Dispersion of passive pollution from a surface source over an urban heat island

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The results of computer simulation of dispersion of passive pollutants from an extended surface source over an urban heat island in a critical meteorological period (gentle wind, stable thermal stratification of the atmosphere, locking inversion) are presented. The Eulerian model of the atmospheric diffusion is constructed based on the three-parameter theory of turbulent transfer. It includes the differential transport equations for the average concentration and correlation between turbulent fluctuations of the concentration and temperature. The fully explicit anisotropic algebraic mass flux model of pollution is formulated. The simulation shows that the pollution plume disperses above the inversion layer. Comparison between the results obtained with the fully explicit algebraic mass flux model, which physically correctly takes into account the buoyancy effects, and the simple Boussinesq model ignoring the buoyancy effects show that the Boussinesq model essentially underestimates both vertical and horizontal pollutant diffusion, that results in accumulation of pollutants near the surface.

Introduction

A large share of urban territories is a permanent source of heat and pollution due to anthropogenic activity, for example, industrial processes, traffic, farming, and so on. Indeed, urban areas are mostly covered with concrete and asphalt, which accumulate and then emit the incoming radiation, thus causing significant heating of the surface air layer as compared to the environment. As a result, urban territories form local heat islands.[1] The urban landscape with high buildings and streets of various sizes together with the ambient orography form a very complex local surface geometry. The local boundary conditions together with thermal stratification form a complex mechanism of interaction between heat transfer and associated emission of pollutants. Description of this complex interaction mechanism is vitally important for estimation of possible dispersion of toxic pollutants potentially hazard to human health. This is also important for monitoring air quality, planning the future development of cities and arrangement of industrial zones, designing and controlling urban traffic, as well as industrial activity in critical meteorological periods.

The present practice[2,3] of describing the pollution dispersion in the environment is based on semiempirical methods and simple integral simulation with preset wind conditions, while the situations on micro- and macroscales being under the dominant effect of buoyancy turn out to be beyond the range of such models. The Large Eddy Simulation (LES) method[4] can be considered as a possible choice, but traditional LES technologies are still inapplicable to large-scale problems with high Reynolds and Peclet numbers.

In this paper, we develop the Eulerian model of atmospheric diffusion of a passive contaminant based on the three-parameter theory of turbulent transport of momentum and scalar in the thermally stratified atmospheric boundary layer.[5] This theory can be considered as a potentially efficient, computationally clear, and physically correct method for simulation of the combined effects of orography and thermal stratification on the pollution dispersion in the atmosphere. Effects of thermal stratification at formation of large-scale circulation over an urban heat island are reconstructed using the three-parameter theory of turbulent transport in accordance with the data of instrumental measurements.[6] They are analyzed based on numerical simulation of dispersion of passive contaminants from a surface source whose size coincides with the size of a surface heat source[5,6] for the critical meteorological period (gentle wind, stable atmospheric stratification, locking inversion).

The developed three-parameter model of the turbulent transport allows us to use realistic boundary conditions. However, detailed measurements in the controlled laboratory experiment[6] were conducted for large-scale circulation over an urban heat island of relatively small size ($z_i/D \ll 1$, where z_i is the height of the mixed layer; D is the diameter of the heat island), that is, with unresolved current details near the aerodynamically smooth surface of a prototype of the actual urban heat island. This circumstance was taken into account in formulation of boundary conditions in Ref. 5 and will be taken into account below in formulation of boundary conditions for dispersion of pollution from a surface source.

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Eulerian diffusion model of the pollution dispersion in the stratified atmosphere

To describe atmospheric dispersion of passive pollution, the basic three-parameter E–ε–$<\theta^2>$ model of turbulence ($E = 1/2 <u_i u_i>$ is the kinetic energy of turbulence; ε is its dissipation; $<\theta^2>$ is the variance of turbulent temperature fluctuations) should be complemented with equations for the average concentration $C(x_i,t)$, the vector of the turbulent pollutant flux $<u_i c>$, and the correlation between the concentration and temperature fluctuations $<c\theta>$. Since the results of simulating the transport of an active pollutant (heat) over an urban heat island[5] agree well with the measurements,[6] for the turbulent flux of a passive scalar (pollutant mass) we also use the fully explicit anisotropic algebraic model[5,7] obtained from simplification of the differential transport equation for $<u_i c>$ in the approximation of a locally equilibrium turbulence.

The governing equations for the concentration field of a passive scalar are written, as in Ref. 5, in the cylindrical coordinate system:

$$\frac{\partial C}{\partial t} + \frac{1}{r}\frac{\partial}{\partial r} rCU_r + \frac{\partial}{\partial z} CU_z = -\frac{1}{r}\frac{\partial}{\partial r} r < u_r c > - \frac{\partial}{\partial z} < u_z c >; \quad (1)$$

$$- < u_i c > = C_T \frac{E^2}{\varepsilon}\sqrt{2R}\frac{\partial C}{\partial x_i} - \frac{\sqrt{R}}{\alpha_{1c}}\frac{E}{\varepsilon} \times [\{2\nu_T + (1-\alpha_{2c}) D_T\} S_{ij} + (1-\alpha_{2c}) D_T \Omega_{ij}](\partial C/\partial x_j) + [(1-\alpha_{2c})/\alpha_{1c}] (E/\varepsilon)\sqrt{R}\, g_i \beta < c\theta > ; \quad (2)$$

$$\frac{\partial < c\theta >}{\partial t} + \frac{1}{r}\frac{\partial}{\partial r} r < c\theta > U_r + \frac{\partial}{\partial z} < c\theta > U_z = -\alpha_{3c}\frac{\varepsilon}{E} < c\theta > + \frac{1}{r}\frac{\partial}{\partial r}\left[r\,\alpha_{2s}\frac{\nu_T}{\mathrm{Sc}_T}\right]\frac{\partial < c\theta >}{\partial r} + \frac{\partial}{\partial z}\left[\alpha_{2s}\frac{\nu_T}{\mathrm{Sc}_T}\right]\frac{\partial < c\theta >}{\partial z} - \left\{< u_r c > \frac{\partial \Theta}{\partial r} + < u_z c > \frac{\partial \Theta}{\partial z} + < u_r\theta > \frac{\partial C}{\partial r} + < u_z\theta > \frac{\partial C}{\partial z}\right\}, \quad (3)$$

where U_r and U_z are the average horizontal and vertical velocities, respectively; u_r and u_z are respectively the horizontal and vertical turbulent velocity fluctuations; Θ is the average temperature; θ is the turbulent temperature fluctuation; $C(x_i, t)$ is the average pollution concentration; $-<u_i c>$ is the vector of turbulent flux of the scalar [the vertical component $-<u_z c>$ and the horizontal (radial) component $-<u_r c>$ are not presented here and can be readily derived from Eq. (2)]; $<c\theta>$ is the correlation between the concentration and temperature fluctuations; $S_{ij} = (1/2)(\partial U_i/\partial x_j + \partial U_j/\partial x_i)$ is the average velocity shear tensor; $\Omega_{ij} = (1/2)(\partial U_i/\partial x_j - \partial U_j/\partial x_i)$ is the average rotation tensor; $\nu_T = C_\mu E^2/\varepsilon$ is the turbulent viscosity coefficient; $D_T = C_T\sqrt{2R}\,E^2/\varepsilon$ is the turbulent diffusion coefficient; Sc_T is the turbulent Schmidt number, $R = \tau_c/\tau$ is the ratio of the characteristic time scales of the scalar (τ_c) and dynamic (τ) turbulent fields; β is the thermal expansion coefficient of the medium; g_i is the vector of acceleration due to gravity. For turbulent stresses, a simple Boussinesq model is used. In this problem, this model keeps some anisotropy for normal Reynolds stresses

$$< u_r^2 > = (2/3)E - 2\nu_T (\partial U_r/\partial r), \quad (4)$$

$$< u_z^2 > = (2/3)E - 2\nu_T (\partial U_z/\partial z), \quad (5)$$

$$< u_\varphi^2 > = (2/3)E - 2\nu_T (U_r/r), \quad (6)$$

$$- < u_r u_z > = 2\nu_T (\partial U_r/\partial z + \partial U_z/\partial r). \quad (7)$$

In Eq. (6), u_φ is the azimuth turbulent velocity fluctuation. In Eqs. (1)–(7) and below, capital letters and <…> denote averaged values, and small letters denote turbulent fluctuations. The axis z is directed vertically upward. Equations (1)–(7) use the same parameters as in Ref. 5 in the dimensionless form.

The constant coefficients in Eqs. (1)–(7) are chosen based on the following reasoning. The value of $\alpha_{1c} = 4.0$ corresponds to the lower boundary of the range of this constant used by different authors in solution of the problems connected with transport of passive pollutants. Variation of its value within 20% had no noticeable effect on the results of simulation of the concentration field of the passive pollutants. The absence of experimental data on the behavior of the correlation $<c\theta>$ does not allow us to estimate its value from the solution of simple limit problems. By this reason, α_{3c} in the dissipative term of Eq. (3) was assumed equal, as in Ref. 8, to $C_{1\theta}$. In Eq. (2), α_{2c} determines the degree of influence of the buoyancy effect on the vertical transport of pollution by the flux $-<u_z c>$ in parameterization of correlation of the scalar field with pressure pulsations. The constant $C_{2\theta}$ in the anisotropic model of the turbulent heat flux $-<u_i \theta>$, similar to the model (2) (see Eq. (31) in Ref. 9), determines, in its turn, the influence of the buoyancy effects on the vertical heat transfer. Its value, calibrated when solving various problems of thermally stratified turbulent currents, is equal to 0.40. The commonly used assumption is that $C_{2\theta} = \alpha_{2c}$. Then, following Ref. 7, in the governing system of equations of diffusion model (1)–(7), the coefficient $(2/3\alpha_{1c})$ in the first term in the right-hand side of Eq. (2) is replaced by C_T for the first term in the right-hand side of Eq. (2) to give the simple Boussinesq model for eddy diffusion. In all other terms in the right-hand side of Eq. (2), α_{1c} remains an independent constant. The coefficients C_μ and C_T have the "standard" values calibrated when simulating the evolution of homogeneous turbulence under the conditions of stable stratification: $C_\mu = 0.095$, $C_T = C_\mu / \mathrm{Sc}_T$ ($\mathrm{Sc}_T = 0.9$). The time scale ratio is taken to be constant and equal to $R = 0.6$.

The penetrating turbulent convection is induced by the constant heat flux from a surface heat source in the form of a round plate of D diameter (Fig. 1). Figure 1 depicts a schematic pattern of circulation over the real urban heat island (*a*) and its model (*b*) in the form of a heated disk used in the laboratory experiment[6] and numerical simulation. The shadgraph in Fig. 1 shows the heat plume in the quasisteady state with a domelike top (a hat) along with the pollution source, whose length is equal to the diameter of the heated disk.

The heat source simulates a prototype of the urban heat island with relatively short length under condition of a gentle wind and stable stratification of the environment. The equations of thermal fluid dynamics describing the circulation over such island can be written ignoring the Coriolis force and radiation in the axisymmetric cylindrical coordinate system. Besides, the hydrostatic approximation can be accepted, while the buoyancy effects are taken into account in the Boussinesq approximation.[5]

The superficial pollutant source with the preset constant emission rate Q has the same linear dimension D_μ as the heat source. Thus, the vertical flux of pollutants is set constant within the source area:

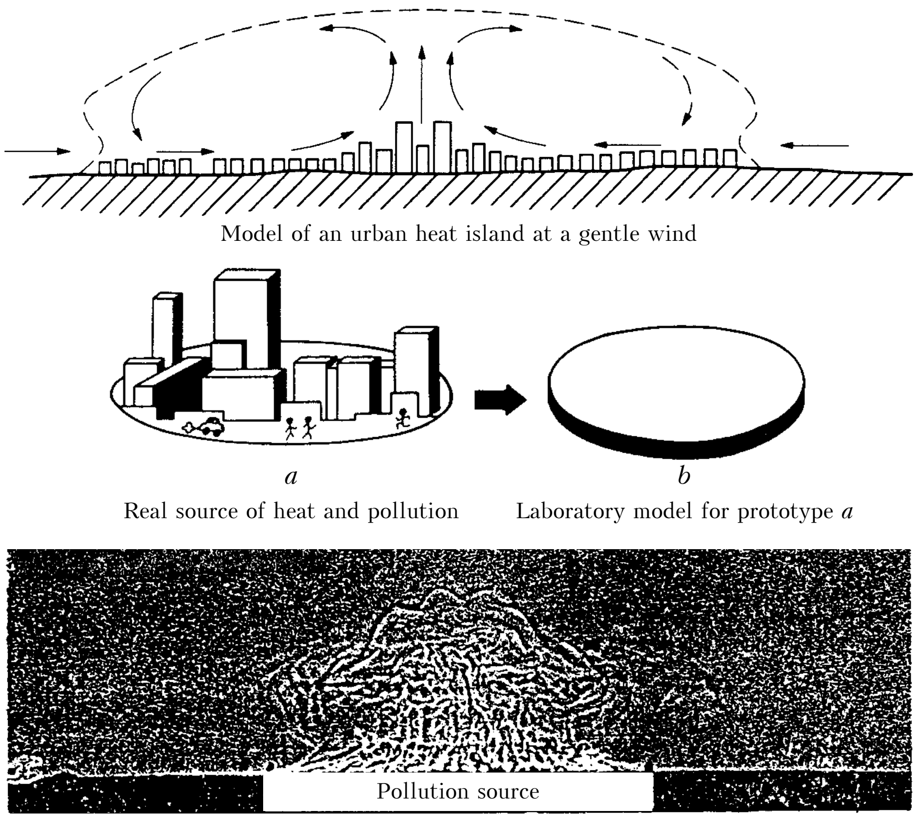
$$-D_\mu\,(\partial C/\partial z) = H_c, \tag{8}$$

where $D_\mu = \nu/\mathrm{Sc}$ is the molecular diffusion coefficient; ν is the kinematic viscosity coefficient; Sc is the molecular Schmidt number, and $H_c = Q/(0.5\, r/D)$. The parameter Q was specified from the condition that the Reynolds number $\mathrm{Re} = Q/\nu$ provides for pollution income from the source without initial momentum and, thus, it was limited by the velocity of the external flux to the source.

At the initial instant of time, the environment is at rest, and the initial fields of the concentration C and correlation $\langle c\theta \rangle$ are zero. At the lower boundary of the cylinder-shaped domain of integration, the conditions of impenetrability for concentration fluxes C (beyond the mass source) and covariance $\langle c\theta \rangle$ are set:

$$E = \langle \theta^2 \rangle = \frac{\partial \varepsilon}{\partial z} = \frac{\partial C}{\partial z} = \frac{\partial \langle c\theta \rangle}{\partial z} = 0\,. \tag{9}$$

The values of the kinetic energy of turbulence E, its dissipation rate ε, and the variance of temperature pulsations $\langle \theta^2 \rangle$ are specified at the first layer of the difference grid above the surface as in Refs. 4 and 6. The conditions of impenetrability (8) for fluxes are set at the top boundary (at $z = Z$). The symmetry conditions are imposed on the central line of the heat island (at $r = 0$). The same conditions are also used on the outer boundary of the domain of integration (at $r/D = 1.8$). Other boundary conditions for the velocity and temperature fields have the same form as in Ref. 5.



Developed turbulent plume over the heated disk *b*

Fig. 1.

The system of equations of diffusion model (1)–(7) was solved numerically with the use of the sweep method and semi-implicit scheme of direction variables (the second scheme with upstream differences[10] that keeps the second order of approximation at certain restrictions) on the biased difference grid. To keep the conservative and transportive properties of the difference scheme, the equations were written in the difference form in the near-boundary grid nodes with the second order and the use of the corresponding boundary conditions.

Results of simulation of passive pollutant dispersion from a superficial source over an urban heat island

The results of simulation of the turbulent circulation structure over the urban heat island (different turbulent values of the turbulent velocity and temperature fields) can be found in Refs. 5 and 9 and, therefore, are omitted here.

Simulation of passive pollution dispersion from an extended surface source over the urban heat island (Fig. 1) was largely aimed at revealing the role of the buoyancy effects on the distribution of average pollution concentration. It should be noted that since experimental measurements of the pollution dispersion from such source over the urban heat island in the considered critical meteorological period are absent, it is impossible to check directly the results of numerical realization of diffusion model (1)–(7). But we can judge the degree of their reliability from indirect indications.

First, a similar in essence model of an active pollutant (heat) transport gives[5,9] the results quite close to the data of direct instrumental measurements.[6]

Second, the accuracy of the numerical solution was checked on the consequently finer grids (25 × 116 nodes and 50 × 232 nodes along the horizontal and vertical, respectively). Therefore, the results presented below should be estimated keeping in mind these notes.

Figures 2 and 3 show the lines of equal concentration [Figs. 2 (I), 3 (I)] and the current streamlines of the circulation current over the urban heat island [Figs. 2 (II), 3(II)] obtained using model (1)–(7) (Fig. 2) and the simple Boussinesq eddy diffusion model for the vector of the turbulent flux of scalar $-\langle u_i c\rangle$ [only the first term in the right-hand side of Eq. (2) is held] (Fig. 3).

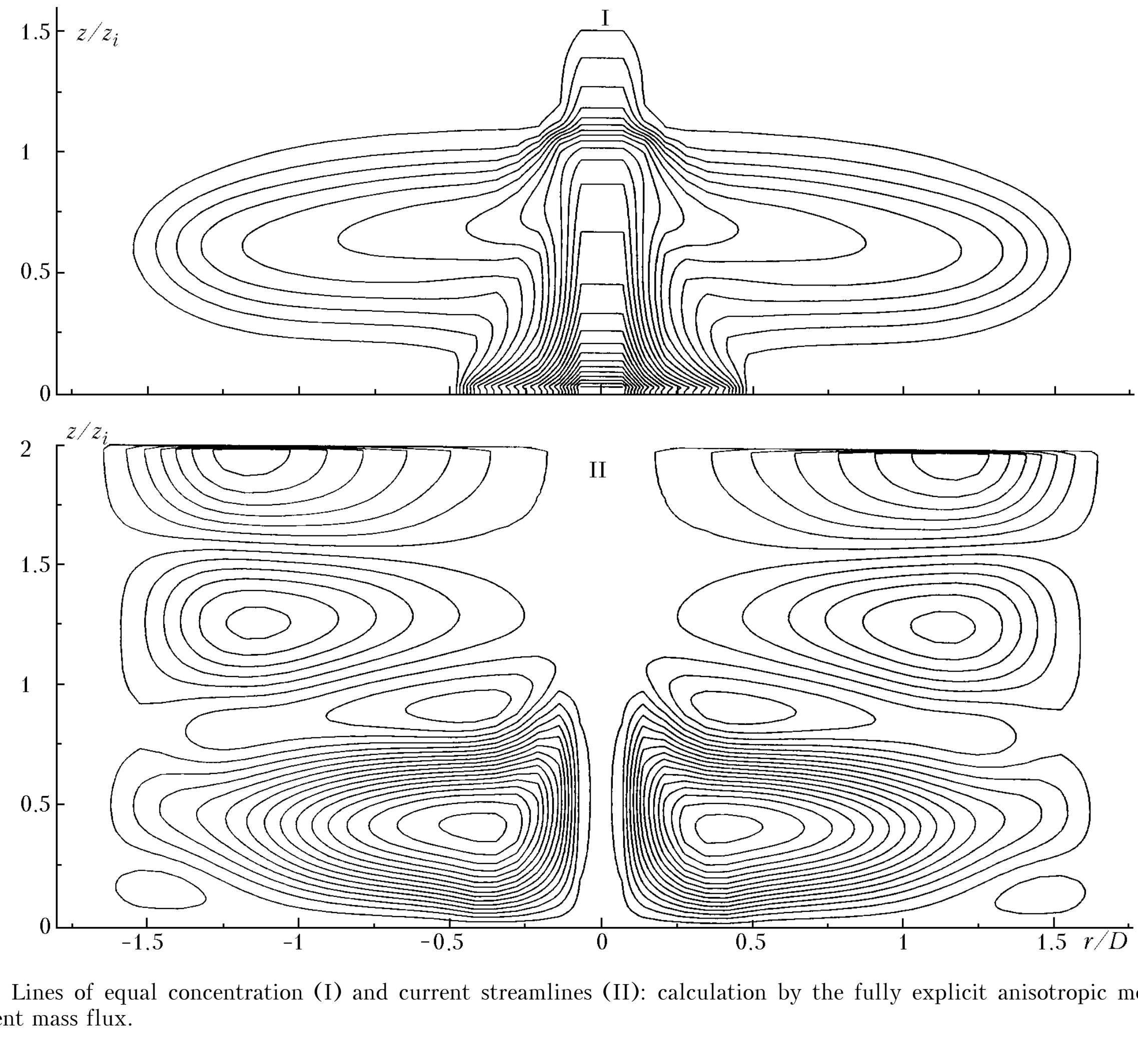


Fig. 2. Lines of equal concentration (I) and current streamlines (II): calculation by the fully explicit anisotropic model for turbulent mass flux.

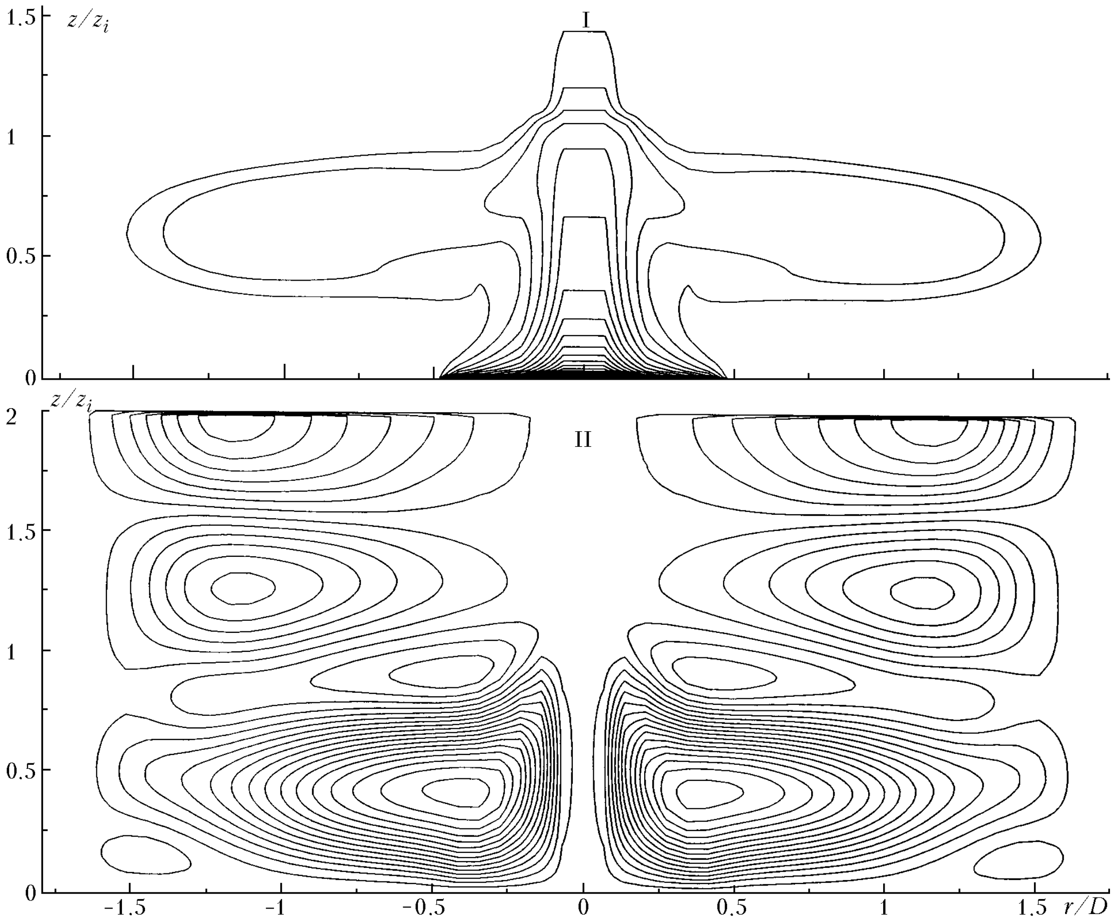


Fig. 3. Lines of equal concentration (I) and current streamlines (II): calculation by the simple Boussinesq model for turbulent mass flux.

Although this model is too rough for adequate allowance for the buoyancy effects on the turbulent transport of passive pollutants, its use could be justified by the fact that the basic three-parameter model of the turbulent transport of momentum and heat for the considered situation[5,7] gives the results on transport of the active pollutant (heat) that well agree with the data obtained in the controlled laboratory experiment.[6]

Figures 2 and 3 show that under the effect of the developing penetrative turbulent convection the pollution from a superficial source is transported by two concentrated eddy formations (in the bottom part of the both figures) upward and then dispersed in the horizontal direction. However, one can see differences in the distribution of the average concentration. The Boussinesq model ignoring the buoyancy effects gives slower pollutant diffusion in the vertical (and, consequently, horizontal) direction as compared to model of turbulent scalar flux (2) accounting for the buoyancy effect. In the latter case, the level of the concentration turns out to be higher both near the surface and all over the mixed layer. In the inversion layer (at $z/z_i \approx 1$), the normalized value of the concentration at the center of the heat island is almost twice as large as for the Boussinesq model.

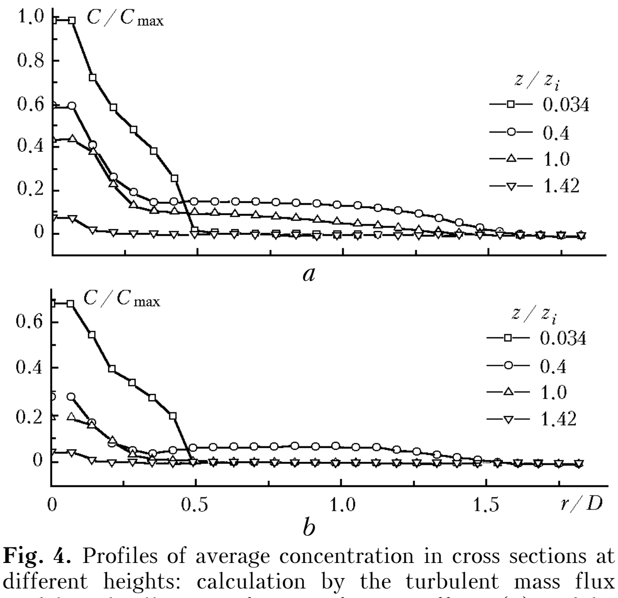


Fig. 4. Profiles of average concentration in cross sections at different heights: calculation by the turbulent mass flux model with allowance for stratification effects (*a*) and by the Boussinesq model ignoring stratification effects (*b*).

Figure 4 depicts the profiles of the normalized concentration along the radial coordinate in different cross sections above the heat island as calculated by model (2) (Fig. 4*a*) and the Boussinesq model (Fig. 4*b*). To be noted is one common feature consisting in the fact that the pollution plume "breaks through" the inversion layer ($z/z_i \approx 1$). This result was observed in recent laboratory experiments on dispersion of passive pollution from continuous and instantaneous sources in the convective boundary layer.[11]

Acknowledgments

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