NUMERICAL SIMULATION OF THE STRUCTURE OF AEROSOL CAPS OVER INDUSTRIAL CENTERS

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Modeling the dispersal of atmospheric aerosol over an industrial center is performed based on the system of equations for dynamics of the atmospheric boundary layer including the equations for the wind velocity components, temperature, humidity, and balance equation for the energy fluxes on the underlying surface. Cities are sources of aerosol pollution of the atmosphere. They can be characterized by a strong thermal inhomogeneity what leads to formation of the specifically urban caps of air pollutants. We discuss some specific features revealed to occur in the aerosol concentration diurnal behavior under different meteorological conditions.

INTRODUCTION

Experimental data[1] and observations show the presence of caps of air pollution over industrial centers where the emissions from plants, motor vehicles, and from other anthropogenic pollution sources do concentrate.

So the pollution level of urban atmospheres becomes higher and, undoubtedly, is hazardous for people living in the city. This effect occurs due to a significant thermal inhomogeneity of the urban areas as compared with those not involved in the process of intensive industrial development and unpopulated ones.

In this paper we discuss the regularities in the aerosol caps diurnal behavior based on mathematical simulation of the admixture diffusion in air over an idealized industrial center in summer.

The city is represented as a square of 100 km^2 area placed at the center of a square calculation domain with the side of 36 km. The vertical coordinate z was limited by the height of the boundary atmospheric layer equal to 1.5 km. Characteristics of the underlying surface out of the city were taken to be typical for a forest-steppe. In this paper, the city differs from the surrounding surface in reflection, roughness, and in thermal properties of soil that were taken from Refs. 7 and 8.

The model that is used in this paper is developed in the Computer Center of the Siberian Branch of the Russian Academy of Sciences.[2,3] Then it has been adapted for the urban conditions at the State Scientific Center «Vektor». The model is based on the nonlinear nonstationary system of equations for the quasi-static boundary layer of the atmosphere as the Boussinesq approximation. To describe the admixture dispersal, the semi-empirical equation of turbulent diffusion was used. After splitting the physical processes and directions, the equations were solved by finite difference method with economical semiimplicit schemes of the second order of Crank–Nicolson type approximation.[3,4] The number of grid points was 19 along the horizontal and 15 along the vertical.

According to Ref. 5, the main sources of atmospheric pollution can be classified into two groups: the surface (motor transport, boiler, chimneys) and high-altitude (big plants, heat and electric power stations). The sources of the first type are situated near the underlying surface (motor transport) or in the 50-m surface layer. The stacks' height of the second group is 100–200 m and higher. For these sources, the temperature of the emitted pollutants is always higher as compared with that in the ambient medium. This circumstance was taken into account by introducing the parameter of the efficient height of the emission sources.[6] It varies from several tens to several hundreds of meters. Motor transport exhaust and other surface sources were modeled by assuming a pollutant flow on the underlying surface within the urban area.

The calculations simulated diurnal variations of wind velocity, temperature, humidity, and turbulence characteristics that are typical for June in the West Siberian region under calm conditions and wind blowing to the city with the speed of 2 m/s at height of 10 m. Then the corresponding concentration fields of aerosol pollutants were determined for particles with the diameter of 10 μm from different sources.

PLANAR SOURCE, CALM CONDITIONS

Figure 1 (a, b) presents the concentration isolines and schematic presentation of the vector field of wind in the vertical plane that is parallel to the x axis and while passing through the center of the calculation domain. The data correspond to night- and day-time conditions at time t = 5 a.m. and 3 p.m. The concentration is in conventional units. Figure 2

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presents vertical profiles of the aerosol concentration in the air over the downtown area of the city (curves *1*), at different time moments; over the outskirts (curves *2*), and in the suburbs at a distance of 4 km from the city (curves *3*). The profiles of concentration are normalized to the corresponding maximum value presented next to the curves. To avoid superposition of the curves, the plots with the number *2* are shifted by unity, and those with the number *3* by two.

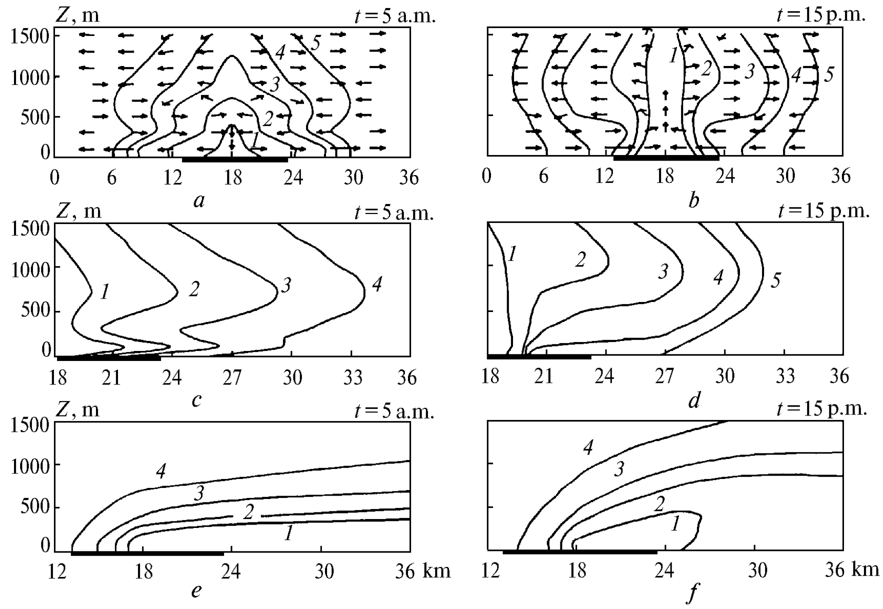

FIG. 1. Schematic representation of the vector field of wind and isolines of pollutant concentration over the city at night and in the afternoon for a planar source and calm weather conditions (a, b); for a point elevated source and calm conditions (c, d); for a point elevated source in the presence of wind (e, f). Isolines 1–5 correspond to concentrations of 3000, 380, 76, 30, *and* 7 *units (a); figures 1–5 correspond to concentrations of* 67, 42, 17, 8.4, *and* 1.7 *units (b); figures 1–4 correspond to pollutant concentrations* $2.2\cdot10^{-3}$, $4.5\cdot10^{-4}$, $9\cdot10^{-5}$, *and* $9\cdot10^{-6}$ *units (c); figures 1–5 correspond to concentrations* $1.5\cdot10^{-3}$, $3.8\cdot10^{-4}$, $1.9\cdot10^{-4}$, $7.5\cdot10^{-5}$, *and* $3.8\cdot10^{-5}$ *units (d); figures 1–4 correspond to concentrations* 10^{-5}, 10^{-6}, 10^{-8}, *and* 10^{-11} *units (e); figures 1–4 correspond to concentrations* 10^{-4}, 10^{-5}, 10^{-6}, *and* 10^{-8} *units (f).*

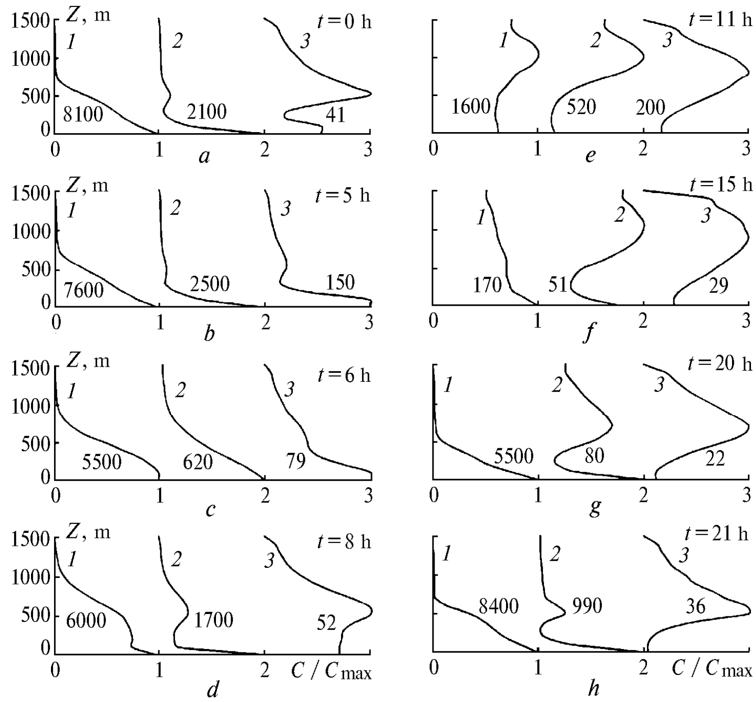

FIG. 2. Vertical profiles of pollutant concentration over the center of the city, its outskirts, and suburbs at different time for a planar source and calm conditions, curves 1, 2, and 3, respectively.

The difference in temperature of the underlying surface between the city and suburbs forms a typical, for a heat island circulation in the boundary layer. In the day-time, in the lower part of the boundary layer over the city, the horizontal air convergence with upgoing vertical flows is observed. In the upper part of the boundary layer, one can observe horizontal air divergence that spreads to the periphery and sinks in the suburbs (see Fig. 1*b*).

At night, the things are happening the opposite way (see Fig. 1*a*). Such an air circulation forms a characteristic field of pollutant concentration as aerosol caps.

In day-time hours, except for $t = 9–11$ h, concentration maximum over the city center is always near the surface (curves *1*). The maximum value of concentration is observed at 9 p.m. and equals $8.4\cdot10^3$ conventional units, then it decreases to $5.5\cdot10^3$ at $t = 6$ p.m. Starting from this moment, with heating of the city surface and increase of vertical turbulent exchange, the aerosol is transported into the upper part of the boundary layer and the concentration profile is smoothed. At the same time, the divergence grows in the upper part of the boundary layer that leads to an increase in the horizontal transfer of pollutants from the center and toward suburbs down to $1.77\cdot10^2$ conventional units at 3:00 p.m. In the evening and at night, the concentration maximum increases and moves into the surface layer due to a decrease in the vertical turbulent exchange and change of the circulation type. Over the suburbs (curves *2*), the maximum concentration is always, except for $t = 9$:00 a.m. to 3:00 p.m. is near the underlying surface. During the day-time (from 9 a.m. and until 8 p.m.) one can observe an unusual *S*-shaped concentration profile with two maxima (Figs. 2, *e–g*). The maximum value of concentration near the surface is obviously explained by the presence of a planar source in this part of the city. As a result of the convergence in the lower part of the boundary layer, clear air of the suburbs spreads to the center and brings there the admixtures from the underlying surface. This, in particular, leads to a local minimum in the concentration in the city outskirts at a height of 300 m (see Fig. 2*f*). In the upper part of the boundary layer, the admixture spreads from the center of the area to its periphery. This leads to accumulation of the pollutants and to the second maximum at a height of 900 m. During the night hours, when horizontal divergence is observed in the lower part of the boundary layer, pollutants are transported from the center of the city to the suburbs. In this time, pollutant concentration in the suburbs is about 50 fold as high as that at day-time (Figs. 2*b*, *f*).

Over the suburbs (curves *3*) the maximum concentration value equals to $1.5\cdot10^2$ units is near surface as observed at 5:00 a.m. In the afternoon and at hours nearer to the evening, the maximum moves to a height of 700–900 m and decreases down to 22 conventional units by 8:00 p.m. Here, as in the suburbs, one can observe an *S*-shaped profile with two maxima, but only at night 0–3 a.m. (Fig. 2*a*).

The Table I presents the ratios of the maximum concentration values over the city to the values near the underlying surface. One can see that the aerosol cap is observed in the suburbs since 7 and until 24 h. In this cap, the concentration can sometimes exceed the surface ones by 2 to 8 times, for instance, at 10:00 p.m., by 40 times. In the outskirts of the city, it is observed at 9–15 h. Over the central part of the city, the aerosol cap occurs only at 10–11 h.

TABLE I.

Time, h	Suburbs	Outskirts	Center
0	1.8	*	*
1	*	*	*
7	1.7	2.2	*
8	1.4	*	*
10	6.7	7.1	1.3
11	5.7	6.0	1.6
12	6.0	2.0	*
14	4.0	1.5	*
15	3.5	1.3	*
16	3.0	*	*
18	2.1	*	*
19	4.9	*	*
20	8.5	*	*
21	27.7	*	*
22	40.8	*	*
23	5.6	*	*

*The maximum value is near the underlying surface.

In the below example the planar source is on at 6 a.m. and off at 8 p.m., i.e., the automobile transport exhaust was absent in the evening and night hours. Day-time concentration profiles in fact do not vary as compared with a constant source. Significant difference is observed in night-time profiles (Figs. 2*a*, *b*; 3*a*, *b*). After switching-off of the source at 8 p.m., the pollutant concentration in the center of the city near the underlying surface decreases approximately by two times as compared with a permanently acting source. In the suburbs, much like in the previous case, the concentration near the underlying surface grows, although much slower, and it is equal to $2.6\cdot10^2$ units by 5 a.m. what is about 10 times less than at the same time in the case considered above. In the suburbs, the surface concentration also grows and reaches 26 units by 5 a.m. what is by 6 times lower as compared with the previous case. The maximum concentration is observed at the height of 600 m and equals 31 units. From midnight and until 5 a.m., the *S*-shaped profile is observed both in the city outskirts and suburbs.

PLANAR SOURCE IN THE PRESENCE OF WIND

Let us consider the influence of the wind blowing toward the city on the structure of the concentration field over the city. In these calculations, the wind was directed along the x axis with speed of 2 m/s at the height of 10 m. Concentration almost reaches its maximum value by 7 a.m. (Fig. 3*d*). The pollutant is localized over the city near the underlying surface. The values of concentration in the center of the city, in the outskirts, and in the suburbs are 24, 31, and 11 units, respectively. With heating of the surface and increasing turbulent exchange, the extension of the aerosol plume increases and grows with the increasing distance from the city. However, the maximum values are still near the underlying surface. They decrease a little bit but then begin to increase by the evening. The maximum is observed at 8 p.m. and it equals 33, 52, and 22 units in the center of the city, in the outskirts, and in the suburbs, respectively.

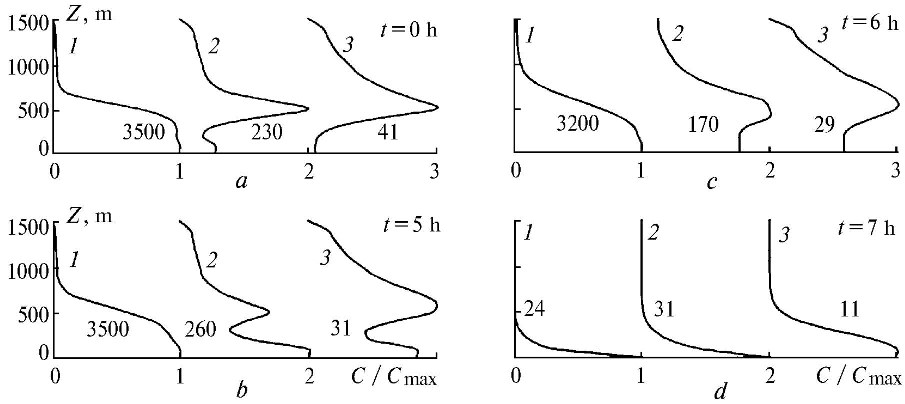

FIG. 3. Ditto as in Fig. 2 but for a planar source active from 6 a.m. *to* 8 p.m. *under calm conditions (a–c) and wind blowing to the city (d).*

The planar source is off at 8 p.m. (termination of the work of the motor transport). Already in an hour, pollutant concentration decreases by a factor of 10^9 in the center of the city, 10^5 in the outskirts, and by 50 times in the suburbs. In the suburbs, it is greater approximately by a factor of 10^3 as compared with the outskirts, and by a factor of 10^7 as compared with the center. By about 10 p.m., the concentration still decreases everywhere by a factor of 10^7 to 10^8.

Thus the planar source of pollutants which is in the surface layer of the city creates a stable aerosol cap at a height of 700–900 m only in the city outskirts since 7 a.m. and until 12 p.m. Within the cap, concentration can be higher by 2 to 8 times (in some moments, up to 40 times) as compared with the concentration near the surface. Over the city outskirts, the aerosol cap is observed since 10 a.m. and until 3 p.m. and it is not observed over the central part of the city. The outer wind, even of a low speed of 2 m/s at a height of 10 m, destroys the cap and completely purifies the city atmosphere during an hour after termination of the motor transport work.

POINT ELEVATED SOURCE

The influence of an elevated point source was considered in the next series of calculations. For this purpose, a permanently acting point source of particles is placed in the center of the city at the effective height of 100 m. Figures 1*c* and *d* present the concentration isolines for t = 5 a.m. and 3 p.m. under calm weather conditions. Figures 4*a–f* show the vertical concentration profiles over the center of the city (curves *1*), over the city outskirts (curves *2*), and over the suburbs at a distance of 4 km from the city (curves *3*) at t = 0, 6, 10, 12, 14, and 19 h. Over the center of the city, the maximum value of concentration equal to $2.4\cdot10^{-2}$ units is observed in night-time and morning hours at the source's height. By t = 10 h the maximum reduces to $7.4\cdot10^{-3}$ units and shifts up to a height of 900 m. At the same time, the vertical concentration profile smoothens. Then, the maximum value becomes lower and reaches the minimum of $3.4\cdot10^{-3}$ units by the moment t = 14 h. By the evening, the concentration maximum shifts back to the height of 100 m, increases in the magnitude, and becomes equal to $2.4\cdot10^{-2}$ units by the moment t = 0 h; then it remains unchanged until t = 5 a.m.

In the outskirts and in the suburbs the zone with the maximum concentration value is at a height of 700 m at night and at 1000 m in the afternoon. Minimal values of the concentration maximum are observed in the afternoon and at the level of $5.2\cdot10^{-4}$ and $2.6\cdot10^{-4}$ units, respectively. By the evening, they increase and reach $1.1\cdot10^{-3}$ and $3.8\cdot10^{-4}$ units at t = 23 h; then they remain constant until t = 6 h.

Calculations with five sources placed in the center of the square and in the centers of the sides do not change the qualitative picture of the concentration distribution over the city and in the suburbs (Figs. 4*g*, *h*). In the outskirts the concentration profiles become similar to those in the center of the city.

In the case when a point source is over the center of the city at a height of 400 m, the maximum of concentration in the center of the area ($2.2\cdot10^{-2}$ units) is observed at night time and found at the source's height (Fig. 4*i*). In the afternoon, the maximum decreases to $8.8{\cdot}10^{-4}$ units at t = 13 h (Fig. 4*j*), and by the evening it increases to $1.9{\cdot}10^{-2}$ units at t = 19 h and to $2.2{\cdot}10^{-2}$ units at t = 0 h. In the outskirts of the city and in the suburbs the concentration maxima are the same as in the case of a source at a height of 100 m and lie at a height of 700 m at night and 1000 m in the afternoon. At t = 10 h they are equal to $1.1{\cdot}10^{-3}$ and $3.2{\cdot}10^{-4}$ units, respectively. It is approximately 3 times higher than at night. Further, they decrease and reach the minimal values of $1.8{\cdot}10^{-4}$ and $1.0{\cdot}10^{-4}$ at t = 16–18 h and then slowly increase to $4.5{\cdot}10^{-4}$ and $1.2{\cdot}10^{-4}$ at t = 21 h. For this variant, in the afternoon, concentration values are approximately 3.7 lower in the center, 2.7 times in the outskirts, and 2.3 times in the suburbs as compared with the case of a single source at a height of 100 m. At night, these ratios are 1.1, 2.8, and 3.0 for the center, the outskirts, and the suburbs, respectively. The decrease in maximum concentration at the increasing height of a source is caused by the extension of the area with a more intense convective and turbulent transfer of pollutants.

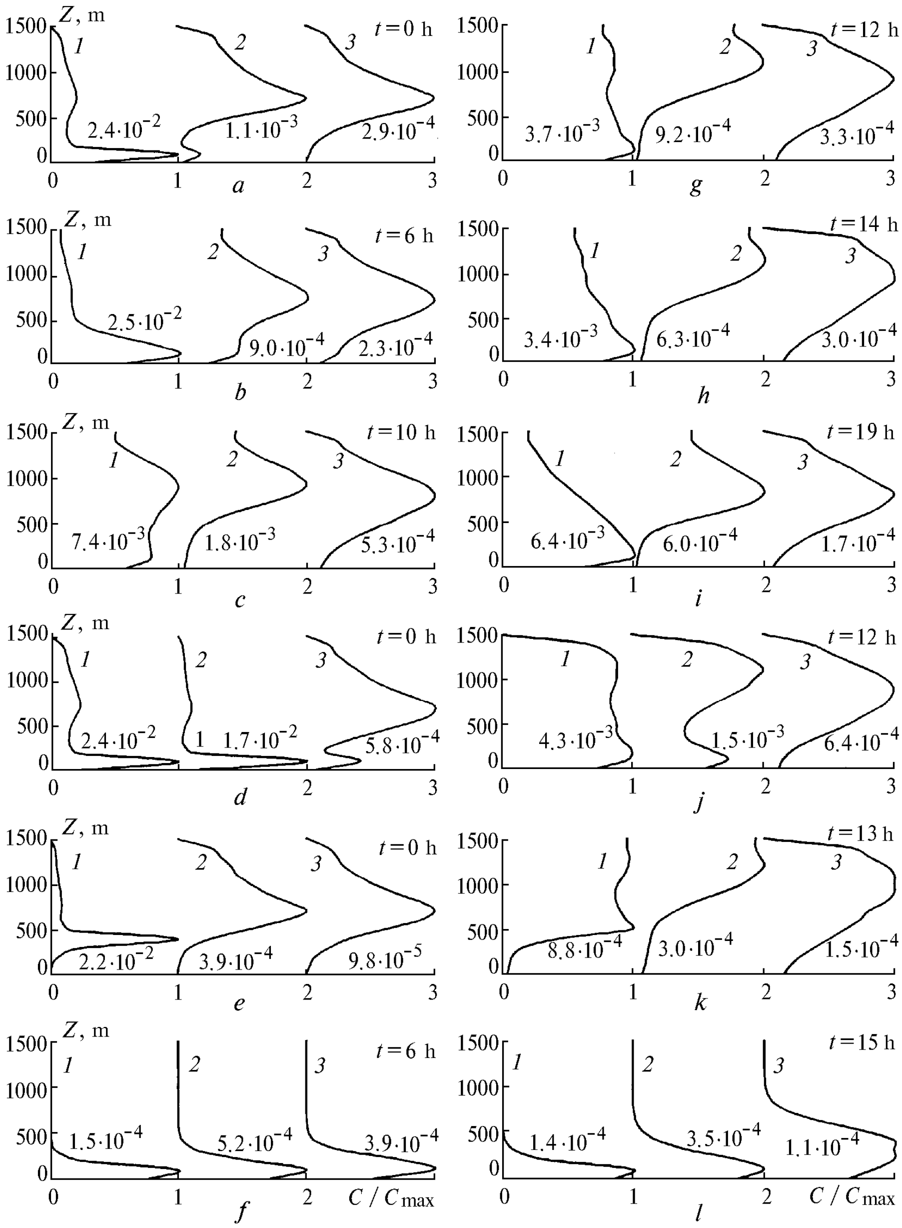

FIG. 4. Ditto as in Fig. 2 but for a point source at a height of 100 m *(a–f), for 5 point sources (g, h), for a point source at a height of* 400 m *(i, j), and for a point source at a height of* 100 m *in the presence of wind blowing to the city (k, l).*

An increase of the number of elevated sources up to five does not qualitatively change the picture of concentration fields over the city and the suburbs. In the outskirts, concentration profiles become similar to those at the center of the city.

ELEVATED POINT SOURCE IN THE PRESENCE OF WIND

Let us consider the influence of wind blowing to the city on the structure of the concentration field for the case of a single source placed at a height of 100 m. Figures 1*e* and *f* present the concentration isolines. The vertical profiles of concentration are presented in Figs. 4*k* and *l*. In the center of the area and in the outskirts of the city, the maximum concentration values are at the source's height during all the days and equal, respectively, to $1.4\cdot10^{-4}$ and $3.5\cdot10^{-4}$ units in the afternoon (t = 12–15 h), and $1.5\cdot10^{-4}$ and $5.2\cdot10^{-4}$ units at night (t = 0–6 h). This means that the areas of maximum values shift along the air flow to the outskirts of the city. In the suburbs, the maximum value is at the height of the source at night time and equals $5.9\cdot10^{-4}$ units at t = 0–4 h. In the afternoon, the maximum value of concentration takes place at 200–300 m and varies from $1.2\cdot10^{-4}$ units at t = 12 h to $4.2\cdot10^{-4}$ units at t = 21 h.

When a point source is at a height of 400 m, in the center of the area and in the city outskirt the maximum values of concentration are at the source's height during all the days and equal, respectively, $5.2\cdot10^{-5}$ and $1.4\cdot10^{-4}$ units in the afternoon during t = 12–15 h, and $8.8\cdot10^{-6}$ and $3.7\cdot10^{-4}$ units at night during t = 0–4 h.

Thus, the maximum values shift along the air flow to the city outskirts. In the suburbs, at night, the maximum value is at the source's height and equals $1.7\cdot10^{-4}$ units during t = 22–4 h. In the afternoon, the maximum value is at a height of 500–600 m and varies from $5.9\cdot10^{-5}$ at t = 12 h to $1.2\cdot10^{-4}$ at t = 21 h. Then the maximum descends to the source's height and increases to $1.7\cdot10^{-4}$ units by the moment t = 22 h.

Qualitative conclusions about the position of the concentration maximum from a single source completely remains valid in the case when five point sources are spread over the city in the center of the area and in the outskirts. In the center and outskirts, the area of maximum concentration values lies at the height of the sources, and in the suburbs in the afternoon it shifts to the height exceeding that of the sources by 100–200 m. At night, the area of maximum values lies at the height of the sources.

Thus, under calm weather conditions, a single point source placed over the central part of the city creates an aerosol cap over the center of the city at the efficient height of the source regardless of time; in the outskirts and suburbs, the cap is created at a height of about 700 m at night and 1000 m in the afternoon. Several pointlike sources create an aerosol «cap» over the city at a certain efficient height. In the suburbs, this height equals 700 m at night and 1000 m in the afternoon. In presence of wind, aerosol cap occurs over the city at the height of the sources during the whole day. At night in the suburbs, it is also observed at the height of the sources, and in the afternoon it ascends to 700 m when moving from the city.

CONCLUSIONS

Comparison of the obtained theoretical results with the data of airborne sounding of atmospheric aerosol over the cities of Russia and Kazakhstan[1] permits one to arrive at a conclusion about a satisfactory (taking into account the simplifying assumptions included in the calculations) coincidence of the main regularities in the formation of aerosol caps. The regularities refer to maximum concentration values normalized by their surface values, position of the aerosol caps, their size and spatial structure. Simulating the processes of aerosol dispersal over real industrial centers containing different sources at different heights, should result in a more complicated dependence of the concentration field and the structure of the aerosol cap on the power, type, and position of the sources. However, it seems so that qualitatively the regularities concerning the height of the aerosol cap, time of its appearance, its lifetime, and spatial structure will not change significantly.

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