Super-short-term forecasting of the atmospheric aerosol evolution based on dynamic-stochastic approach and lidar data

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Methodical foundations and algorithms of solving the problem of super-short-term forecast of the atmospheric aerosol evolution are treated based on the dynamic-stochastic approach. The approach uses the apparatus of the Kalman filtering. The quality of the algorithms is tested by the data of lidar sensing conducted in the vicinity of Tomsk.

Super-short-term forecasting of ecological state of the atmosphere above cities and industrial centers finds wide application in last years, because it helps to take adequate precautions against dangerous subsequences of pollution.

The methods applied now for forecasting technogenic pollution (including aerosol) use the data of the available network of meteorological stations and mesoscale mathematical models based on hydrothermodynamic equations and the turbulent diffusion equation.[1,2] However, modeling of evolution of atmospheric pollution (including aerosol formations) on the basis of the hydrodynamic approach in the mesoscale limits is a quite difficult problem. This is due to the fact that the spectrum of mesoscale atmospheric motions depends on thermal and orographic inhomogeneities of the underlying surface, turbulent characteristics of the atmosphere, and peculiarities of the temperature stratification. Cloudiness also significantly affects spatial distribution of the underlying surface temperature that can result in appearance of different mesoscale phenomena.

It should be also emphasized that, according to Ref. 3, main quantity of admixtures is concentrated in the planetary boundary layer of the atmosphere. So, in order to describe the processes of transfer, diffusion, and transformation of admixtures in more detail, it is necessary to use realistic mathematical models of the boundary layer for precalculation of the thermodynamic regime. The models should, at least, take into account the diurnal behavior of meteorological parameters and pollution, orographic and thermal inhomogeneities of the underlying surface, inhomogeneities of the turbulent characteristics of the atmosphere, and so on.

Last years, in addition to hydrodynamic approach, the dynamic-stochastic approach is also used in solving the problem of the super-short-term forecast. It is based on the supposition that an atmospheric state can be described by random fields related to each other through a system of relationships. However, the dynamic-stochastic approach has small prehistory in meteorology and is quite a new instrument of investigation. The models of transfer and scattering of admixtures in the atmosphere constructed in the framework of this approach make it possible to forecast the fields of concentration of a polluting substance with good quality within the advance interval up to 4 hours (see, foe example, Ref. 4).

The process of forecasting based on the dynamic-stochastic approach is a continuous process realizable in two stages:

– assimilation of collected measurements of the parameters of the atmospheric state and correction of the model parameters;

– forecasting based on the corrected model.

A random factor is an inherent component of the process of admixture transport in the atmosphere in the time intervals of the super-short-term forecasting. Taking into account this fact, the dynamic-stochastic approach to forecasting the aerosol evolution in the atmosphere in small time intervals should be considered as more realistic.

However, to realize such approach, just the same turbulent diffusion equation as well as all boundary and initial conditions necessary for solving it are used when deriving the forecast equations.

Therefore, another version of the dynamic-stochastic approach, based on the use of a simplified model of temporal behavior of a meteorological parameter represented by the stochastic differential equation of the second order, is proposed in this paper for solving the problem of super-short-term forecasting of the atmospheric aerosol evolution. The peculiarity of the approach is the fact that the complicated procedure of solving the turbulent diffusion equation is absent, hence, realization of the forecast algorithm is much simpler.

Let us briefly consider the forecasting algorithm based on the use of the apparatus of Kalman filtering and differential stochastic equations of the second order describing the dynamics of temporal variations of the atmospheric aerosol concentration. Assume that the correlation properties of this parameter evolution can be represented as an exponential function.

It is known[5] that analytical formulae of the following form are commonly used for approximation of

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temporal correlation functions of the atmospheric state parameters:

$$\mu_\xi(\tau) = \exp(-\alpha\tau), \quad \alpha > 0, \tag{1}$$

$$\mu_\xi(\tau) = \exp(-\alpha\tau^2), \quad \alpha > 0, \tag{2}$$

$$\mu_\xi(\tau) = \{\exp(-\alpha|\tau|)\}\cos\beta\tau, \quad \alpha > 0, \tag{3}$$

$$\mu_\xi(\tau) = \{\exp(-\alpha\tau^2)\}\cos\beta\tau, \quad \alpha > 0. \tag{4}$$

Besides, the following formula was proposed[6] for approximation of the empirical correlation functions of the temperature, humidity of air, zonal and meridional wind:

$$\mu_\xi(\tau) = (1 - \alpha\tau)\exp(-\beta\tau), \tag{5}$$

where $\mu_\xi(\tau)$ is the temporal correlation function of the parameter ξ (here τ is the time shift), α and β are the approximating coefficients (in general case they depend on the height h).

As additional investigations, based on real lidar measurements, show, this type of analytical expression enables one to approximate also empirical correlation functions of the atmospheric aerosol concentration. Average approximating coefficients in Eq. (5) for the layer from 140 to 1140 m (for which reliable lidar data were obtained) are the following: $\alpha = 7.5\cdot10^{-6}$ and $\beta = 0.05$. These values of α and β are used as initial conditions when initiating the algorithm of estimating and forecasting the atmospheric aerosol concentration.

According to Ref. 7, a random process with correlation functions of the form (5) can be described by the second-order stochastic differential equation

$$\frac{d^2\xi(t)}{dt^2} + 2\beta\frac{d\xi(t)}{dt} + \beta^2\xi(t) = \frac{d\omega(t)}{dt} - (\alpha-\beta)\omega(t). \tag{6}$$

Formula (6) determines the evolution of the process $\xi(t)$ at some linear system output when its input is affected by the white noise $\omega(t)$. The transmission function of such a system, according to Eq. (5) has the form[8]:

$$H(s) = \frac{s + (\alpha - \beta)}{(s-\beta)^2}, \tag{7}$$

where s is the Laplace transform parameter.

Introducing the vector of state $\mathbf{X}(t) = |X_1(t), X_2(t)|^T$, where T is the transposition operator, $X_1(t) = \xi(t)$ is the atmospheric aerosol concentration, and $X_2(t)$ is the auxiliary variable, one can pass from the differential equation of the second order (6) to the system of two stochastic differential equations of the first order

$$\begin{cases} \dfrac{dX_1}{dt} = X_2(t) - 2\beta X_1(t) + \omega(t); \\ \dfrac{dX_2}{dt} = -\beta^2 X_1(t) + (\beta-\alpha)\omega(t). \end{cases} \tag{8}$$

The system of equations (8) can be used as a model of the space of states when synthesizing the algorithm for estimations of the current values of the atmospheric aerosol concentration based on the Kalman filtering theory. The limitation for using Eq. (8) is an uncertainty of values of α and β and their dependence on the height and time. This limitation can be removed through introducing an additional variable $X_3(t) = \beta(t, h)$ in the vector of states $\mathbf{X}(t) = |X_1(t), X_2(t), X_3(t)|^T$, ignoring the effect of α in the model of state (because of its small value), and passing to the extended system of differential equations

$$\begin{cases} \dfrac{dX_1}{dt} = X_2(t) - 2X_3(t)X_1(t) + \omega_1(t), \\ \dfrac{dX_2}{dt} = -X_3^2(t)X_1(t) + \omega_2(t), \\ \dfrac{dX_3}{dt} = 0, \end{cases} \tag{9}$$

where $\omega_1(t)$ and $\omega_2(t)$ are the equivalent noises of the state.

The space of states (9) is written assuming that $X_3(t)$ is constant on the whole interval of observations. Note that the differential equation for $X_3(t)$ can have a more complicated form depending on the quantity of *a priori* data for β.

Let us write the equations of state (9) in the difference form:

$$\begin{cases} X_1(k+1) = X_1(k) - 2X_1(k)X_3(k)\Delta t_k + X_2(k)\,\Delta t_k + \omega_1(k), \\ X_2(k+1) = X_2(k) - X_1(k)X_3^2(k)\Delta t_k + \omega_2(k), \\ X_3(k+1) = X_3(k), \end{cases} \tag{10}$$

where Δt_k is the time interval between successive measurements $k = 0, 1, 2, \ldots, K$.

The equation of observations at direct measurement of the aerosol concentration can be represented by additive mixture of the true value of $X_1(t)$ and the measurement error

$$\tilde{Y}(k) = X_1(k) + \varepsilon(k), \tag{11}$$

where $\tilde{Y}(k)$ is the current measurements of the atmospheric aerosol concentration at the selected (fixed) height h, $\varepsilon(k)$ is the error (noise) of the measurement.

Let us write Eqs. (10) and (11) in the matrix form:

$$\mathbf{X}(k+1) = \mathbf{\Phi}[\mathbf{X}(k)] + \mathbf{\Gamma}\mathbf{W}(k); \tag{12}$$

$$\tilde{\mathbf{Y}}(k) = \mathbf{H}\mathbf{X}(k) + \mathbf{E}(k); \tag{13}$$

where

$$\mathbf{\Phi}[\mathbf{X}(k)] = \begin{vmatrix} X_1(k) - 2X_1(k)X_3(k) + X_2(k)\Delta t_k \\ X_2(k) - X_1(k)X_3^2(k)\Delta t_k \\ X_3(k) \end{vmatrix}$$

is the transitional vector-function of states, $\mathbf{H} = |1 \ \ 0 \ \ 0|$ is the vector-function of observations, $\mathbf{W}(k)$ is the (2×1) dimensional vector of the state noises, $\mathbf{\Gamma} = \begin{vmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{vmatrix}$

is the matrix of transition for the state noises, $\mathbf{E}(k)$ is the vector of the measurement noises.

Equations (12) and (13) completely determine the structure of the estimation algorithm.[9]

Because of non-linearity of equations (12), one should use the extended Kalman filter as the method for synthesis of the algorithm of estimation. In this case, equations of optimal estimation of the vector of states $\mathbf{X}(k)$ have the form:

$$\hat{\mathbf{X}}(k+1) = \hat{\mathbf{X}}(k+1|k) + \mathbf{G}(\hat{\mathbf{X}}, k+1)\,[\tilde{\mathbf{Y}}(k+1) - \mathbf{H}\hat{\mathbf{X}}(k+1|k)], \qquad (14)$$

where $\hat{\mathbf{X}}^{\mathrm{T}}(k+1) = |\hat{X}_1, \hat{X}_2, \hat{X}_3|$ is the estimate of the vector of state at the moment $(k+1)$; $\hat{\mathbf{X}}(k+1|k)$ is the vector of forecasted estimates at the moment $(k+1)$ by the data at a step k. The estimates are forecasted using the formula

$$\hat{\mathbf{X}}(k+1|k) = \mathbf{\Phi}[\hat{\mathbf{X}}(k)], \qquad (15)$$

$\mathbf{G}(\hat{\mathbf{X}}, k+1)$ is the (3×1)-dimensional matrix of the weight coefficients.

The weight coefficients are calculated in the extended Kalman filter using the recurrent matrix relationships of the form:

$$\mathbf{G}(\hat{\mathbf{X}}, k+1) = \mathbf{P}(k+1|k)\cdot\mathbf{H}^{\mathrm{T}}\cdot[\mathbf{H}\cdot\mathbf{P}(k+1|k)\cdot\mathbf{H}^{\mathrm{T}} + \mathbf{R}_{\varepsilon}(k+1)]^{-1}; \qquad (16)$$

$$\mathbf{P}(k+1|k) = \mathbf{F}[\hat{\mathbf{X}}(k)]\cdot\mathbf{P}(k|k)\cdot\mathbf{F}^{\mathrm{T}}[\hat{\mathbf{X}}(k)] + \mathbf{\Gamma}\cdot\mathbf{R}_{\mathbf{w}}(k)\cdot\mathbf{\Gamma}^{\mathrm{T}}, \qquad (17)$$

$$\mathbf{P}(k+1|k+1) = [\mathbf{I} - \mathbf{G}(\hat{\mathbf{X}}, k+1)\cdot\mathbf{H}]\cdot\mathbf{P}(k+1|k), \qquad (18)$$

where $\mathbf{P}(k+1|k)$ is the (3×3)-dimensional *a posteriori* correlation matrix of the forecasting errors, $\mathbf{P}(k+1|k+1)$ is the (3×3)-dimensional *a priori* correlation matrix of the estimating errors, $\mathbf{R}_{\varepsilon}(k+1)$ is the variance of observation noises, $\mathbf{R}_{\mathbf{w}}(k)$ is the (2×2)-dimensional diagonal correlation matrix of the state noises, $\mathbf{I}$ is the (3×3)-dimensional unit matrix,

$$\mathbf{F}(\hat{\mathbf{X}}(k)) = \frac{\partial \mathbf{\Phi}[\hat{\mathbf{X}}(k)]}{\partial \hat{\mathbf{X}}} =$$

$$= \begin{vmatrix} 1-2\hat{X}_3(k)\Delta t_k & \Delta t_k & -2\hat{X}_1(k)\Delta t_k \\ -\hat{X}_3^2(k)\Delta t_k & 1 & -2\hat{X}_1(k)\hat{X}_3(k)\Delta t_k \\ 0 & 0 & 1 \end{vmatrix}$$

is the (3×3)–dimensional Jakobi matrix of the transitional vector-function.

The procedure of forecasting $X_1(t + \Delta t_k)$ and $X_2(t + \Delta t_k)$ on the interval of advance Δt_k is realized by means of solving the difference equations (15) with the initial conditions

$$\hat{\mathbf{X}}(k) = |\hat{X}_1(k), \hat{X}_2(k), \hat{X}_3(k)|^{\mathrm{T}}$$

and a smaller step of time quantization.

To put the filtering algorithm (14)–(18) into operation at the moment $k = 0$ (initialization moment), it is necessary to set the following initial conditions:

$\hat{\mathbf{X}}(0) = \mathbf{M}\{\mathbf{X}(0)\}$ is the initial vector of estimation, where $\mathbf{M}$ is the operator of mathematical expectation;

$\mathbf{P}(0|0) = \mathbf{M}\{[\mathbf{X}(0) - \mathbf{M}\{\mathbf{X}(0)\}][\mathbf{X}(0) - \mathbf{M}\{\mathbf{X}(0)\}]^{\mathrm{T}}\}$ is the initial correlation matrix of estimation, as well as the values of the elements of correlation matrices of the noises $\mathbf{R}_{\varepsilon}(0)$ and $\mathbf{R}_{\mathbf{w}}(0)$.

In practice, the values $\hat{\mathbf{X}}(0)$ and $\mathbf{P}(0|0)$ can be set based on the minimum of data on the real properties of the system. In the case of the full absence of useful information, the values are set as $\hat{\mathbf{X}}(0) = 0$, and $\mathbf{P}(0|0) = \mathbf{I}$.

The algorithm considered above was used for solving the problem of the super-short-term forecasting of the aerosol concentration in the atmospheric boundary layer.

Let us briefly analyze the results of the statistical estimation of the algorithm quality for the cases of 4-, 8-, and 12-hour forecasting.

The proposed algorithm was examined using the measurements of the vertical distribution of the aerosol scattering coefficient (at total number of measurements $N = 90$) carried out with a three-path correlation lidar in the region of Tomsk city (56°N, 85°E) from June 10 to August 12 of 1994 with the time step of 4 hours. As the vertical resolution of the aforementioned data (after averaging individual measurements) is about 100 m, it is possible to study in detail the peculiarities of the atmospheric aerosol evolution in almost all atmospheric boundary layer (up to the height of 1140 m).

The following formula was used to determine the profiles of the aerosol mass concentration N_{a} (mg·m^{-3}):

$$N_{\mathrm{a}}(h) = 4\alpha(h),$$

where $\alpha(h)$ is the aerosol scattering coefficient, h is the height.

At the same time, the root-mean-square (standard) error

$$\delta_{\xi} = \left[\frac{1}{n}\sum_{i=1}^{n}(\hat{\xi}_i - \xi_i)^2\right]^{1/2} \qquad (19)$$

(here $\hat{\xi}_i$ and ξ_i are respectively the forecasted and measured values of the meteorological parameter, i.e., the atmospheric aerosol concentration, n is the number of realizations), and the relative error

$$\theta_{\xi} = \delta_{\xi}/\sigma_{\xi}, \qquad (20)$$

where σ_{ξ} is the rms deviation characterizing the variability of the same parameter ξ, were used for statistical estimation of the quality of the super-short-term forecast.

The vertical distribution of the rms errors in super-short-term forecasting of the atmospheric aerosol concentration N_{a} (mg·m^{-3}) for different values of the advance τ together with its standard deviations are shown in the Fig. 1 as an example.[11] The values of the relative errors of the same forecast are given in the Table.

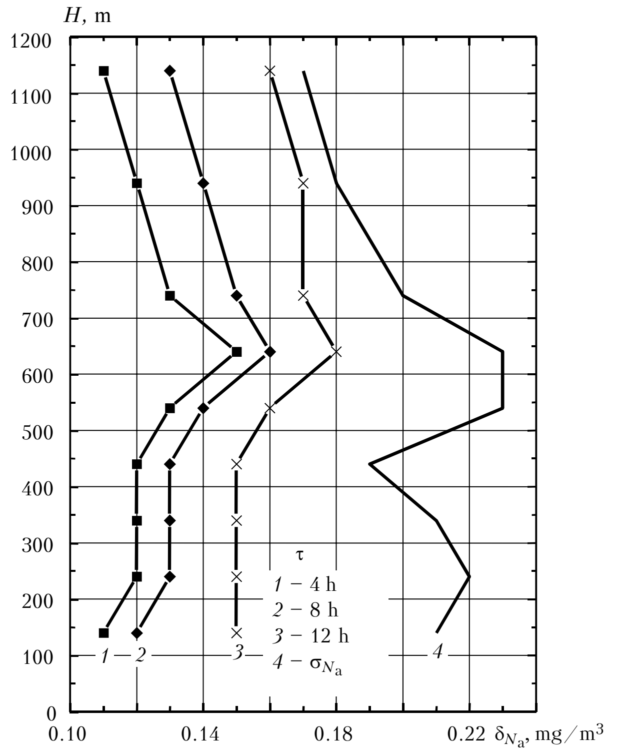

Fig. 1. Vertical distribution of the standard deviation (σ_{N_a}) and rms errors (δ_{N_a}) in forecasting the atmospheric aerosol concentration for different values of the advance (τ).

Table 1. Relative errors (θ, %) in super-short-term forecasting of the atmospheric aerosol concentration for different τ

Shift	Height, m								
τ, hours	140	240	340	440	540	640	740	940	1140
4	52	54	57	58	56	60	65	66	65
8	57	59	62	63	61	65	75	78	76
12	71	68	71	73	69	74	85	86	94

Analysis of the presented data shows that:

– the dynamic-stochastic approach based on the use of the apparatus of Kalman filtering and differential stochastic equations of the second order provides for the results quite acceptable for practice, but only at the value of advance $\tau = 4$ hours. Indeed, the values of the relative error in the super-short-term forecasting of the atmospheric aerosol concentration in the whole considered layer by this method do not exceed the permissible values $\theta_d = 66\%$ commonly used in practice of the statistical forecasting[12];

– the same method can be used in the super-short-term forecasting of the atmospheric aerosol concentration also at $\tau = 8$ hours, but only in the atmospheric layer of 140–640 m, where the condition $\theta < \theta_d$ is fulfilled. Above 640 m the values of the relative error exceed 66%.

Such a peculiarity of the behavior of the relative error θ well correlates with the corresponding behavior of the rms deviation: its maximal values are observed in the layer of 140–640 m, and they dramatically decrease above 640 m.

Thus, the performed numerical experiments on the estimation of the quality of the dynamic-stochastic method based on the use of the apparatus of Kalman filtering have shown it to be quite efficient for super-short-term forecasting of the atmospheric aerosol concentration at $\tau \le 4$ hours. The proposed method can be used at $\tau = 8$ hours only up to the height of 640 m.

It should be noted in conclusion that the obtained estimates of the quality of the dynamic-stochastic forecasting of the atmospheric aerosol concentration need additional examination on the basis of a longer series of experimental observations.

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