Algorithms based on sensitivity operators for analyzing and solving inverse modeling problems of transport and transformation of atmospheric pollutants

Alexey Penenko$^{1,2}$, Alexander Gochakov$^3$, Vladimir Penenko$^{1,2}$,

$^1$Institute of Computational Mathematics and Mathematical Geophysics SB RAS, ICM&MG SB RAS, prospekt Akademika Lavrentjeva 6, Novosibirsk, 630090, Russian Federation
$^2$Novosibirsk State University, NSU, Pirogova st 1, Novosibirsk, 630090, Russian Federation
$^3$Siberian Regional Scientific-Research Hydrometeorological Institute, Sovetskaya s 30, Novosibirsk, 630099, Russian Federation

E-mail: aleks@ommgp.sscc.ru

Abstract. An application of sensitivity operator-based algorithms to an inverse modeling scenario of urban air quality is presented. A source identification problem and a concentration field continuation problem are solved and analyzed. The analysis of the sensitivity operator allows one to obtain a preliminary estimate of the source identification problem solution.

1. Introduction

Problems that are difficult to solve by standard means often arise when studying the processes of transport and transformation of pollutants in the atmosphere. In particular, they may include inverse modeling tasks, when one needs to consider existing representations of ongoing processes in the form of mathematical models and the available observation data sets about these processes. The configuration of such a task depends on the object of study, the volume and quality of available data and a priori information. In addition to classical inverse problems, inverse modeling problems also include sensitivity assessment and data assimilation problems.

An overview of modern data assimilation algorithms can be found in [1, 2] and source identification algorithms are discussed in [3]. The variational (optimization) approach is a comprehensive tool for inverse modeling [4]. In the paper, we consider an alternative basic aggregate for the construction of an inverse modeling framework, namely the sensitivity relation. The approach is based on ensembles of solutions of adjoint equations and sensitivity operators. It consists of constructing families of sensitivity operators of different dimensions based on the inverse problem, linking the observed characteristics with uncertainty functions. The approach is based on an idea proposed by G. I. Marchuk in [5] and methods of sensitivity theory [4]. Sensitivity operators allow formulating a family of quasi-linear operator equations for the inverse problem, the sets of solutions of which contain the set of solutions of the original problem. Hence the sensitivity operators can be used to both solving and analyzing the inverse problems. Analogous algorithms have been applied to the linear passive transport problem [6] and the nonlinear transport-transformation model with point-wise sources and in situ measurements [7].
The paper’s objective is to present an application of sensitivity operator-based algorithms to an inverse modeling scenario of an urban air quality study for the city of Novosibirsk.

2. Methods
2.1. Problem statement
A convection-diffusion-reaction model for \( l = 1, \ldots, N_c \) is considered in a domain \( \Omega_T = \Omega \times (0,T) \), where \( \Omega \) is a sufficiently smooth approximation of a bounded rectangular domain \([0,X] \times [0,Y]\) in \( \mathbb{R}^2 \), \( T > 0 \). The domain \( \Omega_T \) is bounded by \( \partial \Omega_T = \partial \Omega \times [0,T] \).

\[
\frac{\partial \varphi_l}{\partial t} - \nabla \cdot (\text{diag}(\mu_l) \nabla \varphi_l - \mathbf{u} \varphi_l) + P_l(t,\varphi_l) \varphi_l = \Pi_l(t,\varphi_l) + f_l + r_l, \quad (\mathbf{x},t) \in \Omega_T, \quad (1)
\]

\[
\mathbf{n} \cdot (\text{diag}(\mu_l) \nabla \varphi_l) + \beta_l \varphi_l = \alpha_l, \quad (\mathbf{x},t) \in \Gamma_{\text{out}} \subset \partial \Omega \times [0,T], \quad (2)
\]

\[
\varphi_l = \alpha_l, \quad (\mathbf{x},t) \in \Gamma_{\text{in}} \subset \partial \Omega \times [0,T], \quad (3)
\]

\[
\varphi_l = \varphi^0_l, \quad \mathbf{x} \in \Omega, \ t = 0, \quad (4)
\]

where \( N_c \) is the number of considered substances, \( \varphi_l = \varphi_l(x,t) \) denotes the concentration of the \( l \)-th substance at a point \((x,t) \in \Omega_T\), \( \varphi \) is the vector of \( \varphi_l(x,t) \) for \( l = 1, \ldots, N_c \), will be called the state function, \( L = \{1, \ldots, N_c\} \). The functions \( \mu_l(x,t) \in \mathbb{R}^2 \) correspond to the diffusion coefficients, \( \text{diag}(\mathbf{a}) \) is the diagonal matrix with the vector \( \mathbf{a} \) on the diagonal, \( \mathbf{u}(x,t) \in \mathbb{R}^2 \) is the underlying flow speed. \( \Gamma_{\text{in}} \) and \( \Gamma_{\text{out}} \) are parts of domain boundary \( \partial \Omega_T \) in which the vector \( \mathbf{u}(x,t) \) points inwards the domain \( \Omega_T \) and is zero or points outwards the domain \( \Omega_T \) correspondingly, \( \mathbf{n} \) is the outer normal. The functions \( \alpha_l(x,t), \varphi^0_l(x) \) are boundary and initial conditions, correspondingly, \( f_l(x,t) \) is the a priori known source function, \( r_l(x,t) \) is a source function to be determined with the inverse problem solution (the uncertainty function).

In our approach to inverse modeling, model parameters are divided into “predefined parameters” and “uncertainty functions”. Most often, the uncertainty functions in the air quality studies are unknown sources of pollution. Let \( \mathbf{r} \in Q \), where \( Q \) is the set of admissible sources such that a priori given constraints are fulfilled. Loss and production operator elements \( P_l, \Pi_l : [0,T] \times \mathbb{R}^N_c \rightarrow \mathbb{R}_+ \) are defined by the transformation model (in the considered case of the chemical transformations, they are polynomials with positive time-dependent coefficients). We suppose all the functions and model parameters are smooth enough for the solutions to exist and the further transformations to make sense. Let us define the Direct problem: given \( f_l, r_l, \mu_l, \mathbf{u}, \alpha_l, \varphi^0_l \), find \( \varphi \) from (1) – (4).

Let there be an “exact” source function \( \mathbf{r}^{(*)} \) to be found and \( L_{\text{meas}} \) denote the set of indices of the measured substances. Let \( \varphi^{(*)} \) be the solution of the direct problem with the source function \( \mathbf{r}^{(*)} \). We consider the measurement data combined of:

(i) Image-type measurements: The final concentration field image \( \{\varphi_l^{(*)}(x,T)|x \in \Omega, l \in L_{\text{meas}}\} \).

(ii) In situ measurements: The time series of concentrations \( \{\varphi_l^{(*)}(x,t)|t \in [0,T], x \in \chi, l \in L_{\text{meas}}\} \) in a given set of the measurement sites \( \chi \).

We can consider several relevant inverse modeling problems. The obvious one is the uncertainty function \( \mathbf{r}^{(*)} \) identification problem with the measurement data described above. The second one is the “continuation” problem, which consists of reconstructing \( \varphi^{(*)} \) using the inverse source problem as an auxiliary one. In this case, the concentration fields are continued from observable to unobservable sub-domains (in physical space and time, as well as in the space of chemical species) using the advection-diffusion-reaction model. Hence, the obtained concentration field obeys the model equations.
2.2. Sensitivity-operator based algorithm

For the solution of the source identification problem, we use the algorithm based on the ensembles of the adjoint problem solutions, described in [8, 9]. In the abstract form, the relation between the model state function variation and uncertainty function variation is given by the sensitivity relation

\[ \langle S[r^{(2)}, r^{(1)}]; H, r^{(2)} - r^{(1)} \rangle_Q = \langle H, \delta \varphi \rangle_H, \]  

(5)

where \( S[r^{(2)}, r^{(1)}; H] \) denotes the sensitivity function which is calculated by the solution of the adjoint problem (the details can be found in [9]). The solution of the adjoint problem is determined by its source function \( H \), which is defined by the measurement operator.

If we consider a set of functions \( U = \{ H(\xi) \}_{\xi=1}^{\Xi} \), then combining the corresponding relations, we obtain a sensitivity operator relation

\[ M_U \left[ r^{(2)}, r^{(1)} \right] \left( r^{(2)} - r^{(1)} \right) = H_U \varphi \left[ r^{(2)} \right] - H_U \varphi \left[ r^{(1)} \right], \]

(6)

where

\[ M_U \left[ r^{(2)}, r^{(1)} \right] z = \sum_{\xi=1}^{\Xi} e^{(\xi)} \left\langle S[r^{(2)}, r^{(1)}; H^{(\xi)}], z \right\rangle_Q, \quad H_U \varphi = \sum_{\xi=1}^{\Xi} e^{(\xi)} \left\langle H^{(\xi)}, \varphi \right\rangle_H. \]

The adjoint functions needed to compose the sensitivity operator can be evaluated in parallel, as an ensemble.

Combining ensembles of solutions of adjoint equations corresponding to different measurement data types into one sensitivity operator allows us to consider heterogeneous monitoring networks. This is an important feature since the modern monitoring systems provide various types of information: it can be point-wise (in situ) measurements in space and time of concentrations of pollutants [10], time series of concentrations at monitoring stations [8, 11], images of concentration fields (similar to [9,12]), etc.

If \( r^{(*)} \) is the exact solution of the source identification problem, \( I \) is the measurement data, aggregated in the state-function form, and \( \delta I \) is its perturbation, then for any \( U \) and \( r \) the relation holds:

\[ M_U \left[ r^{(*)}, r \right] \left( r^{(*)} - r \right) = H_U I + H_U \delta I - H_U \varphi \left[ r \right]. \]

(7)

This quasi-linear operator equation can be solved based on the regularized TSVD Newton-Kantorovich method [9]. The ensemble of the adjoint problem solutions is optimized according to the maximal projection of the initial discrepancy to the appropriate trigonometric cosine-basis [13].

Using the projection on the orthogonal complement to the sensitivity operator kernel, we can estimate what can be found from the available data without solving the inverse problem [8, 9]. Another useful aggregate is the diagonal of the projector mentioned above, which allows one to assess the “observability” (“illumination” in the terminology of [6]) of the sources on a particular territory by the existing monitoring system. This diagonal has the same dimensionality as the uncertainty function and can be analyzed in the same way.

2.3. Inverse modeling scenario

Let us demonstrate some of the approach’s features using the example of an urban air quality assessment scenario for Novosibirsk city. To prepare the coefficients of the chemical transport model (1)-(4), the meteorological parameters \( u \) and \( \mu \) are calculated with the WRF model [14] in the area limited by geographic coordinates 54.75° - 55.16°, 82.66°- 83.37°, corresponding to Novosibirsk city. The calculations were made for the model period 12:00-14:00 July 09,
Figure 1. “Exact” solution of the source identification problem (a). Projection of the “Exact” solution to the orthogonal complement of the sensitivity operator kernel (b). Illumination function (c). Source identification result (d). The domain where the illumination function value is less than 1% of its maximal value is marked with red.

2019. To obtain 2D spatial wind speed fields, the 3D WRF fields were vertically averaged. The domain parameters for the numerical inverse problem solution are $X = 35613 m$, $Y = 34697 m$, $T = 2 \times 3600 s$ and the grid parameters are: $N_x = 50$, $N_y = 49$, $N_t = 232$.

The sources were located in the places of the city’s roads, marked by contours in figure 1 (a). The sources emitted NO with constant rates, which were proportional to the total number of cars in the specified location for the whole interval. 2GIS Company provided information about the road traffic intensity. The emitted substance name and the constant emission regime are known in the inverse modeling scenario. Emission rates are a priori considered as non-negative. Another information about the sources of emission was considered as unavailable.

The locations of the measurement sites (marked by red circles in figure 1 (a)) were taken from the state report [15]. Measurement sites provide time-series of the concentrations for the model time interval. Image-type data is obtained as the final image of the concentration field.
Figure 2. Relative error versus computation time of source identification problem (a) and continuation problem (b). The computation time is measured in direct problem solution times. The relative error of the “continuation” with respect to model time (c). “Combined,$O_3$” curve corresponds to the case when the source of $NO$ is identified from $O_3$ measurements, i.e., “indirect” measurements. “Combined,$NO$” curve corresponds to the case when the source of $NO$ is identified from $NO$ measurements, i.e., “direct” measurements. “Background” corresponds to the experiment without using the measurement data.

In the numerical experiments, the concentrations of $O_3$ or $NO$ are measured. The reactions set is defined by the RADM2 transformation mechanism [16] with 61 reacting species and time-dependent reaction rates [17,18].

3. Results

In figure 1 we compare the source identification results with “indirect” $O_3$ measurements to the exact solution and the preliminary estimates. Figure 1 (b) shows the “Exact” source function’s projection to the orthogonal complement of the sensitivity operator kernel. Figure 1 (c) shows the illumination for the heterogeneous monitoring system. In figure 1 (d), the source reconstruction result is presented. The domain where the illumination function value is less than 1% of its maximal value is marked with red.

The figures 1 (b) and (c) allow one to evaluate the effectiveness of the inverse problem solution (figure 1 (d)). The computation time for obtaining these estimates is approximately equal to the time of one iteration of the inverse problem solution algorithm.

In figure 2, the convergence parameters of the algorithm are presented. Relative errors with respect to the computation time of the source identification problem and continuation problem are presented in figure 2 (a) and (b) correspondingly. In figure 2 (b), the relative error of reconstructing $NO$ concentration field is presented. The computation time is measured in direct problem solution times. Relative error with respect to the model time is presented in figure 2 (c). “Combined,$O_3$” curve corresponds to the case when the source of $NO$ is identified from $O_3$ measurements, i.e., “indirect” measurements. “Combined,$NO$” curve corresponds to the case when the source of $NO$ is identified from $NO$ measurements, i.e., “direct” measurements. “Background” corresponds to the experiment without using the measurement data.

Analyzing the values in figure 2, we can conclude that the continuation problem solution has lower relative errors than that of the source identification problem.
4. Discussion
An important advantage of the adjoint ensemble approach for inverse modeling is that various problems are reduced in a unified form to a family of quasilinear operator equations, due to the properties of adjoint equations and sensitivity relations. In this case, the choice of the uncertainty functions determines the sensitivity functions used. The latter are calculated with the adjoint equation’s solutions. The adjoint equation structure is determined by a direct problem linearization, i.e., by a process model. In turn, the measurement data determine the sources for the adjoint equation. Another important advantage is that the approach takes the solution of ensembles of independent adjoint problems. Therefore the elaborated algorithm may be naturally parallelized.

The quasi-linear structure of the resulting operator equation admits using linear analysis tools to estimate the inverse problem properties. Since the solving of the inverse problem may take a significant amount of time, compared to the solution of the direct problem, it is advantageous to have an express estimate of the inverse problem solution quality that can be achieved in the given conditions.

5. Conclusion
The sensitivity operator-based approach can be considered as a useful tool for solving and analyzing various inverse modeling problems of air quality.

Acknowledgments
The construction of the modeling scenario, the algorithm’s adaptation to the conditions of Novosibirsk city, and the numerical experiments were carried out with financial support of the Russian Foundation for Basic Research and the Novosibirsk Region Government under scientific project 19-47-540011. 2GIS Company provided information about the road traffic intensity. The continuation problem analysis was supported by the Russian Foundation for Basic Research under project 20-01-00560.

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