Numerical study of climate formation and atmospheric pollution in industrial regions*

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A numerical model for mesoclimate and atmospheric pollution in industrial region is presented. Both anthropogenic and natural factors are included. One of the case studies is discussed.

1. Introduction

The necessary investigations of the climatic changes as well as the need to estimate an ecological future of the industrial regions lead to the construction of mathematical models that describe the corresponding processes [1, 2]. The spreading of the pollutants in the atmosphere of a big city or, in general. of an industrial region, goes on the background of the atmospheric circulation arising under the joint influence of the natural and man-caused factors. The formation of the air masses circulation is realized by the interaction between of the large scale atmospheric motion and the local inhomogeneities of the underlying surface. These inhomogeneities can be the results of the influence of the temperature contrasts between environment and a warmer urban region, reservoirs and land, and also between the different kinds of the underlying surface. For the modeling of the processes of such scales it is necessary to take into account the man-caused factors as artificial heat, moisture and pollutants sources, and the large scale changes of the land surface. The corresponding parameterizations are induced in the model for the description of the underlying surface influence. It needs more exact presentation of the atmospheric motion in the boundary layer. To describe the inhomogeneities of the surface itself the land use categories are introduced. The specific estimations of the land surface parameters for each land use category are given both in their natural form and in the anthropogenic changed form.

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2. Governing system of equations

The numerical model is based on the system of equations of hydrodynamics and transport of pollutants in the atmosphere. Let us consider the system of equations which describes the atmospheric hydrodynamics over inhomogeneous surface in hydrostatic approximation. For the convenient relief description the vertical coordinate is used which follows the relief,

$$\sigma = (p - p_T)/\pi_s, \qquad \pi_s \equiv p_s - p_T, \tag{1}$$

here p is pressure, p_T and p_s are the pressures at the upper air boundary and at the land surface. The coordinates x and y are directed to the East and the North accordingly.

The basic equations of the model are [2, 3]:

the equations of motion

$$\frac{\partial \pi_s u}{\partial t} + \tilde{\mathcal{L}}(\pi_s u) - l \pi_s v = -\pi_s \left[\frac{\partial H}{\partial x} + \frac{\sigma RT}{\Phi} \frac{\partial \pi_s}{\partial x} \right], \tag{2}$$

$$\frac{\partial \pi_s v}{\partial t} + \tilde{\mathcal{L}}(\pi_s v) + l \pi_s u = -\pi_s \left[\frac{\partial H}{\partial v} + \frac{\sigma RT}{\Phi} \frac{\partial \pi_s}{\partial v} \right], \tag{3}$$

where $\Phi \equiv \sigma \pi_s + p_T$;

• the continuity equation

$$\frac{\partial \pi_s}{\partial t} + \mathcal{L}(\pi_s) = 0. \tag{4}$$

Here

$$\mathcal{L}(\pi_s \varphi) = \frac{\partial \pi_s \varphi u}{\partial x} + \frac{\partial \pi_s \varphi v}{\partial y} + \frac{\partial \pi_s \dot{\sigma} \varphi}{\partial \sigma}$$
 (5)

is the transport operator in σ -system of coordinates in the divergent form;

$$\tilde{\mathcal{L}}(\pi_s \varphi) = \mathcal{L}(\pi_s \varphi) + F_{\varphi}^H + F_{\varphi}^B, \tag{6}$$

where F_{φ}^{H} , F_{φ}^{B} are the operators of the turbulent exchange of a substance φ in the horizontal and vertical directions; $\vec{u}=(u,v,\dot{\sigma})$ is the wind velocity vector, $u,v,\dot{\sigma}$ are the components of the velocity vector in the directions of x,y,σ respectively, $\dot{\sigma}\equiv\frac{d\sigma}{dt}$. The equation for the pressure tendency $\pi_{s}\equiv p_{s}-p_{T}$ is

$$\frac{\partial \pi_s}{\partial t} + \int_0^1 \left[\frac{\partial \pi_s u}{\partial x} + \frac{\partial \pi_s v}{\partial y} \right] d\sigma = 0.$$
 (7)

The last equation was derived by vertical integration of the continuity equation (4) under conditions $\dot{\sigma} = 0$ at $\sigma = 0$ $(p = p_T)$ and $\sigma = 1$ $(p = p_s)$.

The equation for the vertical component in σ -coordinates is

$$\dot{\sigma} = -\frac{1}{\pi_s} \int_0^{\sigma} \left[\frac{\partial \pi_s}{\partial t} + \frac{\partial \pi_s u}{\partial x} + \frac{\partial \pi_s v}{\partial y} \right] d\sigma. \tag{8}$$

The expression $\frac{\partial \pi_s}{\partial t}$ is excluded with the help of (7).

The equation for the heat income is

$$\frac{\partial \pi_s T}{\partial t} + \tilde{\mathcal{L}}(\pi_s T) - \frac{RT\tau}{c_p(\sigma + p_T/\pi_s)} = \frac{\pi_s Q}{c_p},\tag{9}$$

$$\tau = \frac{dp}{dt}, \qquad \tau = \pi_s \dot{\sigma} + \sigma \frac{d\pi_s}{dt}, \qquad \frac{d\pi_s}{dt} = \frac{\partial \pi_s}{\partial t} + u \frac{\partial \pi_s}{\partial x} + v \frac{\partial \pi_s}{\partial y}, \quad (10)$$

where T is temperature, c_p is a specific heat at a constant pressure, Q is a heat source term.

The hydrostatic equation has the form

$$\frac{\partial H}{\partial \sigma} = -\frac{\pi_s R}{\Phi} T. \tag{11}$$

The equation of the transport of pollution is

$$\frac{\partial \varphi}{\partial t} + \tilde{\mathcal{L}}(\varphi) = f,\tag{12}$$

where f is the function describing the sources of pollution, φ is the concentration of the pollutant. In general, pollutants are multi-component mixture. The number of components is prescribed as an initial parameter of the model.

The rates of the gravitational settling are taken into account by adding the corresponding values to the vertical component of the velocity vector.

To close the mathematical model it is necessary to give the boundary and initial conditions. The conditions at the low boundary are given with the help of parameterized models of the surface layer and surface boundary layer. The conditions of the approach to the values of the background processes are given at the upper and side boundaries [2].

The discrete approximations are based on the variational principle in the combination with the splitting technique [3]. Following the ideas of splitting according to the physical processes [4], let us divide the problem into two stages:

- 1) transport + diffusion,
- 2) dynamical adjustment of meteo-fields.

In the first stage the monotonic numerical schemes [5-7] are used for the approximation of the advective-diffusive operators of the type (6).

The practical experience in application of splitting methods for the solution to the problems of geophysical hydrodynamics shows that the subproblem of the dynamical adjustment of the fields is the most difficult and laborious stage of the splitting scheme in its realization. The correlation of the space-time scales of the processes under consideration is such that it is necessary to use implicit or explicit-implicit schemes for the correct simulation. It is due to the fact that the operator that adjusts the pressure gradients and wind field (without turbulent exchange) is anti-symmetric. That is why the two-layer explicit schemes are unstable in time for the problems with anti-symmetric operator.

3. The algorithm for the solution to the problem of dynamic adjustment of the fields

If the conditions of approximation are valid the proposed algorithm allows us to provide the energy balance and, as a consequence, the stability of calculations being independent on the temperature stratification of the atmosphere [8]. Let us consider the problem of the dynamic adjustment of the meteo-fields

$$\frac{\partial u}{\partial t} - lv = -\frac{\partial H}{\partial x} + \frac{1}{\pi_c} \frac{\partial H}{\partial \sigma} \frac{\partial \Phi}{\partial x},\tag{13}$$

$$\frac{\partial v}{\partial t} + lu = -\frac{\partial H}{\partial u} + \frac{1}{\pi_{\bullet}} \frac{\partial H}{\partial \sigma} \frac{\partial \Phi}{\partial u},\tag{14}$$

$$\frac{1}{\pi_s} \frac{\partial H}{\partial \sigma} + \frac{RT}{\Phi} = 0,\tag{15}$$

$$\frac{\partial \pi_s}{\partial t} + \frac{\partial \pi_s u}{\partial x} + \frac{\partial \pi_s v}{\partial y} + \frac{\partial \pi_s \omega}{\partial \sigma} = 0, \tag{16}$$

$$\frac{\partial T}{\partial t} - \frac{RT}{\Phi c_p} \tau = \frac{\varepsilon}{c_p},\tag{17}$$

$$\tau = \pi_s \omega + \sigma \frac{d\pi_s}{dt} + \frac{dp_T}{dt} = \pi_s \omega + \sigma \frac{\partial \pi_s}{\partial t} + \left(u \frac{\partial \Phi}{\partial x} + v \frac{\partial \Phi}{\partial y} \right). \tag{18}$$

In the frames of the splitting method the system (13)–(18) is considered within the time interval $[t_j, t_{i+1}]$. The notation $\omega \equiv \dot{\sigma}$ is made for the convenience. The form of the equation is chosen in such a way that it would be possible to construct the discrete analogs of the direct and adjoint problems simultaneously. The solution to the adjoint problem is necessary for the investigation of the sensitivity of the model to the variations of the

input parameters and for the solution to the optimal control problems. The algorithms of the adjoint problem realization could be simplified if the time derivation is not applied to the product of the unknown functions. The scheme of the direct problem realization is the same even in the case when equations (13), (14), (17) are obtained directly by the splitting of (2), (3), (9) and they have the time derivatives of the products of the functions $\pi_s u$, $\pi_s v$, $\pi_s T$.

It is supposed that the functions

$$u^j$$
, v^j , ω^j , T^j , π^j , H^j .

are given at the time moment $t = t_j$.

The continuity equation (16) is nonlinear with respect to the unknown functions \vec{u} and π_s . In order not to use iterations and to provide sufficient accuracy of the solutions let us linearize this equation within the time interval $[t_j, t_{j+1}]$ in the following way:

$$\frac{\partial \pi_s}{\partial t} + \frac{1}{2}\operatorname{div} \pi_s \vec{u}^{j+1} + \frac{1}{2}\operatorname{div} \vec{u}\pi_s^{j+1}. \tag{16a}$$

Here the index (j+1) in the expression div $\vec{u}\pi_s$ denotes the unknown functions. The functions without indices are given.

Further we shall use the splitting method in accordance with the scheme "transport-adjustment". In the stage of the fields adjustment we shall use the equation

$$\frac{\partial \pi_s}{\partial t} + \frac{1}{2} \operatorname{div} \pi_s^j \vec{u}^{j+1} = 0 \tag{16b}$$

with the prescribed π_s^j instead of (16). The following equation

$$\frac{\partial \pi_s}{\partial t} + \frac{1}{2} \operatorname{div} \vec{u}^{j+1} \pi_s^{j+1} = 0, \tag{16c}$$

will be solved in the transport step. Here \vec{u}^{j+1} is the velocity calculated in the adjustment stage.

If problem (13)-(18) is considered as one of the splitting steps, the boundary conditions for it are the consequences of the general statement of the problem and the structure of the splitting schemes.

Usually, for the limited area problems the conditions are accepted which conjugate the modeling processes with the large scale movement. The large scale fields are proposed to be given. These conditions can be realized with the help of the state function derivatives or with the use of the deviations of the components from their background values.

Now let us consider numerical realization of the model. We shall use the method of the numerical model construction based on variational principle in the combination with the splitting technique [3, 8]. In this case, following

[8], let us correspond the system (13)-(18) with the integral identity, which arises from the energy balance. Then the integral identity will be used for the construction of the discrete approximations and numerical algorithms. For this goal equations (13)-(17) are scalar multiplied by the components of the vector $\vec{\varphi}^* = (u^*, v^*, \tau^*, H^*, T^*c_p)$ respectively and integrated in the region D_t . Here u^* , v^* , H^* , T^* are arbitrary, sufficiently smooth functions and

$$\tau^* = \pi_s \omega^* + \sigma \left(\frac{\partial \pi_s^*}{\partial t} + u^* \frac{\partial \pi_s^*}{\partial x} + u^* \frac{\partial \pi_s^*}{\partial y} \right). \tag{19}$$

As a result we can obtain

$$\begin{split} I\left(\vec{\varphi},\vec{\varphi}^{*}\right) &\equiv \int_{D_{t}} \left\{ \left(\frac{\partial u}{\partial t} - lv + \frac{\partial H}{\partial x} - \frac{1}{\pi_{s}} \frac{\partial H}{\partial \sigma} \frac{\partial \Phi}{\partial x} \right) u^{*} + \right. \\ &\left. \left(\frac{\partial v}{\partial t} + lu + \frac{\partial H}{\partial y} - \frac{1}{\pi_{s}} \frac{\partial H}{\partial \sigma} \frac{\partial \Phi}{\partial y} \right) v^{*} + \right. \\ &\left. \left(\frac{1}{\pi_{s}} \frac{\partial H}{\partial \sigma} + \frac{RT}{\Phi} \right) \left[\pi_{s} \omega^{*} + \sigma \left(\frac{\partial \pi_{s}^{*}}{\partial t} + u^{*} \frac{\partial \pi_{s}^{*}}{\partial x} + v^{*} \frac{\partial \pi_{s}^{*}}{\partial y} \right) \right] + \\ &\left. \frac{1}{\pi_{s}} H^{*} \left(\frac{\partial \pi_{s}}{\partial t} + \frac{\partial \pi_{s} u}{\partial x} + \frac{\partial \pi_{s} v}{\partial y} + \frac{\partial \pi_{s} \omega}{\partial \sigma} \right) + \right. \\ &\left. c_{p} T^{*} \left(\frac{\partial T}{\partial t} - \frac{RT}{\Phi c_{p}} \tau - \frac{\varepsilon}{c_{p}} \right) \right\} dD dt = 0, \quad dD = \pi_{s} dx dy d\sigma. \quad (20) \end{split}$$

Integrating the expression

$$\vec{u}^* \operatorname{grad} H = u^* \frac{\partial H}{\partial x} + v^* \frac{\partial H}{\partial y} + \omega^* \frac{\partial H}{\partial \sigma}, \tag{21}$$

from (20) by parts we can write down the antisymmetric pair of the addends

$$(H^*\operatorname{div}\pi_s\vec{u} - H\operatorname{div}\pi_s\vec{u}^*). \tag{22}$$

Here $\vec{u}^* = (u^*, v^*, \omega^*)$.

Then, after obvious transformations we obtain

$$I(\vec{\varphi}, \vec{\varphi}^*) \equiv \int_{D_t} \left\{ \left(u^* \frac{\partial u}{\partial t} + v^* \frac{\partial v}{\partial t} + c_p T^* \frac{\partial T}{\partial t} \right) - l(vu^* - uv^*) + \frac{1}{\pi_s} (H^* \operatorname{div} \pi_s \vec{u} - H \operatorname{div} \pi_s \vec{u}^*) - \frac{RT}{\Phi} (\tau T^* - \tau^*) - \varepsilon T^* + \frac{\sigma}{\pi_s} \left(\frac{\partial H}{\partial \sigma} \right) \left[u^* \left(\frac{\partial \pi_s^*}{\partial x} - \frac{\partial \pi_s}{\partial x} \right) + v^* \left(\frac{\partial \pi_s^*}{\partial y} - \frac{\partial \pi_s}{\partial y} \right) \right] + \frac{\sigma}{\pi_s} \left(\frac{\partial H}{\partial \sigma} \right) \frac{\partial \pi_s^*}{\partial t} + \frac{1}{\pi_s} H^* \frac{\partial \pi_s}{\partial t} \right\} dD dt + \int_{\Omega_t} H u_n^* d\Omega dt = 0.$$
 (23)

Here $\Omega_t = \Omega \times [0, \vec{t}], \Omega$ is the lateral boundary of the domain D, $d\Omega \equiv \{\pi_s dx d\sigma, \pi_s dy d\sigma\}$ is the square element on the lateral boundary, u_n^* is the normal component of $\vec{u^*}$ to the boundary Ω . Here the conditions $\omega = 0$ at $\sigma = 0$ and $\sigma = 1$ are taken into account.

Prescribing $\vec{\varphi}^* = (u, v, \tau, H, 1)$ in (23), we can obtain the equation of energy balance

$$\int_{D_{t}} \left[\frac{\partial}{\partial t} \left(\frac{u^{2} + v^{2}}{2} + c_{p} T \right) - \varepsilon \right] dD dt + \int_{S_{t}} H_{s} \frac{\partial \pi_{s}}{\partial t} dS dt + \int_{\Omega_{t}} H u_{n} d\Omega dt = 0, \quad (24)$$

where $H_s = gZ_s$, Z_s is the relief of the surface; dS = dx dy. $S_t = S \times [0, \bar{t}], a, S$ is the projection of the region D to the surface (x, y).

Comparing the expressions (23) and (24), we can conclude that it is enough to fulfill the following conditions for the providing the energy balance of the discrete approximations.

- 1. The pressure gradients in the motion equations must be calculated in the same way as in the formula for the function τ .
- 2. The approximation of the gradient operator in (13)-(15) must agree with the approximation of the divergence operator in the continuity equation (16), (16b) as it is dictated by the antisymmetric expression (22); (16b) is used in the calculations.
- 3. The approximations of $\frac{\partial H}{\partial \sigma}$ in the hydrostatic equation and σ in the expression for τ have to be chosen in such a way that the correlations like these

$$\sigma \frac{\partial H}{\partial \sigma} + H = \frac{\partial \sigma H}{\partial \sigma},\tag{25}$$

$$\int_{0}^{1} \left(\sigma \frac{\partial H}{\partial \sigma} + H \right) d\sigma = \sigma H \Big|_{0}^{1} = H_{s} \equiv q Z_{s}. \tag{26}$$

must be valid for them.

In the most simple way this goal is reached when piecewise-polynomial or finite-element approximations for H are used. Then the operations of differentiation and integration are carried out analytically.

The divergent central-difference schemes possess the characteristics of the type (25), (26) as well.

4. We shall construct the time discretization basing on (23), (24). These relations show that it is unnecessary to take geopotential and surface pressure at the implicit step. In this case they can be taken from the previous step. It is the condition of energy balance that is important here. We have to eliminate the corresponding addends in the discrete analog (23) when the same values of $\bar{\varphi}^*$, used to obtain (24), are substituted into it. It is also important that the temperature does not change the sign.

As it is seen in (24), for the scheme to be stable in time it needs the substitution $u^* = v^{j+1}$, $v^* = v^{j+1}$ in (23) to get the implicit scheme and $u^* = u^{j+1/2}$, $v^* = u^{j+1/2}$ to get the Kranck-Nickolson scheme. As for the terms with Coriolis parameter in (13), (14) they have to be approximated at the implicit step. Equation (16b) and formula (18) for τ should be approximated with the use of the values u, v obtained from the motion equations at $t = t_{j+1}$. The monotonic numerical schemes obtained by means of variational approach with the use of the local adjoint problems [6] are applied at the transport stage.

4. Scenarios for the modeling of mesoclimate and atmospheric quality

For the modeling of mesoregional atmospheric processes it is necessary to know the state functions at the initial time moment. Besides, we need continuous information about large scale atmospheric processes which are the background motion for our problems. The lack of such data makes doubtful the correctness of the boundary conditions In practice, the initial and background data are either absent or irregular in space and time. That is why initialization of the models and their closure by boundary conditions are crucial points when the problems are solved in the real time regimes. As our goal is to learn the conditions of mesoclimate formation we can work in the frames of scenario approach.

Taking the Novosibirsk industrial region and Novosibirsk Scientific Center (Academgorodok) as the examples we have made the development of the constructive aspects of model realization and the choice of the appropriate scenarios. Specifically, the typical scenarios of hydrometeorological regime have been calculated. Basing on them, the series of calculations has been made allowing us to evaluate anthropogenic loads for the given regions, to reveal zones that are the most unfavourable from the ecological point of view for the placing of new industrial objects. Sensitivity functions of the functionals defining the mean values of pollutants concentrations over the given regions within the definite time period have been used for the estimation of the intensity and configuration of the influence regions of anthropogenic sources.

More detailed description of the models and results concerned with the scenarios for some industrial regions is done in [9, 10]. The results of the scenarios are presented as the computer movies. As a whole, their analysis shows that the estimations of atmospheric quality and ecological future of Academgorodok have to be done taking into account the fact that Academgorodok is the part of the climatic system of the Novosibirsk industrial region.

As a result of interaction between the local structure of the city heat island and the reservoir and the background flow, the complex atmospheric circulation system arises. The system is characterized by the upward air flows over the more heated areas of the surface and by the backward currents directed against background flow. The latter is the most important fact. That is why it is not recommended to estimate ecological situations and to plan environmental protection measures near the heat islands by means of the methods based on wind rose as these methods do not give correct results.

The calculations show that quality of the atmosphere in Academgorodok is affected by sources placed in the region with the character scale of 30 km. Naturally, the relative values of influence function and configuration of the influence domain itself depend on the structure of the atmospheric circulation. They are generally oriented against the air mass moving. As it is seen from the behavior of the influence functions, the relative contribution of the sources placed in the Academgrodok region is approximately one order higher than the same power sources placed out of the region. Generation of the backward currents in the lee side of Academgorodok as well as the presence of breeze circulations and downward flows give the preconditions for accumulation of pollutions in the housing estates of Academgorodok and in the surrounding forests.

It is worth mentioning that at the North-West type of atmospheric circulation the influence function for the functional that describes the air quality within the housing districts of Academgorodok has the maximum values domain that geometrically covers the "household" territory of the research institutes. Since such a type of atmospheric circulation predominates in summer time, the medical and ecological services should be very attentive to this zone as that of increased potential danger for the air quality in Academgorodok. The calculations give the maximum relative contribution of the sources placed there into atmospheric pollution of the "upper" zone of Academgorodok.

Figures 1-4 show the fragments of the scenario on mesoclimate and transport of pollutants for Novosibirsk industrial region. The scales of the domain are 50 km×50 km (Figures 1, 2). The more detailed region has been used for Academgorodok – 12 km×12 km (Figures 3, 4). Input data for the scenario are: summer season, July, 12-15 o'clock of the local time, southern background flow of 5 m/s at the height corresponding to the pressure of 700 mb. Six pollutant sources are considered: four heat power plants – HPP-1, 2, 3, 4, and two aggregate city sources – Iskitim and Berdsk.

The fragments present two dimensional cross sections at the height of 50 m of the wind vectors and pollution concentration. The maximum wind speed is about 8 m/s. The arrows show the directions of the moving. The length of arrows are proportional to the wind speed. Concentrations of

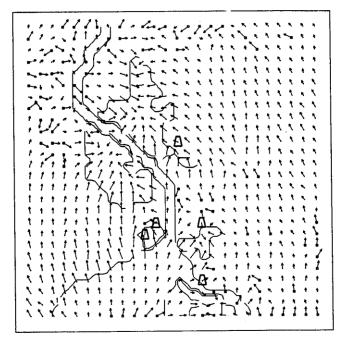


Figure 1. Horizontal structure of atmospheric circulation in Novosibirsk industrial region: height 50 m, southern background flow, July, 12.00-15.00 of local time

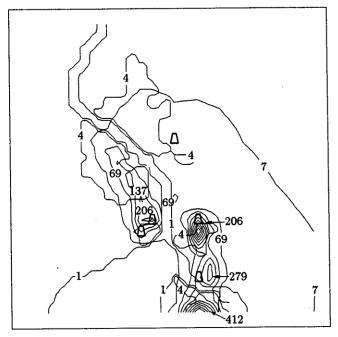


Figure 2. Horizontal section at 50 m of concentrations field from 6 sources

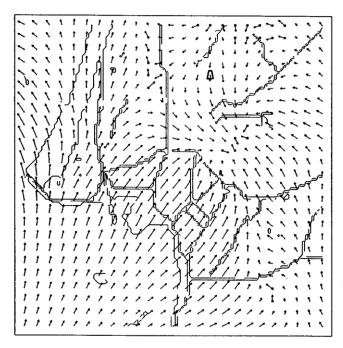


Figure 3. More detailed atmospheric circulation in Academgorodok (the conditions are the same as in Figure 1)

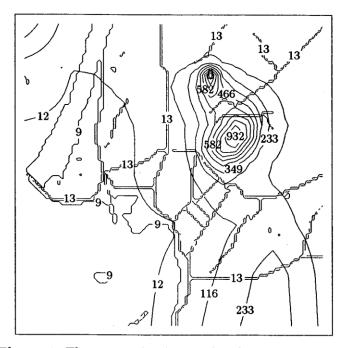


Figure 4. The same as in Figure 2, but for Academgorodok

pollution are given in relative units. The capacities of all sources have been normalized on the capacity of HPP-2. For the convenience, the main inhomogeneities of underlying surface are drawn. For example, line 1 shows the rivers and the reservoirs, line 4 bounds the city districts (see Figures 1 and 2), line 9 marks water-land boundary, line 13 indicates the main roads (see Figures 3 and 4).

Figures 1-3 show the horizontal structure of atmospheric circulation which are the result of interaction between background flow and the inhomogeneities of the landscape. The influence on the air flow formation of the city heat islands and the water objects are seen in Figure 1.

In Figure 3, the breeze circulation is strictly expressed. Water is colder than land at that time. Breeze circulation interacts with the local heat island. The system of backward flows are seen in the northern part of Academgorodok.

In the comparison with Academgorodok, the heat island of the main part of Novosibirsk generates the more intensive structure of vertical flows and backward flows from the lee side (see Figure 1). The consequence of such structure of atmospheric motion is the distribution of the pollution concentration (see Figures 2 and 4). It is seen in Figures 3 and 4 that there are all prerequisites for arising of ecologically unfavourable situations.

5. Conclusion

Analysis of the results confirm our main point again that it is insufficient to use simplified "engineering" methods, commonly used in practice for the solution to the environmental problems, for ecological planning and prediction. It is necessary to take into account the features of the regions and their potential possibilities to generate ecologically unfavourable situations.

Our experience shows that the socially admissible estimations of ecological perspective can be obtained just with the help of rather full, in physical content, mathematical models which take into account the interconnections between hydrothermodynamical, chemical and biospherical processes in the climatic system of cities and industrial regions under the different kinds of anthropogenic loads. One of the basic versions of the model of such a class is presented here. Following such approach to the problems of environmental forecasting, the troubles connected with "suddenly" arising ecological catastrophes might be avoided.

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