J. KOSAE Vol. 19, No. E2 (2003) pp. 75~81
Journal of Korean Society for Atmospheric Environment

Variational Data Assimilation for Optimal Initial Conditions in Air Quality Modeling

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(Received 6 March 2003, accepted 22 May 2003)

Abstract

Variational data assimilation, which is recently introduced to the air quality modeling, is a promising tool for obtaining optimal estimates of initial conditions and other important parameters such as emission and deposition rates. In this paper, two advanced techniques for variational data assimilation, based on the adjoint and quasi-inverse methods, are tested for a simple air quality problem.

The four-dimensional variational assimilation (4D-Var) requires to run an adjoint model to provide the gradient information in an iterative minimization process, whereas the inverse 3D-Var (I3D-Var) seeks for optimal initial conditions directly by running a quasi-inverse model.

For a process with small dissipation, I3D-Var outperforms 4D-Var in both computing time and accuracy. Hybrid application which combines I3D-Var and standard 4D-Var is also suggested for efficient data assimilation in air quality problems.

Key words : Air quality modeling, Data assimilation, Variational methods, Adjoint model, Quasi-inverse model

1. INTRODUCTION

Air quality modeling, used for predicting future states of atmospheric pollutants, inherently includes uncertainties in input parameters (e.g., meteorological conditions, emissions, initial and boundary conditions for pollutants, empirical constants, etc.) (see, e.g., Seinfeld, 1988). Especially, tropospheric chemistry is largely affected by emissions and the absorption of constituents by surface interactions. Therefore, providing accurate estimates of the initial states and emission rates is essential for improving the air quality prediction.

Accurate initial states and emissions can be estimated by solving the *inverse* problems. For given measurements of observable quantities, an inverse problem aims at obtaining the values of model parameters, including initial states (Tarantola, 1987). The inverse problems in meteorology often involve solving variational problems for *data assimilation*, which denotes a process that blends all available observations with model to produce an accurate estimate of initial states.

Until recently, assimilations in atmospheric chemistry have favorably employed simple methods such as optimal interpolation and nudging (e.g., Collins *et al.*, 2001; Austin, 1992). An advanced assimilation, using the variational inverse modeling, was first introduced

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in stratospheric chemistry simulation by Fisher and Lary (1995) and was expanded to tropospheric gas phase mechanism by Elbern *et al.* (1997).

One of the most important inverse modeling applications in atmospheric chemical transport is to estimate emissions or surface fluxes using observed concentrations, mainly due to the uncertainties involved in emission estimation. There exist several different approaches for inverse modeling of airborne emissions such as the Green's function (Enting, 2000), Bayesian inversion (Bergamaschi *et al.*, 2000), the adjoint of a chemical transport model (Pudykiewicz, 1998), and the four-dimensional variational data assimilation (4D-Var; Elbern *et al.*, 2000a, b).

Another category of advanced data assimilation is represented by Kalman filter, in which forecast error covariances are computed every time step. This method will not be covered in this study; for interested readers, several references related to this category can be found for a review (Ghil and Malanotte-Rizzoli, 1991) and for applications to air quality problems (e.g., van Loon *et al.*, 2000; Zhang *et al.*, 1999; Hartley and Prinn, 1993).

Unlike meteorological prediction, the issue of finding correct initial conditions with the aid of observations (i.e., data assimilation) has received relatively less attention until now. Two major reasons for this, as indicated by Elbern *et al.* (1997), are: 1) measurement sites of chemical constituents are very sparse (i.e., highly localized), and 2) chemistry-transport simulations are mostly controlled by emission and deposition process rather than by initial values. However, these problems can be treated by adopting advanced data assimilation methods that can handle with all available observations distributed in both space and time. Especially, in the 4D-Var framework, parameters (e.g., emission and deposition rates, surface fluxes, etc.) as well as initial and/or boundary conditions can be optimized simultaneously.

The feasibility of 4D-Var for comprehensive tropospheric chemistry problem has been demonstrated for initial conditions (Elbern *et al.*, 1997), for emissions of various chemical species (Elbern *et al.*, 2000a, b), and for synthetic conditions (Elbern and Schmidt, 1999). The 4D-Var allowed to obtain initial states for air pollution modeling even when only sparse observations are available (Elbern *et al.*, 1997). Elbern *et al.* (2000b) analyzed the emission rates of unobserved NO by applying the 4D-Var with observations of ozone only. As demonstrated, the 4D-Var has been successfully applied to deduce emission estimates for specific time periods of interest as well as optimized initial conditions for air quality models.

Originally the variational approach has been introduced into meteorology by Sasaki (1958). The 4D-Var, which is the most advanced framework of the variational approach, has been recognized as a promising tool for yielding dynamically-balanced optimal initial conditions for numerical forecast problems (see reviews by Talagrand, 1997; Park and Županski, 2003). In the 4D-Var, a *cost function*, which is defined as the weighted squared distance between model solutions and observations, is minimized via iterative processes.

At each iteration, the 4D-Var requires to run the forward model (e.g., nonlinear air quality model), its corresponding adjoint model and a minimization algorithm. Integration of the adjoint model provides the gradient information required by minimization algorithms (see Gill *et al.*, 1981 for a review). In minimizing the cost function, most algorithms require several tens of iterations to reach a local minimum of the cost function. This causes the most unfavorable problem in operational application of the standard 4D-Var due to a huge computational demand.

Recently an efficient variational assimilation scheme, called the *inverse 3D-Var* (I3D-Var), is developed based on the inverse model integration (Kalnay *et al.*, 2000). In the I3D-Var, the observational increment at initial time is obtained by a backward integration of the tangent linear model, in which the sign of time step is changed (i.e., *inverse*). Here, the sign of dissipative terms is also changed in order to avoid computational blow-up (i.e., *quasi-inverse*).

It is demonstrated that the I3D-Var solves the minimization problem close to the 4D-Var at much less computational cost (e.g., Kalnay *et al.*, 2000; Leslie *et al.*, 2000).

In this study, application of variational data assimilation will be illustrated to obtain optimal initial conditions for an air quality problem represented by a simple transport (advection) and diffusion process, using both the adjoint approach (standard 4D-Var) and the quasi-inverse approach (I3D-Var). Although estimation of other parameters can be also obtained by the variational assimilation, it is not covered here. Section 2 provides theoretical background on the adjoint and quasi-inverse approach in variational assimilation, and section 3 describes model and experiment design. Results and conclusions appear in section 4 and 5, respectively.

2. BRIEF THEORETICAL BACKGROUND

Let us assume that a forward model describing time evolution of pollutants is represented by a nonlinear propagator M operating on the initial state vector $\mathbf{X}_0$ (i.e., nonlinear model):

$$\mathbf{X}_t = M\mathbf{X}_0. \tag{1}$$

Taking the first-order (linear) term of the Taylor expansion of (1), for small perturbations $\delta\mathbf{X}_0$ in the vicinity of $\mathbf{X}_0$, yields the tangent linear model:

$$\delta\mathbf{X}_t = L\delta\mathbf{X}_0 \tag{2}$$

where L is a tangent linear operator. Using the adjoint approach, the gradient of any scalar function of the output state vector, $\mathrm{J}(\mathbf{X}_t)$, with respect to input parameters is given by

$$\nabla_{\mathrm{X}_0}\mathrm{J} = L^{*}\nabla_{\mathrm{X}_t}\mathrm{J} \tag{3}$$

where L^{*} is the adjoint operator of L (see Friedman, 1956). This is the adjoint model of (2). In practice, the state vector $\mathbf{X}$ is extended to include all parameters (physical/computational) of the model and J itself (Park and Droegemeier, 1997; Waelbroeck and Louis, 1995).

Using the quasi-inverse approach, one can obtain the initial perturbation fields ($\delta\mathbf{X}_0$) by solving directly (2):

$$\delta\mathbf{X}_0 = L^{-1}\delta\mathbf{X}_t \tag{4}$$

where L^{-1} is the inverse of L. With this formulation, one can trace the short-range forecast error back to ini-tial time. Since the small dissipative terms are irreversible, it is not possible to obtain the "exact-inverse" linear model. In practice, L^{-1} is approximated by the "quasi-inverse" linear model by either changing the sign of dissipative terms to avoid computational instability or neglecting the dissipative terms (Kalnay *et al.*, 2000).

The above-derived adjoint and quasi-inverse linear models can be used to solve an optimization problem such as variational data assimilation. By definding J as the cost function, the adjoint model provides the gradient information (i.e., $\nabla_{\mathrm{X}_0}\mathrm{J}$) which is essential for most minimization (or optimization) algorithms (see Gill *et al.* 1981 for a review on various algorithms).

For example, $\nabla_{\mathrm{X}_0}\mathrm{J}$ is used to obtain optimal initial conditions from uncertain initial analysis fields ($\mathbf{X}_0$) (e.g., Ayotte, 1997; Elbern *et al.*, 1997). The quasi-inverse model produces an increment in initial conditions $\delta\mathbf{X}_0$ that optimally corrects a perceived forecast error at the final time t (see Kalnay *et al.*, 2000).

3. MODEL DESCRIPTION AND EXPERIMENT DESIGN

A simple advection-diffusion model including a passive scalar transport is employed to represent a simplified air quality problem. Here the chemical reaction processes are omitted for simplicity. For an advection velocity u and a passive scalar q, the model equation is given by:

$$\frac{\partial \mathrm{u}}{\partial t} = -\mathrm{u}\frac{\partial \mathrm{u}}{\partial \mathrm{x}} + \nu\frac{\partial^2 \mathrm{u}}{\partial \mathrm{x}^2}$$

$$\frac{\partial q}{\partial t} = -u\frac{\partial q}{\partial x} + \nu\frac{\partial^2 q}{\partial x^2} \tag{5}$$

where

$$u = \bar{u} + \delta u, \quad q = \bar{q} + \delta q$$

and ν is diffusion coefficient. Note that the interaction bewteen u and q in Eq. (5) occurs in one way, i.e., only from u to q. The adjoint and quasi-inverse linear models are developed for this nonlinear model.

In this experiment, numerical computations are conducted by employing the leapfrog/DuFort-Frankel scheme (see Anderson *et al.*, 1984). The initial conditions are given by the sine functions and the boundaries are fixed to zero.

The assimilation period is set to N = 101 or 121, where N is the number of time steps. The validity of tangent linear and quasi-inverse linear models has been tested in various aspects. For this experiment, the diffusion coefficient is set to $\nu = 1 \times 10^{-3}$. For the minimi-zation process in the standard 4D-Var, the limited-memory Broyden-Fletcher-Goldfarb-Shanno (LB-FGS) algorithm (Liu and Nocedal, 1989) is used. The quasi-inverse linear model is solved by changing the sign of diffusion terms.

4. RESULTS

Variational data assimilation experiments were performed using both standard 4D-Var and I3D-Var methods for simulated observations. The iterative 4D-Var process is provided in Fig. 1. As illustrated, one iteration of 4D-Var involves running a forward non-linear model and a backward adjoint model, and conducting a minimization process. Meanwhile, iterative process of I3D-Var does not include the minimization process, thus saving computing time.

Figure 2 represents the performance of two methods (i.e., standard 4D-Var vs. I3D-Var) for assimilation period N = 121. Here, the 4D-Var incorporates observations at all time steps while the I3D-Var takes observation only at the end of the assimilation period. With the I3D-Var the cost function converges to 10^{-14} of its original value after 7 iterations. However, the 4D-Var with complete observations requires 45 equi-

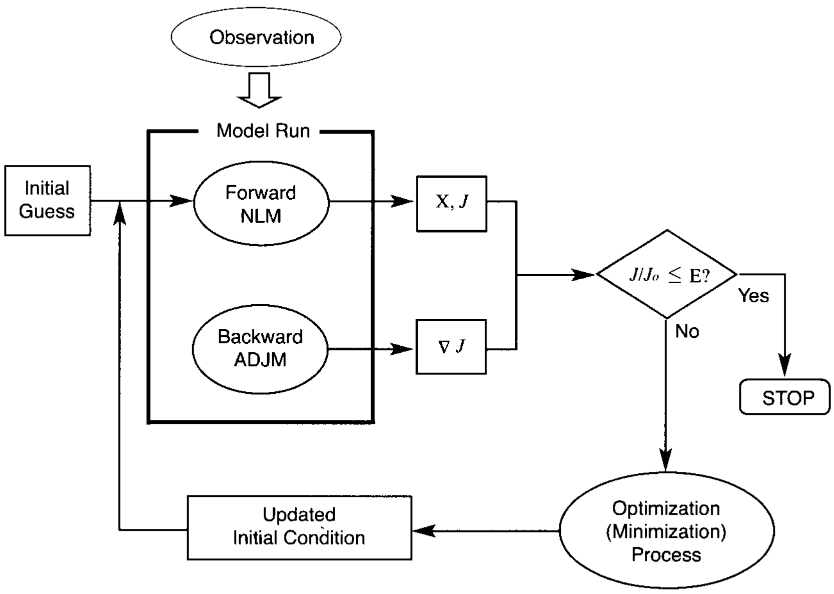

Fig. 1. Iterative process in standard 4D-Var.

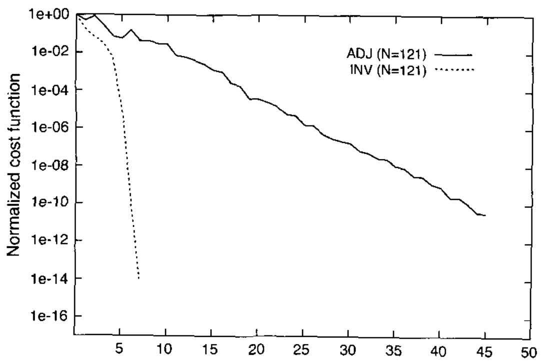

Fig. 2. Convergence rate of cost functions using adjoint 4D-Var (ADJ) and inverse 3D-Var (INV) as a function of ICALL (*number of calls for the nonli-near* model and adjoint or inverse model). For the adjoint 4D-Var, observations are incorporated at all time steps time steps. *The initial error magnitude* is 50 % for u. The diffusion coefficient is set to ν = 1 × 10^{-3} and the assimilation period is N = 121 time stpes.

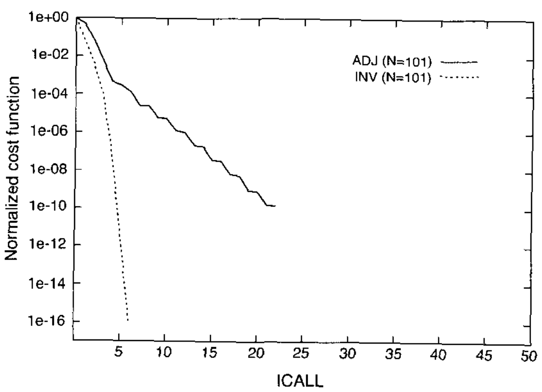

Fig. 3. Same as in Fig. 2 but for N = 101.

valent model integrations for the cost function converges to 10^{-10}. That is, even with much less observations, the I3D-Var achieves the minimization with less computing time and better accuracy than the 4D-Var does.

In Fig. 3, the same experiment is performed for a shorter assimilation period (N = 101). The I3D-Var requires 6 iterations to minimize the cost function at the accuracy of 10^{-16} while the 4D-Var with full observations requires 22 iterations at the accuracy of 10^{-10}. Overall, with a shorter assimilation period, both the I3D-Var and 4D-Var show better performance in computing time, especially with 4D-Var. The I3D-Var outperforms the 4D-Var in accuracy when the assimilation period becomes shorter.

Leslie *et al.* (2000) has recently compared the performance of 4D-Var and I3D-Var for forecasting more than 40 cases of tropical cyclones using a three-dimensional meteorological model. They demonstrated that the I3D-Var is 8 times faster than the 4D-Var with similar accuracy. This saving in computing time implies significant saving in computational resources in operational applications.

Recently, Park and Županski (2003) proposed a hybrid method which combines the I3D-Var and the standard 4D-Var. This is based on the idea that, although the I3D-Var may not replace the full 4D-Var due to problems with dissipation and microphysics, it may serve as a preconditioner when carrying minimization in the framework of the 4D-Var. That is, one may employ the I3D-Var for the first few iterations then switch to the 4D-Var using the I3D-Var results as the initial guess field. With this strategy, the computing time is still much less compared to the cases using just standard 4D-Var.

5. CONCLUSIONS

In this study, two variational assimilation techniques are tested for an air quality problem represented by a simple advection-diffusion model that includes a passive transport variable. Here, the standard 4D-Var is based on the adjoint approach while the inverse 3D-Var (I3D-Var) is based on the quasi-inverse approach. Both are advanced assimilation methods that combine observations scattered in both space and time, climatological and other a priori knowledge, and numerical model in dynamically consistent way.

In the standard 4D-Var, the cost function is minimized by employing an iterative minimization algorithm which requires the gradient information. Thus an adjoint model run is required to provide such gradient information into the minimization algorithm. In I3D-Var, a quasi-inverse linear model is run to minimize the cost function by directly obtaining the optimal increment.

Our results show that, for not too large diffusion process, the performance of I3D-Var is much better than that of standard 4D-Var. For a model with complex microphysics and large diffusion process, the hybrid method combining I3D-Var and 4D-Var can be employed to accelerate the minimization of the cost function. Especially in the air quality prediction system in which the diffusion process is very important, it is strongly recommended to apply the hybrid strategy in designing and performing the four-dimensional variational data assimilation.

There exist several factors that are essential for successful 4D-Var and/or I3D-Var (see a review by Park and Županski, 2003). Especially, in applying variational methods to air quality models, one should pay special attention when chemical reactions are strongly *nonlinear*. Since the adjoint and quasi-inverse linear models are based on the tangent linear approximation, a strongly nonlinear process causes this approximation to be invalid (Park and Droegemeier, 1997). Thus it may induce incorrect gradient and increment information through the adjoint and quasi-inverse linear model, respectively, in the variational optimization. Nonlinearity may also cause alteration in the geometry of cost function by generating multi-minima, plateau, and even a forbidden region (see Park and Županski, 2003). One possible way to alleviate this problem is to make the assimilation window short enough to suppress excessive increase of nonlinearity.

Overall, the variational data assimilation is a promising tool in air quality modeling for optimal estimation of important parameters (e.g., emission rates) as well as initial and boundary conditions. The problem with a large amount of computational resources required by the standard 4D-Var can be alleviated by adopting efficient alternative methods such as I3D-Var or combining both 4D-Var and I3D-Var (i.e., hybrid approach). Although this study has focused on obtaining optimal initial states, the variational assimilation method is also capable of estimating several important parameters in air quality modeling such as emission and deposition rates, surface flux, etc. Further studies are necessary to investigate the usefulness of I3D-Var in estimating such parameters.

ACKNOWLEDGMENT

The author acknowledges graduate students, especially Ms. Eunsue Jo, of the Hydrometeorology Laboratory, Ewha Womans University for their help.

This research is partly supported by the Advanced Basic Research Laboratory Program (R14-2002-031-01002-0) of the Korean Science and Engineering Foundation.

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