heat flux $<u_j\theta>$ are calculated using the three-parameter model of turbulent transport.[1] Equations (1), (3), and (4) form the DC-model of the atmospheric diffusion of a pollutant.

2. Eulerian algebraic model for turbulent mass fluxes

The algebraic model of the turbulent fluxes of concentration can be derived from the transport equation (3), assuming weak-equilibrium turbulence. This assumption states that the turbulence is, approximately, in equilibrium with the mean current having the imposed parameters. If this approximation is taken for both the velocity field and the scalar (temperature, concentration) field, then we obtain from Eq. (3) the algebraic equation for the vector of turbulent flux of the scalar:

$$-<u_i c> = \frac{1}{\alpha_{1c}}\sqrt{\frac{E}{\varepsilon}\frac{<c^2>}{\varepsilon_c}} \times$$

$$\times\left[<u_i u_j>\frac{\partial C}{\partial x_j} + (1-\alpha_{2c})<u_j c>\frac{\partial U_i}{\partial x_j}\right] +$$

$$+\frac{1}{\alpha_{1c}}\sqrt{\frac{E}{\varepsilon}\frac{<c^2>}{\varepsilon_c}}(1-\alpha_{2c})g_i\beta<c\theta>. \quad (5)$$

It can easily be seen that Eq. (5) is implicit for the flux $-<u_i c>$, because its right-hand side includes the flux $<u_j c>$. The simplest way to make Eq. (5) fully explicit is to accept the gradient Boussinesq hypothesis in the right-hand side of Eq. (5) for the momentum and scalar fluxes, although the inconsistency of this procedure is obvious. Thus, it is stated that

$$-<u_i u_j> = 2\nu_t S_{ij} - \frac{2}{3}E\delta_{ij}, \quad (6)$$

$$-<u_i c> = D_t\frac{\partial C}{\partial x_i}, \quad (7)$$

where $S_{ij} = (\partial U_i/\partial x_j + \partial U_j/\partial x_i)/2$ is the tensor of mean deformation rates; $\nu_t = c_\mu E^2/\varepsilon$ is the turbulent viscosity; $D_t = c_\mu\sqrt{2R}(E^2/\varepsilon)$ is the coefficient of turbulent diffusion; δ_{ij} is the Kronecker tensor. The substitution of Eqs. (6) and (7) into Eq. (5) yields the following fully explicit equation for the vector of turbulent flux of scalar:

$$-<u_i c> = c_\mu(E^2/\varepsilon)\sqrt{2R}(\partial C/\partial x_i) - \alpha_{1c}^{-1}(E/\varepsilon)\sqrt{2R}\times$$

$$\times\left[\{2\nu_t + (1-\alpha_{2c})D_t\}S_{ij} + (1-\alpha_{2c})D_t\Omega_{ij}\right](\partial C/\partial x_j) +$$

$$+\left[(1-\alpha_{2c})/\alpha_{1c}\right](E/\varepsilon)\sqrt{2R}g_i\beta<c\theta>, \quad (8)$$

where Ω_{ij} is the mean tensor of rotations. The comparison of Eq. (5) with Eq. (8) shows that the buoyancy effects in the final equation (8) have the exact form, which, in a certain sense, justifies the used procedure of explicit representation of the equation for turbulent fluxes of concentration. The tests on calibration of the model constants yielded the following values: $c_\mu = 0.095$, $\alpha_{2c} = \alpha_{3c} = 0.40$. The algebraic anisotropic model of the atmospheric diffusion (AC-model) includes Eq. (1) for the mean concentration and Eq. (8) for the turbulent fluxes of concentration.

3. Tests of DC- and AC-models of the turbulent mass fluxes. Boundary and initial conditions. Numerical method

The DC- and AC-models have been tested for the critical meteorological situation arising in the nighttime UABL under conditions of gentle wind and stable atmospheric stratification. Such a situation is typical of formation of the turbulent air circulation over a city – the phenomenon called the urban heat island.

In the laboratory experiment,[11] penetrating turbulent convection is induced by the constant heat flux generated by the surface heat source in the form of a circular plate of the given diameter. This heat source models the prototype of the urban heat island with the small elongation (vertical linear scale much smaller than the horizontal one). Fluid-dynamics equations describing the circulation over the urban heat island with the small relative elongation can be written neglecting the Coriolis force and radiation in the cylindrical coordinate system. In addition, the hydrostatic approximation can be applied, and the buoyancy effects can be taken into account in the Boussinesq approximation.[11]

The meteorological parameters needed, such as the mean wind, temperature, turbulent velocity and temperature fields were calculated using the three-parameter model of turbulent transport. The distributions of these parameters in the turbulent thermal plume obtained for the cylindrical geometry of turbulent circulation over the urban heat island can be found in Ref. 1. In these tests they were used as the input information for diffusion calculations. Equations (1), (3), and (4) of the DC-model and equations (1), (4), (8) of the AC-model are written in cylindrical coordinates for the mean concentration

$C(r,z,t)$ sought and the second-order moments of the pollutant concentration field $<u_r c>$, $<u_z c>$, and $<c\theta>$ (r is the coordinate in the horizontal direction, z is the coordinate directed vertically upwards). The equations (1), (3), (4) in the cylindrical coordinates are presented in the Appendix. Equations for the turbulent heat fluxes $<u_r\theta>$ and $<u_z\theta>$ have the form (see Refs. 1 and 10) similar to the form of equations for the turbulent concentration fluxes $<u_r c>$ and $<u_z c>$ with the only difference that the term describing the effects of buoyancy on the turbulent transport of the concentration in the vertical direction uses the covariance $<c\theta>$ in place of the correlation. The equations for the concentration fluxes in the cylindrical coordinates can be easily derived from Eq. (8) and are omitted.

3.1. Boundary and initial conditions

The boundary conditions for the equation of the mean concentration on the surface are realized in the form of a surface pollutant source given the constant productivity Q. The linear dimension of the pollutant source coincides with the linear dimension of the heater – the plate of the given diameter. The constant vertical flux of the pollutant is specified at the source

$$-D_t(\partial C/\partial z) = H_c, \tag{9}$$

where $H_c = Q/(0.5r/D)$. The value of Q was specified from the condition that the Reynolds number $\mathrm{Re} = Q/\nu$ ensures the income of the pollutant from the source without the initial momentum and, thus, is limited by the velocity of the external flux.

At the initial moment in time, the ambient medium is at rest, the initial fields of the concentration C, correlation $<c\theta>$, and concentration fluxes $<u_r c>$, $<u_z c>$ are zero. At the bottom boundary of the domain of integration shaped as a cylinder, the boundary conditions at $z = 0$ are as follows:

$$E = <\theta^2> = \frac{\partial \varepsilon}{\partial z} = \frac{\partial C}{\partial z} = \frac{\partial <c\theta>}{\partial z} = 0,$$
$$-<u_z c> = H_c,\ \ -<u_r c> = 0; \tag{10}$$

while at the top boundary, $z = Z$:

$$\frac{\partial C}{\partial z} = \frac{\partial <c\theta>}{\partial z} = \frac{\partial <u_r c>}{\partial z} = \frac{\partial <u_z c>}{\partial z} = 0.$$

The symmetry conditions are imposed at $r = 0$. The same conditions are also used at the external boundary of the domain of integration (at $1.8r/D$). The other boundary conditions for the velocity and temperature fields have the same form as in Ref. 1.

3.2. Numerical method

The systems of equations of the diffusion DC- and AC-models were solved numerically using the semi-implicit scheme (second scheme with the upstream differences[14] imposing certain restrictions on the second-order approximation) and the method of alternating directions at the shifted difference grid. The difference equations were solved by the sweep method. To preserve the conservative and transportation properties of the difference scheme, the equations were written in the difference form at the near-boundary second-order grid nodes and using the corresponding boundary conditions.

4. Numerical results of the tests of the DC- and AC-models: dispersal of a passive pollutant in the UABL

The results of modeling the structure of turbulent circulation over the urban heat island (different parameters of the turbulent velocity and temperature fields) were obtained earlier and can be found in Refs. 1 and 10.

The dispersal of a passive pollutant from an extended surface source over the urban heat island was modeled in order to verify the numerical results obtained with the use of DC- and AC-models. It should be noted that because the experimental data on the pollutant dispersal from the surface source over the urban heat island in the considered critical meteorological period are lacking, it is impossible to directly check the results of numerical realization of the diffusion models by comparing them with the measurement data. The validity of the models can be judged on from indirect evidences. First, the analogous model of active pollutant (heat) transport gives the results,[1] which are in a rather good agreement with the data of direct instrumental measurements.[11] Second, the accuracy of numerical solution was checked at the successively divided 25×116 grids and 50×232 grid.

The results obtained by numerical simulation are shown in Figs. 1–3, where z_i is the height of the mixing layer, D is the diameter of the hot plate (linear dimension of the urban heat island).

Figure 1 depicts the mean concentration of the passive pollutant normalized to the maximum value as calculated by the AC- and DC-models. One can notice the common effect of the dispersal under conditions of stable stratification of the ambient medium, namely, penetration of a pollutant outside the boundary layer ($z/z_i > 1$). This effect has been observed in recent measurements of the buoyant plumes ascending in the convective boundary layer.[15] It is worthy to note that the lines of equal concentration in Fig. 1*a* are smoother as compared to those in Fig. 1*b*. In general, the distributions are quite similar, as can be seen from Fig. 2, where the concentration profiles from Figs. 1*a* and *b* are shown together. The maximum difference in the mean concentration near the source does not exceed 10%, which confirms the validity of using the algebraic AC-model, which is simpler in realization, for turbulent fluxes in the practice of atmospheric dispersal calculations. This is an encouraging conclusion for the development of the mesoscale model of the urban boundary layer with resolution of the detailed morphology of the urban surface, because the AC-model of diffusion, as compared to the model of transport equations for turbulent fluxes of scalar (DC-model), requires no additional input information, which is often lacking. Figure 3*a* depicts the lines of flow showing the production of two large-scale formations, rotating in the opposite directions, with concentrated vorticity, which extend from the surface to the inversion layer ($z/z_i \sim 1$). At the island center, these eddies produce an intense upward motion, carrying out the pollutant upwards from the source with its dispersal into the mixing layer and then into the inversion layer with the diffusion in the horizontal direction within the inversion layer. The vector field of the vertical $\langle u_z c \rangle$ and horizontal $\langle u_r c \rangle$ concentration fluxes calculated by the DC-model (see Eqs. (A.1)–(A.4) in Appendix) and shown in Fig. 3*b* along with the profiles of the mean concentration shows the usefulness of the model used to describe the dispersal of the passive pollutant in the stably stratified atmosphere over the urban heat island at the gentle wind (for illustration, the vector field is shown by arrows of the same lengths).

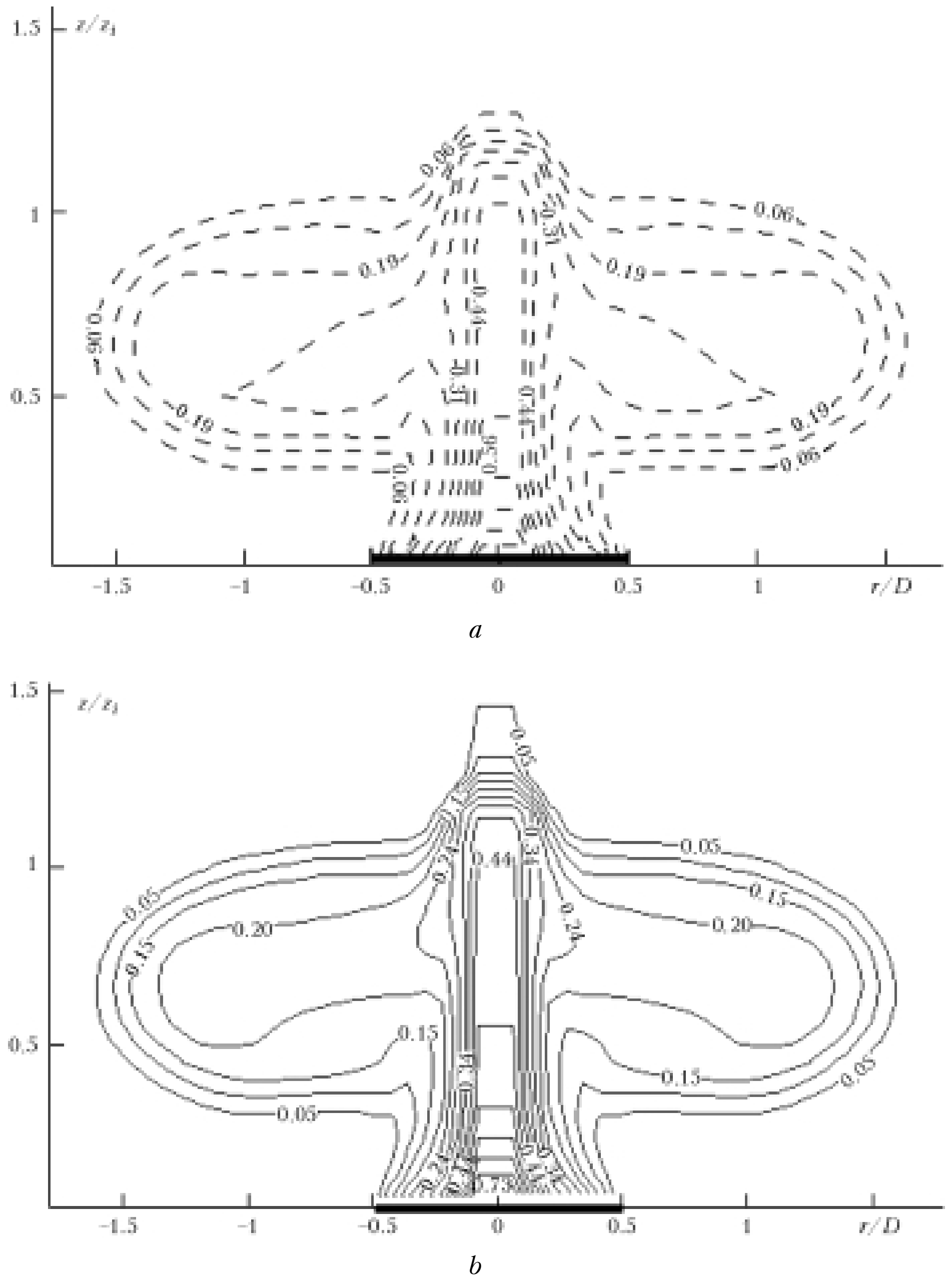


Fig. 1. Field of the mean concentration of a passive pollutant over the urban heat island as calculated by the AC (*a*) and DC (*b*) models.

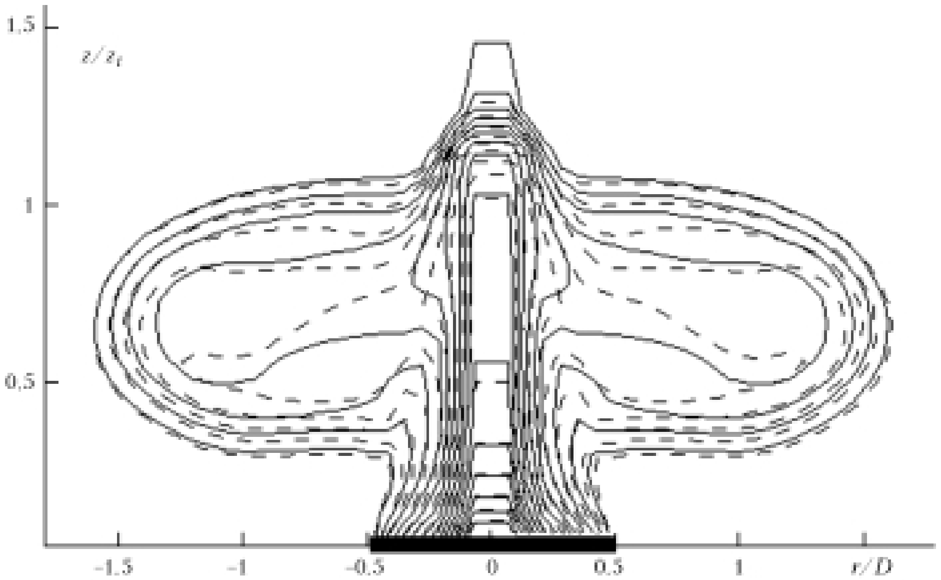
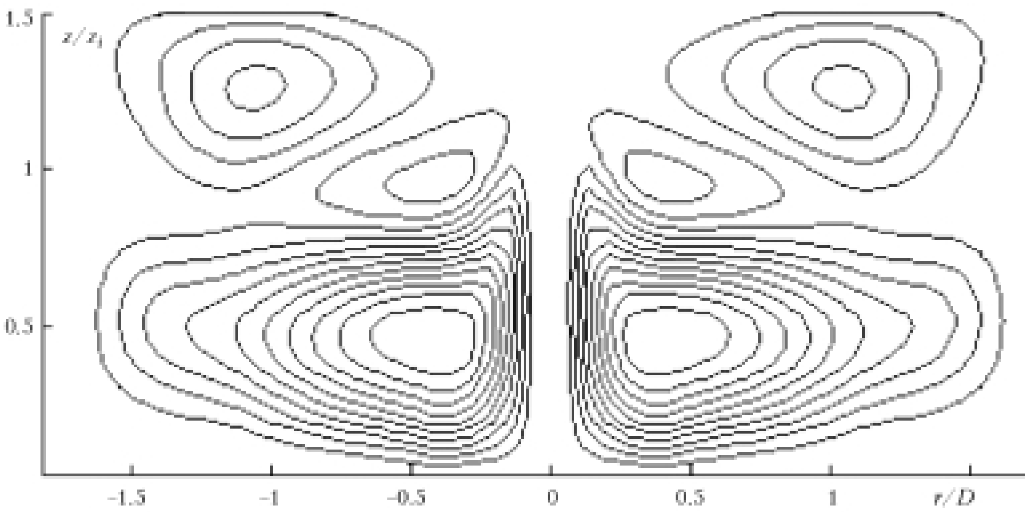
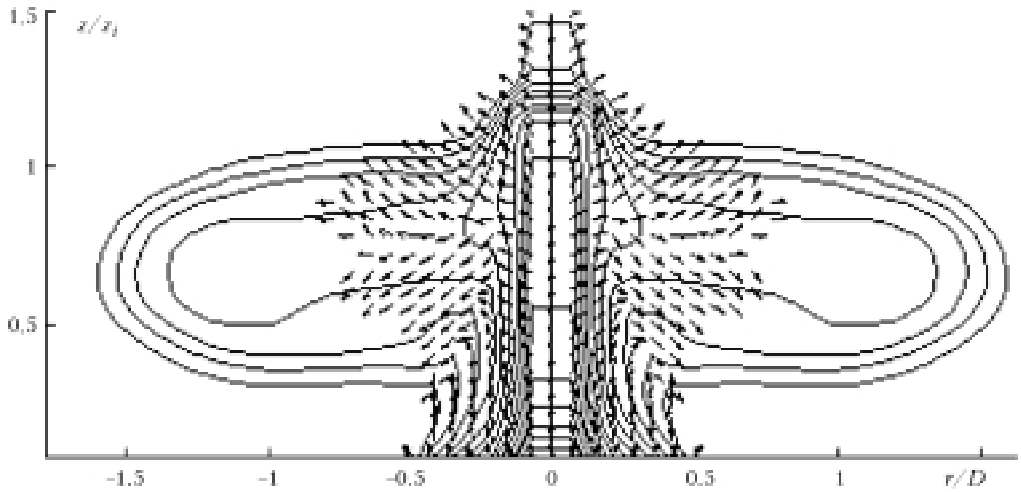


Fig. 2. Field of the mean pollutant concentration as calculated by the AC- and DC-models (superposition of Figs. 1*a* and *b*).



a



b

Fig. 3. Lines of flow (*a*) and the vector field of turbulent vertical $\langle u_z c \rangle$ and horizontal $\langle u_r c \rangle$ fluxes of the pollutant concentration with the superimposed mean concentration profiles (*b*) (superposition of Fig. 1*b*).

Appendix

This Appendix presents the complete system of equations of the DC-model of atmospheric diffusion in the cylindrical coordinates, whose dimensionless form has been obtained using the same parameters, as in the three-parameter model.[1] In the corresponding transport equations for the turbulent fluxes, the molecular transport terms and the effect of the Coriolis force on the covariance were neglected.

The transport equation for the mean pollutant concentration is

$$\frac{\partial C}{\partial t}+\frac{1}{r}\frac{\partial}{\partial r}[rCU_r]+\frac{\partial}{\partial z}[CU_z]=$$

$$=\frac{1}{r}\frac{\partial}{\partial r}r(-<u_rc>)+\frac{\partial}{\partial z}(-<u_zc>). \qquad \text{(A.1)}$$

The transport equation for the radial (horizontal) turbulent flux of the concentration

$$\frac{\partial <u_rc>}{\partial t}+\frac{1}{r}\frac{\partial}{\partial r}[r<u_rc>U_r]+\frac{\partial}{\partial z}[<u_rc>U_z]=$$

advection

$$=\frac{1}{r}\frac{\partial}{\partial r}\left[r\alpha_{1s}\frac{E}{\varepsilon}<u_r^2>\frac{\partial}{\partial r}<u_rc>\right]+$$

$$+\frac{1}{r}\frac{\partial}{\partial r}\left[r\alpha_{1s}\frac{E}{\varepsilon}<u_ru_z>\mathrm{Fr}^{-1}\frac{\partial}{\partial z}<u_rc>\right]+$$

horizontal diffusion

$$+\mathrm{Fr}^{-1}\frac{\partial}{\partial z}\left[\alpha_{1s}\frac{E}{\varepsilon}\{<u_ru_z>\frac{\partial}{\partial r}<u_rc>+\right.$$

$$\left.+\mathrm{Fr}^{-1}<u_z^2>\frac{\partial}{\partial z}<u_rc>\}\right]-$$

vertical diffusion

$$-\{<u_r^2>\frac{\partial C}{\partial r}+<u_zu_r>\mathrm{Fr}^{-1}\frac{\partial C}{\partial z}+$$

$$+<u_rc>\frac{\partial U_r}{\partial r}+\mathrm{Fr}^{-1}<u_zc>\frac{\partial U_r}{\partial z}\}-$$

generation

$$-\alpha_{1c}\frac{\varepsilon}{E}<u_rc>+\alpha_{2c}(<u_rc>\frac{\partial U_r}{\partial r}+<u_zc>\frac{\partial U_r}{\partial z}) \qquad \text{(A.2)}$$

"pressure–concentration gradient" correlation.

The equation for the vertical turbulent concentration flux

$$\frac{\partial <u_zc>}{\partial t}+\frac{1}{r}\frac{\partial}{\partial r}[r<u_zc>U_r]+\frac{\partial}{\partial z}[<u_zc>U_z]=$$

advection

$$=\frac{1}{r}\frac{\partial}{\partial r}\left[r\alpha_{1s}\frac{E}{\varepsilon}<u_r^2>\frac{\partial}{\partial r}<u_zc>\right]+$$

$$+\frac{1}{r}\frac{\partial}{\partial r}\left[r\alpha_{1s}\frac{E}{\varepsilon}<u_ru_z>\mathrm{Fr}^{-1}\frac{\partial}{\partial z}<u_zc>\right]+$$

horizontal diffusion

$$+\mathrm{Fr}^{-1}\frac{\partial}{\partial z}\left[\alpha_{1s}\frac{E}{\varepsilon}\{<u_ru_z>\frac{\partial}{\partial r}<u_zc>+\right.$$

$$\left.+\mathrm{Fr}^{-2}<u_z^2>\frac{\partial}{\partial z}<u_zc>\}\right]-$$

vertical diffusion

$$-\{<u_zu_r>\frac{\partial C}{\partial r}+<u_z^2>\mathrm{Fr}^{-1}\frac{\partial C}{\partial z}+$$

$$+\mathrm{Fr}<u_rc>\frac{\partial U_z}{\partial r}+<u_zc>\frac{\partial U_z}{\partial z}\}+$$

generation

$$+(1-\alpha_{3c})\mathrm{Fr}^{-1}<c\theta>-\alpha_{1c}\frac{\varepsilon}{E}<u_zc>+$$

$$+\alpha_{2c}(<u_zc>\frac{\partial U_z}{\partial z}+<u_rc>\frac{\partial U_z}{\partial r}) \qquad \text{(A.3)}$$

buoyancy + "pressure–concentration gradient" correlation.

Equation for covariance $<c\theta>$

$$\frac{\partial <c\theta>}{\partial t}+\frac{1}{r}\frac{\partial}{\partial r}[r<c\theta>U_r]+\frac{\partial}{\partial z}[<c\theta>U_z]=$$

advection

$$=\frac{1}{r}\frac{\partial}{\partial r}\left[r\alpha_{2s}\frac{E}{\varepsilon}<u_r^2>\frac{\partial}{\partial r}<c\theta>\right]+$$

$$+\frac{1}{r}\frac{\partial}{\partial r}\left[r\alpha_{1s}\frac{E}{\varepsilon}<u_ru_z>\mathrm{Fr}^{-1}\frac{\partial}{\partial z}<c\theta>\right]+$$

horizontal diffusion

$$+\mathrm{Fr}^{-1}\frac{\partial}{\partial z}\left[\alpha_{2s}\frac{E}{\varepsilon}\{<u_ru_z>\frac{\partial}{\partial r}<c\theta>+\mathrm{Fr}^{-2}<u_z^2>\frac{\partial}{\partial z}<c\theta>\}\right]-$$

vertical diffusion

$$-\{<u_r\theta>\frac{\partial C}{\partial r}+<u_z\theta>\mathrm{Fr}^{-1}\frac{\partial C}{\partial z}+<u_rc>\frac{\partial \Theta}{\partial r}+$$

$$+\mathrm{Fr}^{-1}<u_zc>\frac{\partial \Theta}{\partial z}\}-$$

generation

$$-\alpha_{3c}\frac{\varepsilon}{E}<c\theta> \qquad \text{(A.4)}$$

molecular destruction.

In Eqs. (A.1) to (A.4), the following designations are used: $<u_z c>$, $<u_r c>$ are the vertical and horizontal turbulent concentration fluxes; U_r and U_z are the horizontal and vertical mean velocities; $E = <u_i^2>/2$ is the kinetic energy of turbulence (KET); ε is its dissipation rate; $<u_r^2>$, $<u_z^2>$ are the horizontal and vertical KET components; $<u_z\theta>$, $<u_r\theta>$ are the vertical and horizontal turbulent heat fluxes; Θ is the mean temperature; $\mathrm{Fr} = w_D/ND$ is the Froude number (D is the horizontal dimension of the heat island; w_D is the turbulent convective velocity scale; $N = (g\beta\partial\Theta/\partial z)^{1/2}$ is the Brunt–Vaisala frequency). The values of the model constants α_{1c}, α_{2c}, α_{3c}, α_{1s}, and α_{2s} are presented in the text.

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