Numerical experiments on estimation of methane emission based on the data assimilation system for passive impurity in the atmosphere of the Northern hemisphere

E.G. Klimova and N.V. Kilanova

Institute of Computational Technologies,
Siberian Branch of the Russian Academy of Sciences, Novosibirsk

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We propose a technique of data assimilation in solving the problem on estimating the concentration and total outcome of a passive impurity. The forecast of changes in the impurity concentration fields in time is given using semi-Lagrangian model of a passive impurity transfer and diffusion applied to the Northern hemisphere. The algorithm of data assimilation being used in the problem on estimating the fields of concentration and total outcome of a passive impurity is based on the Kalman theory of optimal filtering. In calculating the covariance matrices assumption is made of the ergodicity of the random fields of errors considered. In this paper we present the results of numerical experiments with model data on the passive impurity concentration using methane as an example. Efficiency of the approaches to the assimilation problem proposed is shown.

Introduction

The problem on assimilation of the results of observations is of great demand nowadays in modeling various processes in the atmosphere, ocean, water bodies, etc. The problem on the joint analysis of the observation data and a forecast model is solved either by use of the general optimization approach assuming variational statement of the problem or by using the estimation theory. In the first case, the so-called 4DVAR assimilation method is being developed, in the second one – the assimilation algorithm based on Kalman filter. In this paper we present the data assimilation technique intended for use in problems on estimating of the concentration of a passive impurity. The forecast of changes in the impurity concentration fields with time is performed using a semi-Lagrangian model of the transfer and diffusion of a passive impurity considered for the Northern hemisphere.

The data assimilation algorithm is based on the Kalman theory of optimal filtering. Realization of the Kalman filter algorithm, in its full form, on a computer is impossible since the order of the covariance matrices for modern global models achieves 1 million. One of the approaches to solving this problem is the use of simplified models in calculating matrices of the forecast errors covariances. Such an algorithm is called the suboptimal algorithm of the Kalman filtering.[1,2] Numerical experiments on assimilation of the data on a passive impurity using the above-mentioned algorithm have been described in Refs. 3 and 4. The second approach to organization of the covariance matrix calculations is based on the assumption of ergodicity of the random fields of the error considered. In this case, the probabilistic averaging can be replaced by averaging over time.[5]

Assimilation of the observation data in the problem on transfer and diffusion of a passive impurity

Preliminary estimation of the impurity concentration fields is being done using a model of transfer and diffusion of a passive impurity. The model used is described in detail in Refs. 3 and 6. For solution of transfer and diffusion equation, the quasi-monotonic semi-Lagrangian scheme is applied. Let us briefly state the main idea of this scheme. First, we apply the splitting method to physical processes.[7] According to this method, solutions are being sought, successively at each time step, to the problems on: a) impurity transfer along trajectories and b) for turbulent diffusion.

At the first stage, the problem of impurity transfer is solved in Lagrangian coordinates. At interpolation from the Eulerian to the Lagrangian coordinates, the monotonization procedure, described in detail in Ref. 8, is used. At the second stage, the problem of turbulent diffusion is considered in Eulerian coordinates. Diffusion equation is approximated using Crank-Nicholson scheme. Then the directional splitting method is applied to the difference equation obtained, and the factorization method is used in solving the set of difference equations.

The algorithm of data assimilation used in the problem of estimating the fields of a conservative admixture concentration is based on the Kalman theory of optimal filtering. Statement of the optimal filtering problem can be found in Refs. 9 and 10 and the linear case of a discrete Kalman filter algorithm, in application to transfer and diffusion of a conservative admixture, is described in Refs. 3, 11, and 12.

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The main difficulty in realization of Kalman filter algorithm appears at calculating the covariance matrices of forecast errors due to very high order of these matrices. One of the ways to overcome this computational difficulty is in applying suboptimal algorithms of the Kalman filter. These are the algorithms, which use simplified models in calculations of the covariance matrices of the forecast errors.[1,2,4,13]

Numerical experiments

We have considered the variant of suboptimal algorithm as applied to the problem on estimating the field of methane emission. The algorithm is based on the assumption of ergodicity of the fields of forecast errors. Covariance of the forecast errors have been calculated using the equations for these errors. A description of such an algorithm and numerical experiments on estimation of the field of concentration are presented in Ref. 3.

The "true" concentration field was set in these numerical experiments as follows

$$x_k^{\mathrm{tr}} = A_{k-1}x_{k-1}^{\mathrm{tr}} + \eta_{k-1}^{\mathrm{tr}} + \varepsilon_{k-1}; \quad (1)$$

$$\eta_0^{\mathrm{tr}} = \bar{\eta}, \quad (2)$$

where A_{k-1} is the model operator, x_{k-1}^{tr} is the "true" methane concentration, η_{k-1}^{tr} is the "true" methane emission at time t_{k-1}, ε_{k-1} is the random vector of model "noises."

The concentration forecast by the model x_k^{f} (preliminary estimation of the concentration field) was set as:

$$x_k^{\mathrm{f}} = A_{k-1}x_{k-1}^{\mathrm{f}} + \eta_{k-1}^{\mathrm{f}}; \quad (3)$$

$$\eta_0^{\mathrm{f}} = 0, \quad (4)$$

where η_{k-1}^{f} is the methane emission at time t_{k-1}. The data were modeled for the moments of observations

$$y_k^0 = M_k x_k^{\mathrm{tr}} + \xi_k, \quad (5)$$

where M_k is the matrix interpolating the value of x_k^{tr} from those at nodes of the grid to the observation points, ξ_k is the random value with normal distribution, zero mean, and the variance σ_0^2.

The following numerical experiments on methane emission have been carried out.

In the first experiment, the initial emission field was taken zero, the emission error was set as a random value with zero mean and with root-mean-square error equal 10% of the mean emission value.

The emission field reconstruction was carried out during the assimilation of data on the concentration. The second experiment dealt not with the estimation of the emission itself, but with the estimation of the correction factor in the emission model. It was assumed that time variation of the emission field could be presented in the form

$$\eta_k = \tilde{\eta}(1 + \delta\eta_k), \quad (6)$$

where $\tilde{\eta}$ is the background emission value; $\delta\eta_k$ is the correction factor at the kth moment in time. Thus,

$$\delta\eta_{k+1} = \alpha\delta\eta_k + \sqrt{1-\alpha^2}\,\chi_k, \quad (7)$$

where $\alpha = 0.95$, χ_k is the normally distributed random value with zero mean and the variance equal to 0.01. Such a model was proposed in Ref. 14.

In the experiment #1 we have an equation system for the forecast errors in concentration Δx_k and emission $\Delta\eta_k$:

$$\Delta x_k = A_{k-1}\Delta x_{k-1} + \Delta\eta_{k-1} + \varepsilon_{k-1}; \quad (8)$$

$$\Delta\eta_k = \Delta\eta_{k-1}; \quad (9)$$

$$\Delta\eta_0 = \Delta x_0. \quad (10)$$

Estimates of the concentration and emission fields at the assimilation were calculated by the following formulas:

$$x_k^{\mathrm{a}} = x_k^{\mathrm{f}} + \overline{\Delta x_k(\Delta x_k)^{\mathrm{T}}}\left(M_k P_k^{\mathrm{f}} M_k^{\mathrm{T}} + R_k\right)^{-1}\left(y_k^0 - M_k x_k^{\mathrm{f}}\right); \quad (11)$$

$$\eta_k^{\mathrm{a}} = \eta_k^{\mathrm{f}} + \overline{\Delta x_k(\Delta\eta_k)^{\mathrm{T}}}\left(M_k P_k^{\mathrm{f}} M_k^{\mathrm{T}} + R_k\right)^{-1}\left(y_k^0 - M_k x_k^{\mathrm{f}}\right). \quad (12)$$

In calculating the covariance matrix, we have used the assumption that the probability averaging can be replaced by averaging over time[5]:

$$P_k^{\mathrm{f}} = \overline{\Delta x_k(\Delta x_k)^{\mathrm{T}}} \cong \frac{1}{N-1}\sum_{i=1}^{N}\Delta x_i(\Delta x_i)^{\mathrm{T}}. \quad (13)$$

By analogy with formula (13), the crosscovariance matrix of concentration and emission errors was calculated. Here again the assumption on the possibility of replacing the probability averaging by averaging over time has been the basis:

$$\overline{\Delta x_k(\Delta\eta_k)^{\mathrm{T}}} \cong \frac{1}{N-1}\sum_{i=1}^{N}\Delta x_i(\Delta\eta_i)^{\mathrm{T}}. \quad (14)$$

Thus, using the calculated fields of errors in the concentration and emission, we have estimated covariance of errors in the forecasted fields of methane concentration and emission. After that the field of concentration was calculated, using observation data, by the formula (11) and the emission field by the formula (12).

The initial emission for the second experiment was set as follows:

$$\eta_0^{\mathrm{tr}} = \tilde{\eta}(1 + \delta\eta_0^{\mathrm{tr}}), \quad (15)$$

$$\eta_0^{\mathrm{f}} = \tilde{\eta}(1 + \delta\eta_0^{\mathrm{f}}), \quad (16)$$

and for calculations of the correction factor we took the values $\delta\eta_0^{\mathrm{tr}} = 0.1$, $\delta\eta_0^{\mathrm{f}} = 0.2$. Between the assimilation moments, the change in correction factors was calculated by formula (7), namely:

$$\delta\eta_{k+1}^{\mathrm{tr}} = \alpha\delta\eta_k^{\mathrm{tr}} + \sqrt{1-\alpha^2}\,\chi_k, \quad (17)$$

$$\delta\eta_{k+1}^{\mathrm{f}} = \alpha\delta\eta_k^{\mathrm{f}} + \sqrt{1-\alpha^2}\,\chi_k. \qquad (18)$$

During the assimilation, the concentration was calculated by formula (15) and correction factor $\delta\eta_k^{\mathrm{a}}$ by the formula below

$$\delta\eta_k^{\mathrm{a}} = \delta\eta_k^{\mathrm{f}} + \overline{\Delta x_k(\Delta\delta\eta_k)^{\mathrm{T}}}\left(M_k P_k^{\mathrm{f}} M_k^{\mathrm{T}} + R_k\right)^{-1}\left(y_k^0 - M_k x_k^{\mathrm{f}}\right), \qquad (19)$$

where $\Delta\delta\eta_k$ is the difference vector between the correction factors for the emission forecast and actual emission at the kth step in time:

$$\Delta\delta\eta_k = \delta\eta_k^{\mathrm{tr}} - \delta\eta_k^{\mathrm{f}}.$$

Thus, the crosscovariance matrix of concentration errors and the emission correction factor is calculated in formula (19), by analogy with the Eq. (12).

In numerical experiments, the calculations were performed on the 2.5×2.5° horizontal grid at 15 levels along vertical, in Δt = 15 min time intervals. Also we used data of objective analysis from the Russian Hydrometeorological Center on the wind velocity fields, temperature and pressure for August 1–3, 2002 and model distribution of methane concentration for August.[15] The calculations were made for two days with the assimilation every 12 hours, with the observation data being modeled by the formula (5). The data on orography were taken from the corresponding site.[16] The data on emission were taken from Ref. 17.

For estimation of the parameter characterizing the interaction of the atmosphere and the underlying surface, we have used the parameterization computation code presented by V.A. Shlychkov in description of the lower boundary condition in the model of an impurity transfer and diffusion.

Figure 1 presents the results of the first numerical experiment.

Figure 1*a* shows the relative error in concentration obtained at the data assimilation by use of suboptimal algorithm of the Kalman filter. The emission field is estimated, during the assimilation, by formula (12). The "true" emission value set constant at every step in time, at every grid point at two lower levels along vertical. Time steps are presented on abscissa. Figure 1*b* demonstrates the root-mean-square error in emission.

Figure 2 presents the results of the second numerical experiment. Figure 2*a* demonstrates the root-mean-square error in the concentration estimate obtained in the experiment. Figure 2*b* shows the time variation of the root-mean-square error in the emission estimate obtained in the second experiment. Figure 2*c* depicts time behavior of the root-mean-square error in the estimate of the correction factor of the emission model.

As follows from Fig. 2*b*, the general reduction of the root-mean-square error in estimate of the emission is achieved. Insignificant increase of the estimate after two or three assimilations was conditioned by oscillations of the correction factor.

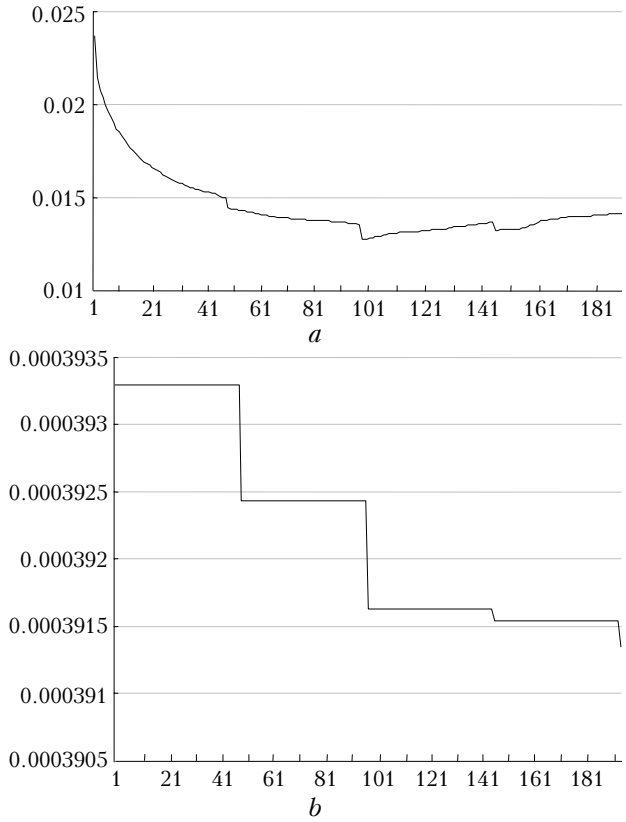

Fig. 1. Root-mean-square error in the estimate of the methane concentration, ppm (*a*), and emission, ppm (*b*). Experiment 1.

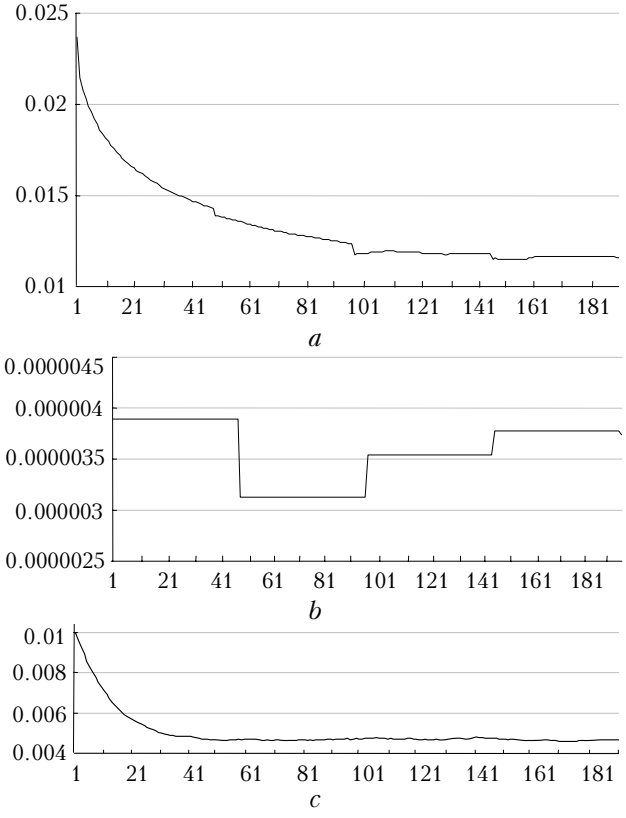

Fig. 2. Root-mean-square error in estimate of the concentration, ppm (*a*), emission, ppm (*b*), and correction factor (*c*); experiment 2.

It should be noted that general level of errors in the concentration field is lower in the second experiment and the emission value is closer to the "true" one in the experiment 2 too.

Conclusion

The numerical experiments discussed enable one to conclude that it is possible to estimate, during the data assimilation, such model parameters as emission.

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