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Sensitivity analysis applied to a variational data assimilation of a simulated pollution transport problem

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SUMMARY

Understanding the impact of the changes in pollutant emission from a foreign region onto a target region is a key factor for taking appropriate mitigating actions. This requires a sensitivity analysis of a response function (defined on the target region) with respect to the source(s) of pollutant(s). The basic and straightforward approach to sensitivity analysis consists of multiple simulations of the pollution transport model with variations of the parameters that define the source of the pollutant. A more systematic approach uses the adjoint of the pollution transport model derived from applying the principle of variations. Both approaches assume that the transport velocity and the initial distribution of the pollutant are known. However, when observations of both the velocity and concentration fields are available, the transport velocity and the initial distribution of the pollutant are given by the solution of a data assimilation problem. As a consequence, the sensitivity analysis should be carried out on the optimality system of the data assimilation problem, and not on the direct model alone. This leads to a sensitivity analysis that involves the second-order adjoint model, which is presented in the present work. It is especially shown theoretically and with numerical experiments that the sensitivity on the optimality system includes important terms that are ignored by the sensitivity on the direct model. The latter shows only the direct effects of the variation of the source on the response function while the first shows the indirect effects in addition to the direct effects. Copyright © 2016 John Wiley & Sons, Ltd.

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1. INTRODUCTION

The ability to know with accuracy the effect of the change of pollutant emission from a foreign region onto a target region would help decision-makers to improve public health and protect the environment. Also, the knowledge of the exact location where change in emission could impact a target region within a given time scale is an asset in choosing the right place for some events, the storage location or the transit route for delicate products. Studies have shown that the change in pollutant emission from a foreign region could have a significant impact on a target or response region, even at the intercontinental level. This is the case for the degradation of air quality over remote continents [1–4]. Some air pollution episodes in the USA were reported to be associated with transpacific transport events [5, 6]. During the last decades, ground-based measurements and satellites remote sensing have provided evidence for foreign influence of pollutants [6–9]. The time scale for the influence of a remote source on a receptor region is highly dependent on weather conditions: [5] shows that under certain weather conditions, Asian emissions can be transported to North America

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within 5 to 8 days. As underlined by [10–13], attributing a given pollution to a specific source is complicated by the interplay of processes influencing the transport (export from the source region, the evolution in transit because of chemical and the depositional losses, dilution, and mixing with local species over the receptor region). As it is difficult to diagnose source–receptor relationships from observation, such analysis rely on models: [13] uses a set of 21 numerical models to estimate the intercontinental source–receptor relationships for ozone pollution; [14] made a similar study based on a high resolution model.

In classical approaches, the analysis of the source–receptor relationship, also known as the sensitivity of the receptor to the sources, is limited to direct simulations: simulations are carried out based on a given state of the source and some perturbation of the same state. The variability over the receptor is considered as the sensitivity of the response region to this source. Examples of such studies include [13–19]. Such approaches have some limitations: the computed sensitivity is a rough approximation of the true sensitivity that is mathematically defined as the gradient of the response function (defined over the response region) with respect to the source. The number of simulations grows with the numbers of sources or groups of sources considered in the sensitivity problem. Classical approaches are computationally limited in the number of sources for point sources and the spatial resolution for extended sources. Those limitations can be remedied by the adjoint approach, which is a mathematically rigorous and efficient algorithmic framework for the sensitivity analysis, especially when the quantity of interest (response function) is known only implicitly as a function of the parameters (source function), with respect to which the sensitivity is needed. This is the case for the pollution with all the intermediate processes mentioned earlier. The adjoint approach allows, in a single run of the adjoint model, the computation of the sensitivity of a given response function (defined on a space-time point or domain) to the global distribution of sources over the physical and temporal domain of the model. The adjoint approach has been used for the problem of pollutant transport to Hawaii [20, 21], intercontinental transport of aerosol to the USA [22], regional sensitivity analysis for ozone pollution episodes [23–25], and intercontinental source analysis of ozone pollution in some US sites [26–28]. Additional applications of the adjoint approach of the sensitivity can be found in [29–35]. The general theory and application of the sensitivity analysis using adjoint and non-adjoint methods can be found in [36–39] and references therein.

Usually, the adjoint approach as stated earlier and found in the literature implicitly supposed that the dynamics (e.g., transport velocity) of the system transporting the pollutant is known exactly. The same implicit assumption is made for the initial state of the pollutant. However, this is not the case in practice. The dynamic and the initial state of the pollutant and perhaps some other parameters of the model are given as the solution of a data assimilation problem. For example, satellite observation of CO_2 are used in the estimation of carbon source/sink/fluxes [40–43]. The observation of CO_2 is sometimes used indirectly in the derivation of Atmospheric Motion Vector that are subsequently used in atmospheric data assimilation systems, see [44] and the references therein. The absorption properties of CO_2 are also intensively used to derive observations that are routinely used in data assimilation, for example, temperature profile. The sensitivity with respect to the source must account for all these processes and can only be performed if the sensitivity is applied to the optimality system [45–47], involving the second-order adjoint. A number of studies pointed out that the second-order adjoint method is more accurate than the first-order adjoint method in the presence of data, see for example [45, 47–49].

It is important to mention that [38, 39] use the second-order adjoint to compute sensitivities. The author proposes a method to compute the second-order functional derivatives of physical response systems using the second-order forward and adjoint sensitivity analysis procedures. The difference with the present work is that we focus on the first-order sensitivity (first-order derivatives) in the presence of variational data assimilation. The second-order adjoint is the consequence of the derivation of the optimality system of variational data assimilation, which is based on the first-order adjoint of the model.

Hereafter, direct model sensitivity refers to the sensitivity analysis applied to the direct model and optimality system sensitivity refers to the sensitivity analysis applied to the optimality system of variational data assimilation. In both cases, we are interested only in the sensitivity analysis based on the adjoint method. In this paper, we give a thorough analysis of the theoretical differences between

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the direct model sensitivity and the optimality system sensitivity for the general case of the problem of pollution and a verification through numerical examples for a particular case. We also verify that features captured only by the optimality system sensitivity are factual.

The remaining part of the paper is organized as follows: In Section 2, we state the general problem and give the summary of the direct model sensitivity and the optimality system sensitivity in a problem of pollution. In Section 3, we analyze the differences between the direct model sensitivity and the optimality system sensitivity. In Section 4, a one-dimensional example is given. Results of the direct model sensitivity and the optimality system sensitivity are compared, and Section 5 concludes the paper.

2. SENSITIVITY ANALYSIS

2.1. Statement of the problem

Let us consider a geophysical system (e.g., ocean, atmosphere, and river) in which the state X evolves according to a given mathematical model F. By state of the system, we mean the set of variables that describes the system at any time and at every point of the physical space (Ω). For example, the system state in ocean models includes but is not limited to temperature, surface elevation, salinity, and horizontal components of the velocity. We further consider a passive tracer or pollutant evolving under the dynamic of the geophysical system. By passive, we mean that the tracer/pollutant has no effect on the dynamic of the system. The case of an active tracer follows the same methodology. The passive tracer is quantified by its concentration C that is a function of the physical space and of the time. The evolution of C is given by a mathematical model G and its emission is given by a space-time source function S. We define the response region (A), a subdomain of Ω, to be the region of interest and the response window to be the time window of interest. Let the function r be the measure of some effect of the pollutant in the response region during the response window. r is hereafter referred to as the response function. For example, r can be the measure of the contamination of the response region during the response window. Another example of r is the number of cases of a disease in the population (of human, animals, or vegetation) due to the pollutant, or equivalently the cost of treatment of such diseases. The development in this paper will consider the response function to be an aggregation function over the response region and the response window. For instance, the illustrations in this paper define the response r to be the average of the concentration C of the pollutant over the response region during the response window.

This paper aims to determine the sensitivity of the response function r to the source function S in the sensitivity window, the latter being the time window in which the gradient of S is of interest. We assume that X and C are the solution of a data assimilation problem. The observations used in the data assimilation problem are measurements of X and of C. We will require the functions F and G to be twice differentiable in all their variables, and the response function r to be differentiable with respect to all its variables. The Gâteaux differentiability is sufficient in this study.

The source function being an input of the data assimilation problem, if the assimilation window intersects the sensitivity window, then a change in the source function also induces a change in X and in C that must be accounted for in the sensitivity analysis. This can only be performed when the sensitivity analysis is applied to the optimality system. However, if the assimilation window does not intersect the response window, the direct model sensitivity can be used to determine the sensitivity of the response function with respect to the source function.

2.2. Mathematical considerations

For the developments in this section, we consider X to be given. The evolution model for X in the general case will be given in Section 2.4.

2.2.1. Evolution model. The pollutant, considered as a passive tracer, is described by its concentration whose evolution is given by the following equations:

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$$\frac{dC}{dt} = G(X, C, S) \text{ in } \Omega \times [0, T], \tag{1}$$

$$C(0) = V, \tag{2}$$

where C is the concentration of the pollutant, S is the space-time source function of the pollutant, X is the state of the geophysical system, G is a function that describes the evolution of the concentration C under the dynamics defined by X, Ω is the physical domain of the system, and $[0, T]$ is the time interval of interest. For example, Equations (1)–(2) can be the transport and diffusion of the pollutant by the velocity fields of the atmosphere.

2.2.2. Sensitivity problem. Let Ω_A, a sub-domain of the physical space Ω be the response region, and φ the function giving the measure of the effect of interest, or the 'effect of the pollutant', of which we want to evaluate the sensitivity with respect to the source. φ is a function of the concentration C and of the source S. We define the response function as

$$r_A(C, S) = \int_0^T \left\langle 1_{\Omega_A}, \varphi(C, S) \right\rangle dt. \tag{3}$$

where 1_{Ω_A} is the indicator function of Ω_A defined as:

$$1_{\Omega_A}(x) = \begin{cases} 1, x \in \Omega_A \\ 0, x \notin \Omega_A \end{cases} \tag{4}$$

In the simplest case, $\varphi(C, S) = C$ and r is the integral of C over the response region and the response window.

2.3. *Sensitivity analysis applied to the direct model*

By definition, the sensitivity with respect to the source S is the gradient of the response function r with respect to S.

It can be shown (e.g., [47, 50]) that this gradient is given by

$$\nabla_S r_A = \left[\frac{\partial G}{\partial S}\right]^t \Lambda_1 + \left[\frac{\partial \varphi}{\partial S}\right]^t 1_{\Omega_A} \tag{5}$$

where Λ_1 is the solution of the first-order adjoint of the model given by

$$-\frac{d\Lambda_1}{dt} = \left[\frac{\partial G}{\partial C}\right]^t \Lambda_1 + \left[\frac{\partial \varphi}{\partial C}\right]^t 1_{\Omega_A}, \tag{6}$$

$$\Lambda_1(T) = 0, \tag{7}$$

Equation (5) gives the solution of the sensitivity problem on the direct model alone. It uses the first-order adjoint of the transport model and shows the direct effects of the variation of the source on the response function. It is assumed that the state of the geophysical system and the initial concentration of the pollutant are known exactly. However, this is not the case for real-life problems as mentioned in Section 1. Most of the time, X and C are the solution of a data assimilation problem. In those cases, if the assimilation window intersects the sensitivity window, then the change in the source function also induces a change in X and in C that must be accounted for in the sensitivity analysis. This can only be performed if the sensitivity analysis is applied to the optimality system.

2.4. *Sensitivity analysis applied to the optimality system*

In this section, we consider the general case where the state of the system and the concentration of the pollutant are given by the solution of a data assimilation problem.

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2.4.1. Data assimilation problem. Let us assume that the state variable X satisfies, between time 0 and time T the differential system:

$$\frac{dX}{dt} = F(X), \tag{8}$$

$$X(0) = U \tag{9}$$

and the concentration C of the pollutant evolves according to Equation (1), which is rewritten for convenience:

$$\frac{dC}{dt} = G(X, C, S), \tag{10}$$

$$C(0) = V. \tag{11}$$

As defined by Equations (8) and (10), X and C also depend on their initial state $X(0)$ and $C(0)$. Given observation X_{obs} of X and C_{obs} of C, data assimilation defines the optimal initial state U^* and V^* as the argument of the minimum of the following cost function:

$$\begin{aligned} J(U,V) =& \frac{1}{2}\|U - U_b\|^2_{\mathbf{B_u}^{-1}} + \frac{1}{2}\|V - V_b\|^2_{\mathbf{B_v}^{-1}} \\ &+ \frac{1}{2}\int_0^T \|H_{\mathbf{x}}X - X_{obs}\|^2 dt + \frac{1}{2}\int_0^T \|H_{\mathbf{c}}C - C_{obs}\|^2 dt, \end{aligned} \tag{12}$$

where $H_{\mathbf{x}}$ is the observation operator that maps the variable X to the space of observations X_{obs} and $H_{\mathbf{c}}$ is the observation operator that maps the space of concentration toward the space of observations of concentration, $\|U - U_b\|^2_{\mathbf{B_u}^{-1}}$ and $\|V - V_b\|^2_{\mathbf{B_v}^{-1}}$ are regularization terms introduced for the well posedness of the problem, U_b and V_b are the first guess also known as background in data assimilation given by previous forecasts. $\mathbf{B_u}$ and $\mathbf{B_v}$ are the background covariance matrices corresponding to U_b and V_b, respectively; the background errors are assumed Gaussian. For the simplicity of the presentation, the observation operators H_X and H_C are assumed to be linear. However, observation operators are not linear in the general case. Without theoretical or practical difficulty, nonlinear observation operators can be accounted for by developing their tangent linear and adjoint counterpart.

The optimal initial conditions U^* and V^* that minimize J are solutions of the optimality system which is the Euler–Lagrange equation involving the gradients of J with respect to U and V. The optimality system is given by

$$\frac{dX}{dt} = F(X), \tag{13}$$

$$X(0) = U_b - \mathbf{B_u}P(0), \tag{14}$$

$$\frac{dC}{dt} = G(X, C, S), \tag{15}$$

$$C(0) = V_b - \mathbf{B}_v Q(0), \tag{16}$$

$$-\frac{dP}{dt} = \left[\frac{\partial F}{\partial X}\right]^t P + \left[\frac{\partial G}{\partial X}\right]^t Q + H_{\mathbf{x}}^t(H_{\mathbf{x}}X - X_{obs}), \tag{17}$$

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$$P(T) = 0, \tag{18}$$

$$-\frac{dQ}{dt} = \left[\frac{\partial G}{\partial C}\right]^t Q + H_{\mathbf{c}}^t (H_{\mathbf{c}} C - C_{obs}), \tag{19}$$

$$Q(T) = 0, \tag{20}$$

where Equations (15) and (17) are the combination of Equations (9), (11), and the Euler–Lagrange equation associated with the cost function, Equation (12). It is worthwhile to point out that the optimality system contains all the available information. In practice, solving the adjoint model allows the computation of the gradient of the cost function, which is then used in an optimization algorithm (Newton-type methods, limited memory Broyden–Fletcher–Goldfarb–Shanno, etc.) to compute the optimal initial conditions for both the state and pollutant concentration.

2.4.2. Sensitivity problem. Let the response function be defined as follows:

$$r(X, C, S) = \int_0^T \left\langle 1_{\Omega_A}, \varphi(X, C, S) \right\rangle dt. \tag{21}$$

By definition, the sensitivity with respect to the source S is the gradient of the response function r with respect to S. Following [45, 47, 50, 51], it can be shown that this sensitivity is given by

$$\nabla_S \Phi_A = \left[\frac{\partial G}{\partial S}\right]^t \Lambda + \left[\frac{\partial^2 G}{\partial S \partial X}\Phi + \frac{\partial^2 G}{\partial S \partial C}\Psi\right]^t Q + \left[\frac{\partial \varphi}{\partial S}\right]^t 1_{\Omega_A}, \tag{22}$$

where Γ, Λ, Φ, and Ψ are the second-order adjoint variables given by

$$\begin{aligned} -\frac{d\Gamma}{dt} = {} & \left[\frac{\partial F}{\partial X}\right]^t \Gamma + \left[\frac{\partial G}{\partial X}\right]^t \Lambda + \left[\frac{\partial^2 F}{\partial X^2}\Phi\right]^t P \\ & + \left[\frac{\partial^2 G}{\partial X^2}\Phi + \frac{\partial^2 G}{\partial C \partial X}\Psi\right]^t Q \\ & + H_{\mathbf{x}}^t H_{\mathbf{x}} + \left[\frac{\partial \varphi}{\partial X}\right]^t 1_{\Omega_A} \Phi, \end{aligned} \tag{23}$$

$$\begin{aligned} -\frac{d\Lambda}{dt} = {} & \left[\frac{\partial G}{\partial C}\right]^t \Lambda + \left[\frac{\partial^2 G}{\partial C \partial X}\Phi + \frac{\partial^2 G}{\partial X^2}\Psi\right]^t Q \\ & + H_{\mathbf{c}}^t H_{\mathbf{c}} \Psi + \left[\frac{\partial \varphi}{\partial C}\right]^t 1_{\Omega_A}, \end{aligned} \tag{24}$$

$$\frac{d\Phi}{dt} = \left[\frac{\partial F}{\partial X}\right]\Phi, \tag{25}$$

$$\frac{d\Psi}{dt} = \left[\frac{\partial G}{\partial C}\right]\Psi + \left[\frac{\partial G}{\partial X}\right]\Phi, \tag{26}$$

$$\Gamma(T) = 0, \tag{27}$$

$$\Lambda(T) = 0, \tag{28}$$

$$\mathbf{B_u}\Gamma(0) + \Phi(0) = 0, \tag{29}$$

$$\mathbf{B_v}\Lambda(0) + \Psi(0) = 0. \tag{30}$$

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It is important to recall that this is still the first-order sensitivity analysis applied to the optimality system, which can be considered as a generalized model. The second-order adjoint is the consequence of the derivation of the optimality system, which is based on the first-order adjoint of the model.

Equations (29) and (30) can also be written as

$$\Gamma(0) + \mathbf{B}_{\mathbf{u}}^{-1}\Phi(0) = 0 \tag{31}$$

$$\Lambda(0) + \mathbf{B}_{\mathbf{v}}^{-1}\Psi(0) = 0. \tag{32}$$

The system of Equations (23)–(30) is made up of four differential equations of first order with respect to time; with final conditions on two variables and two constraints Equations (29) and (30) on the solution at time zero. The system can not be solved as it is, it requires additional informations, an approach to solve such a problem is introduced in Section 3.

2.5. Extension and potential development

Without any theoretical difficulty, the development carried out earlier can be extended to the case of pollutant with kinetic chemistry. The same methodology can be applied with the concentration of many species of pollutant in the place of a single specie; $C = (C_1, C_2, \cdots, C_m)$ where C_i is the concentration of the $i^t h$ specie. Some numerical difficulties may arise if the characteristic time of the kinetic chemistry are very heterogeneous.

3. DIFFERENCE BETWEEN THE DIRECT MODEL AND THE OPTIMALITY SYSTEM SENSITIVITIES

A thorough analysis of the differences between the sensitivity analysis applied to the direct model and the sensitivity analysis applied to the optimality system requires a solution method for the second-order adjoint system Equations (23)–(30).

3.1. Solving the second-order adjoint system

One method to solve the system Equations (23)–(30) is to turn it into the following optimal control problem: Find $\Phi(0)$ and $\Psi(0)$ such that the solution of the system of Equations (24)–(28) satisfies the constraints given by Equations (29) and (30)

Following [47, 50], the system of Equations (24)–(28) can be split into the following two independent systems:

$$-\frac{d\Gamma_1}{dt} = \left[\frac{\partial F}{\partial X}\right]^t \Gamma_1 + \left[\frac{\partial G}{\partial X}\right]^t \Lambda_1 + \left[\frac{\partial \varphi}{\partial X}\right]^t 1_{\Omega_A}, \tag{33}$$

$$-\frac{d\Lambda_1}{dt} = \left[\frac{\partial G}{\partial C}\right]^t \Lambda_1 + \left[\frac{\partial \varphi}{\partial C}\right]^t 1_{\Omega_A}, \tag{34}$$

$$\Gamma_1(T) = 0, \tag{35}$$

$$\Lambda_1(T) = 0 \tag{36}$$

and

$$\begin{aligned} -\frac{d\Gamma_2}{dt} = {} & \left[\frac{\partial F}{\partial X}\right]^t \Gamma_2 + \left[\frac{\partial G}{\partial X}\right]^t \Lambda_2 + \left[\frac{\partial^2 F}{\partial X^2}\Phi\right]^t P \\ & + \left[\frac{\partial^2 G}{\partial X^2}\Phi + \frac{\partial^2 G}{\partial C\,\partial X}\Psi\right]^t Q + H_{\mathbf{x}}^t H_{\mathbf{x}}\Phi, \end{aligned} \tag{37}$$

$$-\frac{d\Lambda_2}{dt} = \left[\frac{\partial G}{\partial C}\right]^t \Lambda_2 + \left[\frac{\partial^2 G}{\partial C \partial X}\Phi + \frac{\partial^2 G}{\partial C^2}\Psi\right]^t Q + H_{\mathbf{c}}^t H_{\mathbf{c}}\Psi, \tag{38}$$

$$\frac{d\Phi}{dt} = \left[\frac{\partial F}{\partial X}\right]\Phi, \tag{39}$$

$$\frac{d\Psi}{dt} = \left[\frac{\partial G}{\partial C}\right]\Psi + \left[\frac{\partial G}{\partial X}\right]\Phi, \tag{40}$$

$$\Gamma_2(T) = 0, \tag{41}$$

$$\Lambda_2(T) = 0 \tag{42}$$

with

$$\Gamma = \Gamma_1 + \Gamma_2, \tag{43}$$

$$\Lambda = \Lambda_1 + \Lambda_2. \tag{44}$$

The system of Equations (33)–(36) contains all the information and can be solved as it is. In addition, given C, the subsystem formed by Equations (34) and (36) is identical to Equations (6)–(7); hence, the same variable name is used. The system of Equations (37)–(42) lacks initial conditions on the variables Φ and Ψ. The optimal control approach to solve Equations (23)–(30) becomes: Find $\Phi(0)$ and $\Psi(0)$ such that the solution of the system of Equations (37)–(42) satisfies the constraints given by Equations (29) and (30).

Given initial conditions

$$\Phi(0) = \Phi_0, \tag{45}$$

$$\Psi(0) = \Psi_0, \tag{46}$$

on Φ and Ψ, the solution of the system (37)–(42) can be obtained by a forward integration of Equations (39)–(40) followed by a backward integration of Equations (37)–(38). It is shown in [51] that this process defines $\Gamma_2(0)$ and $\Lambda_2(0)$ as

$$\begin{pmatrix} \Gamma_2(0) \\ \Lambda_2(0) \end{pmatrix} = \mathbf{H}(U^*, V^*) \begin{pmatrix} \Phi_0 \\ \Psi_0 \end{pmatrix}, \tag{47}$$

where $\mathbf{H}$ is the Hessian of the cost function Equation (12) with respect to the initial conditions U and V, simply named Hessian hereafter. $\mathbf{H}(U^*, V^*)$ is the Hessian evaluated at the solution (U^*, V^*) of the optimality system Equations (13)–(20). Because

$$\Gamma = \Gamma_1 + \Gamma_2, \tag{48}$$

$$\Lambda = \Lambda_1 + \Lambda_2, \tag{49}$$

the conditions

$$\mathbf{B_u}\Gamma(0) + \Phi(0) = 0, \tag{50}$$

$$\mathbf{B_v}\Lambda(0) + \Psi(0) = 0 \tag{51}$$

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become

$$\left(\mathbf{BH}(U^*, V^*) + \mathbf{I}\right)\begin{pmatrix}\Phi_0\\ \Psi_0\end{pmatrix} = -\mathbf{B}\begin{pmatrix}\Gamma_1(0)\\ \Lambda_1(0)\end{pmatrix}, \tag{52}$$

where $\mathbf{I}$ is the identity matrix of the same size as the Hessian and the matrix $\mathbf{B}$ is defined as

$$\mathbf{B} = \begin{pmatrix}\mathbf{B_u} & 0\\ 0 & \mathbf{B_v}\end{pmatrix}. \tag{53}$$

Equation (52) can also be written as

$$\left(\mathbf{H}(U^*, V^*) + \mathbf{B}^{-1}\right)\begin{pmatrix}\Phi_0\\ \Psi_0\end{pmatrix} = -\begin{pmatrix}\Gamma_1(0)\\ \Lambda_1(0)\end{pmatrix}. \tag{54}$$

The Hessian and the matrix of background error covariance are by definition symmetric and positive semi-definite. If one is positive definite then the matrix of the linear system Equation (54) is symmetric and positive definite. Therefore, the system has a unique solution and can be solved using the well-known conjugate gradient algorithm.

3.2. *Difference between the direct model and the optimality system sensitivities*

Let us rewrite the gradient of the response function according to the direct model and the optimality system sensitivities. In the direct model sensitivity, the gradient of the response function is given by

$$\nabla_{1S} r_A = \left[\frac{\partial G}{\partial S}\right]^t \Lambda_1 + \left[\frac{\partial \varphi}{\partial S}\right]^t 1_{\Omega_A} \tag{55}$$

In the optimality system sensitivity, it is given by

$$\nabla_{2S} r_A = \left[\frac{\partial G}{\partial S}\right]^t \Lambda + \left[\frac{\partial^2 G}{\partial S \partial X}\Phi + \frac{\partial^2 G}{\partial S \partial C}\Psi\right]^t Q + \left[\frac{\partial \varphi}{\partial S}\right]^t 1_{\Omega_A} \tag{56}$$

Taking into account the definition of Λ as given by Equation (44), Equation (56) becomes

$$\nabla_{2S} r_A = \nabla_{1S} r_A + \left[\frac{\partial G}{\partial S}\right]^t \Lambda_2 + \left[\frac{\partial^2 G}{\partial S \partial X}\Phi + \frac{\partial^2 G}{\partial S \partial C}\Psi\right]^t Q \tag{57}$$

where Λ_2, Φ, and Ψ are given by the solution of the systems of Equations (33)–(36) and (37)–(42). It is clear that the direct model sensitivity misses the additional terms in (57). Those terms show the indirect effects of the variation of the source on the response function. Although the terms with the second-order derivatives will vanish in some cases (e.g., if S is simply an additive term in G,) the term in Λ_2 will always be there to make the difference between the direct model and the optimality system sensitivities.

3.2.0.1. On the second-order terms in the optimality system sensitivity. When the data assimilation process is accounted for, the response function becomes implicitly a function of the first-order partial derivatives of the model functions F and G with respect to X and C as shown by Equations (23)–(30). Because of the interplay of different terms in the optimality system, the gradient of the response function becomes a function of the second-order partial derivatives of the model functions F and G and expressed implicitly in the term $\left[\frac{\partial G}{\partial S}\right]^t \Lambda_2$ and explicitly in the term $\left[\frac{\partial^2 G}{\partial S \partial X}\Phi + \frac{\partial^2 G}{\partial S \partial C}\Psi\right]^t Q$ of Equation (57).

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3.3. Computational cost

To make an estimation of the computationl cost of the method, let us assume that the system state model, the pollutant model, their tangent linear, their first-order and second-order adjoint counterparts have similar computational cost that we note $\mathcal{N}$. It means that the solution of the direct coupled model costs $2\mathcal{N}$ because it is made up of the system state model and the pollutant model. Assuming that p iterations are needed for the minimization in the data assimilation process, the cost of solving the data assimilation problem is $(4p+2)\mathcal{N}$. The sensitivity analysis applied to the direct model can be performed using the background initial conditions or using the optimal initial conditions that accounts for the observations. The cost of the first approach is $2\mathcal{N}$ while the cost of the later is $(4p+2)\mathcal{N}+2\mathcal{N}$, which includes the cost of the data assimilation that is used to compute the optimal initial conditions. Assuming that q iterations are needed for the minimization process to solve the second-order adjoint system as described in Section 3.1, the cost of the optimality system sensitivity is $2\mathcal{N}+4q\mathcal{N}$, which is made up of the costs of solving the systems Equations (33)–(36) and Equations (37)–(42).

4. EXAMPLE: APPLICATION TO ONE-DIMENSIONAL SYSTEM

In this section, we consider the application to one-dimensional problem.

4.1. Mathematical formulation of the problem

The physical space is the interval $\Omega = [-1, 1]$ and the time domain is the interval $[0, T]$ with $T = 2$. The assimilation window and the sensitivity window are identical to the time domain $[0, T]$. The response region and the response window will be explicitly shown for each case. We consider the problem of pollution by a single species with a given source function.

The one-dimensional velocity field $u = u(x, t)$ evolves according to the Burgers equation given by

$$\begin{cases} \frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} - \nu\frac{\partial^2 u}{\partial x^2} = f, x \in \Omega =]-1, 1[, t \in [0, T]; \\ \qquad u = u_0, t = 0, \text{ initial condition;} \\ \qquad u = u_1, x \in \{-1, 1\}, \text{ boundary conditions} \end{cases}, \tag{58}$$

the evolution of the pollutant concentration is modeled by a one-dimensional advection diffusion equation:

$$\begin{cases} \frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = \eta\frac{\partial^2 c}{\partial x^2} + s, x \in]-1, 1[, t \in [0, T] \\ \qquad c = c_0, t = 0; \\ \qquad c = c_1, x \in \{-1, 1\}. \end{cases} \tag{59}$$

and the response function is defined as

$$r_A(c) = \frac{1}{(t_2 - t_1) \times \mathrm{mes}(\Omega_A)} \int_{t_1}^{t_2} \int_{-1}^{1} 1_{\Omega_A} c(x, t)\, dx\, dt, \tag{60}$$

where the response window is given by $[t_1, t_2]$, $\mathrm{mes}(\Omega_A)$ is the measure of the response region Ω_A. The response function defines the mean value of the concentration c of the pollutant over the space-time region $\Omega_A \times [t_1, t_2]$. The function φ is equal to the concentration of the pollutant.

Background The initial concentration of the pollutant is given by the Gaussian function centered at $x = 0$. The source function s is a step function in x (0 for $x <= 0$ and 0.001 for $x > 0$) and constant along t. The background velocity field is defined by setting f in Equation (58) as defined in [52], which makes it possible to derive an exact solution for the background.

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Observations To sample observations, a 'true' initial condition is defined by adding a Gaussian perturbation of mean zero to the background initial condition. The pertubation has a squared exponential covariance with characteristic length scale 0.3 and standard deviation 0.05 for both variables u and c. The observations of u and c are sampled on a regular grid and perturbed with a Gaussian noise of standard deviation 0.01.

4.2. *Validation of the tangent linear and of the adjoint*

The validation of the tangent linear and of the adjoint is very important for nonlinear models, see [53–55] and references therein. Among others, the following methods can be use to check the validity of the tangent linear model (TLM) and/or of the adjoint codes: the test of the tangent linear, the test of the adjoint and the test of the gradient. The test of the tangent linear is defined by [54] as the investigation of the ability of the TLM to describe the true nonlinear evolution of perturbations and to specify the range of this validity in terms of integration time and the magnitude of the perturbations. The test of the adjoint checks that the adjoint code is actually the adjoint of the tangent linear code. The test of the gradient checks the validity of the gradient computed by the adjoint code. This test is very important in the context of data assimilation because the ultimate goal of the adjoint code if to compute the gradient of the cost function that is used in an optimization process to compute the best initial condition (or parameters) of the model. It is a validation tool for both the TLM and the adjoint. Because the sensitivity is by definition a gradient, the test of the gradient is also a validation of the sensitivity based on the adjoint.

Those tests can be used to validate both the first-order and the second-order adjoint models. However, it should be noted that the second-order adjoint model has very few additional terms compared with the first-order adjoint. Most of those terms are second-order terms that vanish in most cases thanks to the linearity as explained in Section 3. That is the case for the test problem used in this paper. From a valid first-order adjoint model, a valid second-order adjoint model is straightforward. For that reason, the subsequent part of this subsection provides the validation of the tangent linear and of the first-order adjoint of the coupled model (58)–(59). However, for counterintuitive features like negative sensitivities given by the optimality system sensitivity (Section 4.3.2), a specific validation is provided by Table I.

For the test problem presented in this section, we use the test of the gradient to validate the tangent linear and the adjoint models. The test of the gradient is based on the Taylor expansion of the cost function, which writes

$$J(\mathbf{k} + \alpha\delta\mathbf{k}) = J(\mathbf{k}) + \alpha \left\langle \nabla_{\mathbf{k}} J(\mathbf{k}), \delta\mathbf{k} \right\rangle + O(\alpha\|\delta\mathbf{k}\|), \tag{61}$$

where J is the cost function and $\mathbf{k}$ is a symbolic representation of the initial condition and or parameters of the models. A rearrangement of Equation (61) leads to

$$\lim_{\alpha\to 0} \frac{J(\mathbf{k} + \alpha\delta\mathbf{k}) - J(\mathbf{k})}{\alpha \left\langle \nabla_{\mathbf{k}} J(\mathbf{k}), \delta\mathbf{k} \right\rangle} = 1. \tag{62}$$

A correct implementation of the tangent linear code and its adjoint must satisfy the test given by (62) where $\nabla_{\mathbf{k}}\mathbf{J}(\mathbf{k})$ is computed by the adjoint code. There is an infinity of choices for the perturbation vector $\delta\mathbf{k}$. We did the test with a pertubation vector based on the gradient $\delta\mathbf{k} = \dfrac{\nabla_{\mathbf{k}} J(\mathbf{k})}{\|\nabla_{\mathbf{k}}\mathbf{J}(\mathbf{k})\|}$ as well as a random perturbation $\delta\mathbf{k} = \dfrac{\mathbf{r}}{\|\mathbf{r}\|}$ (where $\mathbf{r}$ is a random vector). The perturbation based on the gradient is available once the TLM and the adjoint are available, and most importantly, it is

Table I. Validation of the negative response.

Source	1.0E-3	2.0E-3	3.0E-3	4.0E-3
Response	4.1939E-2	4.1930E-2	4.1928E-2	4.1921E-2

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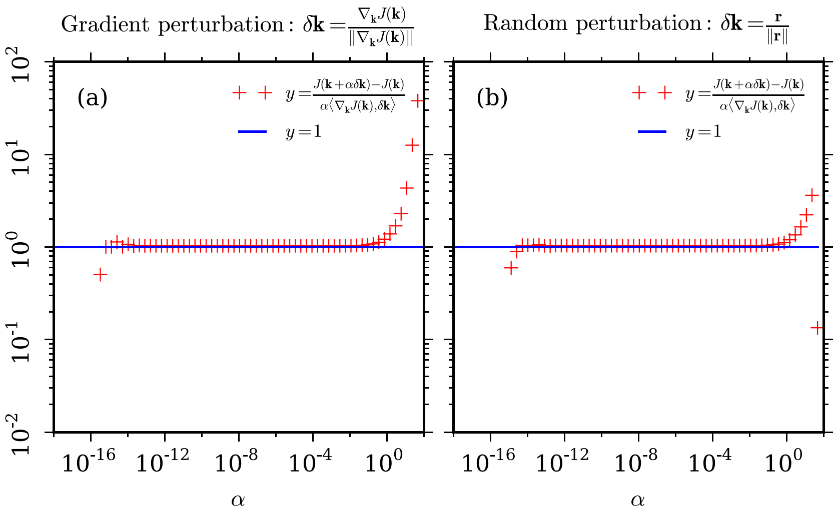

Figure 1. Test of the gradient: (a) perturbation based on the gradient and (b) random perturbation .

used as the increment (or in its definition) in variational data assimilation, so that the test also provides the range of validity of the optimization step around the background. Figure 1 shows the test of the gradient for the coupled model with the perturbation given by the gradient (Figure 1(a)) and a random perturbation (Figure 1(b)). The gradient is valid for α ranging from 10^{-15} to 10^{-1}in both cases. The interpretation is that the adjoint and the TLM are valid and stable for perturbations of norm up to 10^{-1} for the coupled model. It is important to mention that the range of validity of the gradient depend both on the problem and on the perturbation vector. All those test are computed for the time window $[0, 2]$.

4.3. *Numerical results*

The sensitivity analysis applied to the direct model can be performed using the background initial conditions or the optimal initial conditions that accounts for the observations. This distinction is important because the computed sensitivity is also a function of the initial conditions.

4.3.1. Data assimilation problem. Figure 2 shows the full trajectory of the background, the truth and the optimal solutions in the assimilation window. The truth here refers to the solution from which the observations are sampled. The data assimilation process recovers the truth very well. Figure 3 shows the background, the truth, and the optimal solutions at times 0 and 0.5. For time 0.5, we also have the observations that are used in the data assimilation process. There is no observation at time 0.

4.3.2. Gradient of the response function. Figure 4 shows three cases of sensitivity analysis: the direct model sensitivity using the background solution (left column), direct model sensitivity using the optimal solution (middle column), and the optimality system sensitivity (right column) for four different response windows. The data assimilation window and the sensitivity window are the same for all cases. The space-time response region is delimited by a black rectangle in each case (Figure 4). From top to bottom, the response windows are: $[0.5, 0.6]$, $[1.0, 1.1]$, $[1.9, 2.0]$, and $[0.0, 2.0]$.

The direct model sensitivity using the background solution shows that the pollution in the response region comes slightly from the left. This is in agreement with the background transport velocity that is positive (transport from the left to the right) around the response region with low intensity. The sensitivity is positive or null everywhere. It means that any increase of the emission results in no effect or an increase of the pollution in the response region. The positive sensitivity is only at time in or below the response window: the method shows only the direct effect (transport from the source location) of the source on the response function. For limited response windows

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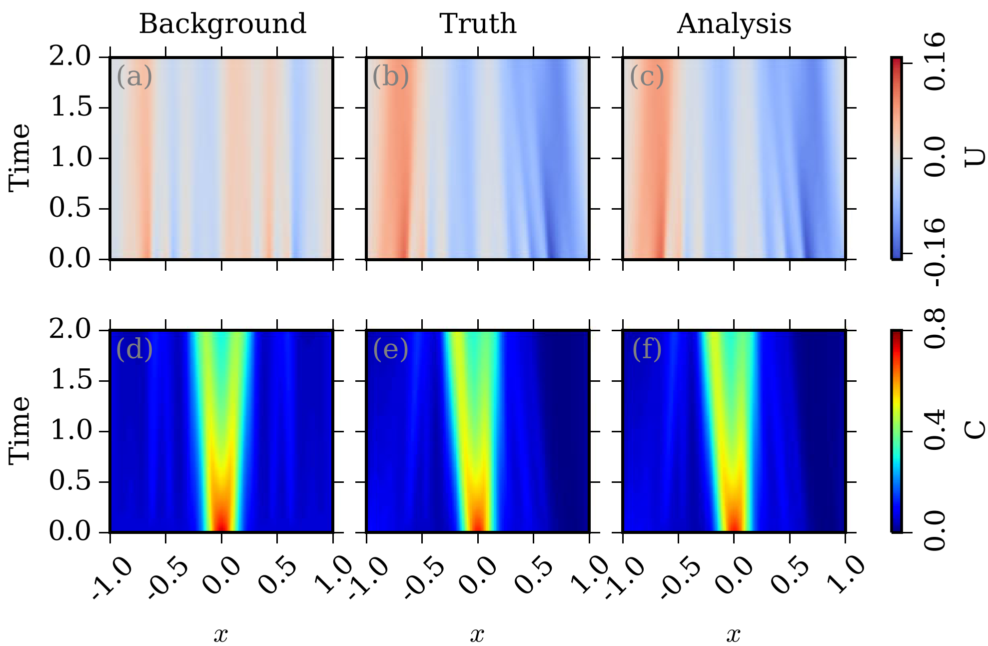

Figure 2. Solution of the data assimilation problem.

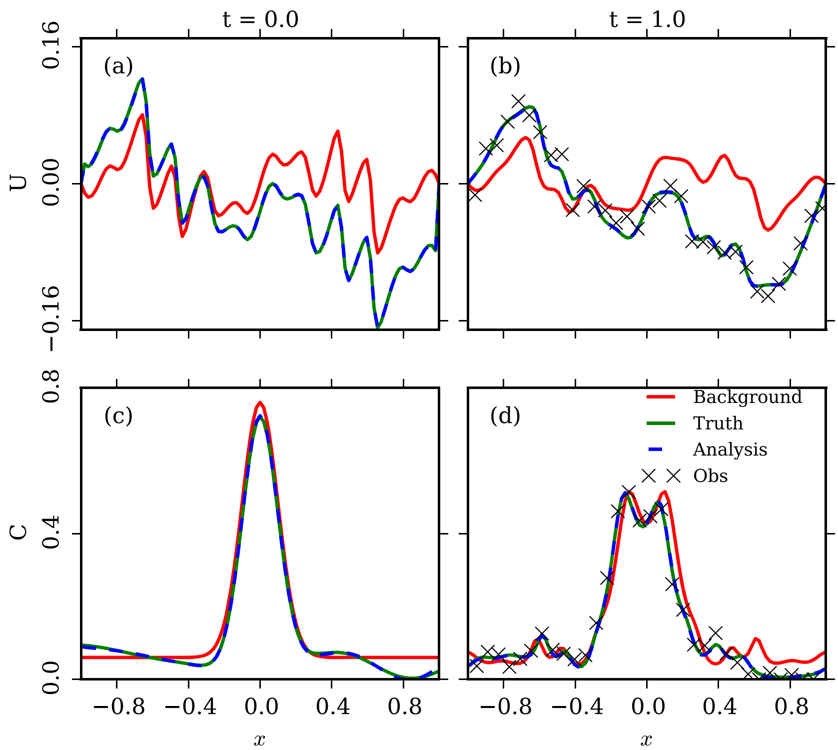

Figure 3. Time slices of the solution of the data assimilation problem.

(Figure 4(a), (d), and (g)), the highest sensitivity (high intensity in the plot) is in the immediate vicinity of the response window. When the response window is extended to match the assimilation window (Figure 4(l)), the highest sensitivity is close to time 0.

The direct model sensitivity using the optimal solution (Figure 4(b), (e), (h), and (k)) shares all the qualitative characteristics of the direct model sensitivity using the background solution with

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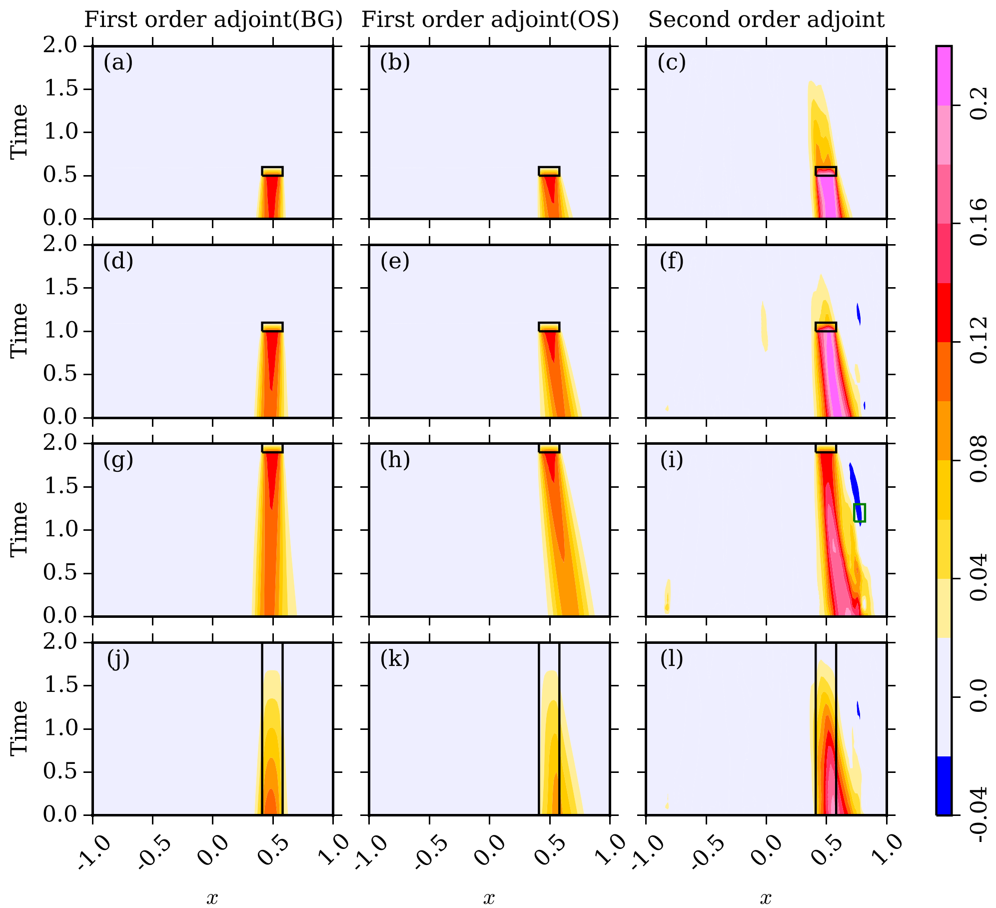

Figure 4. Comparison of the first-order and the second-order adjoint sensitivity. From top to bottom, the response windows are: [0.5, 0.6], [1.0,1.1], [1.9, 2.0], and [0.0, 2.0]. The green box in (i) is the region used to validate negative sensitivities.

the only difference that the pollution in the response region comes slightly from the right thanks to a corrected transport velocity from the prior data assimilation process. Because of the strongest transport velocity, the region with positive sensitivity extends a little farther away from the response region. Despite the prior data assimilation process, the method also shows only the direct effect (transport from the source location) of the source on the response function.

The direct model sensitivity using the background or the optimal solution is strongly dependent on the response region and the transport velocity used.

When it comes to the optimality system sensitivity, the dependence on any transport velocity (background or optimal solution) is less obvious. There is a sensitivity to the future (Figure 4(c) and (f)) and there are also negative sensitivities (blue colors in Figure 4(f), (i), and (l)). In the expression 'sensitivity to the future', the future is relative to the response window and by sensitivity to the future, we mean nonzero sensitivity beyond the upper bound of the response window. There is a sensitivity to the future when the upper bound of the response window is strictly lower than the upper bound of the assimilation window (Figure 4(c) and (f)). It is a direct consequence of the nature of the optimality system of variational data assimilation that enables to account for the variation with respect to the source beyond the response window, which is only possible if the gradient of the response function is derived from the optimality system.

The sensitivity to the future shows that in the presence of data assimilation, any overestimation or underestimation of the source even above the response window can have an effect in the response region. This is possible because the solution of the optimality system will assign stronger or weaker

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transport velocity to some geographic regions at some previous time in order to have a concentration of pollutant that matches the observations.

As it is the case for the sensitivity to the future, the negative sensitivity is also a direct consequence of the presence of data assimilation. For example, the solution of the optimality system can locally change the direction of the transport velocity, which results in the reduction of the number of particles that reach the response region. Because negative sensitivity seems counterintuitive, we carried out a validation experiment in which we computed the response function based on the solution of the optimality system. The setup is identical to the one used for Figure 4(i). The source is increased by a constant value in the region $1.1 \leqslant t \leqslant 1.2$ and $0.75 \leqslant x \leqslant 0.8$, which is a subdomain of the negative response domain (see the green box in Figure 4(i)). Table I summarizes the result of the validation. As the source increases from 1×10^{-3} to 4×10^{-3}, the response decreases.

Another important note on the optimality system sensitivity is that the magnitude is twice as large as that of the direct model sensitivity (background and optimal solution) for the test problem.

To supplement the present analysis, we computed and plotted the difference between the optimality system sensitivity and the direct model sensitivity (background and optimal solution); the result is shown in Figure 5. For convenance, the negative sensitivity in the optimality system sensitivity is set to zero before the computation. The shades of red color indicate the region where the direct model sensitivity underestimate the sensitivity, and the shades of blue indicate the region where it overestimate the sensitivity. The combined presence of the red and blue shades (Figure 5(a), (c), (e), and (g)) shows that the direct model sensitivity using the background solution does not agree with the optimality system sensitivity on the provenance of the pollution in the target region. For a limited response windows, the disagreement is amplified as the response window is moved away from time 0 (Figure 5(a), (c), and (e)). The direct model sensitivity using the optimal solution agrees with the optimality system sensitivity on the provenance of the pollutant in the response region but disagree on the intensity (Figure 5(b), (d), (f), and (h)).

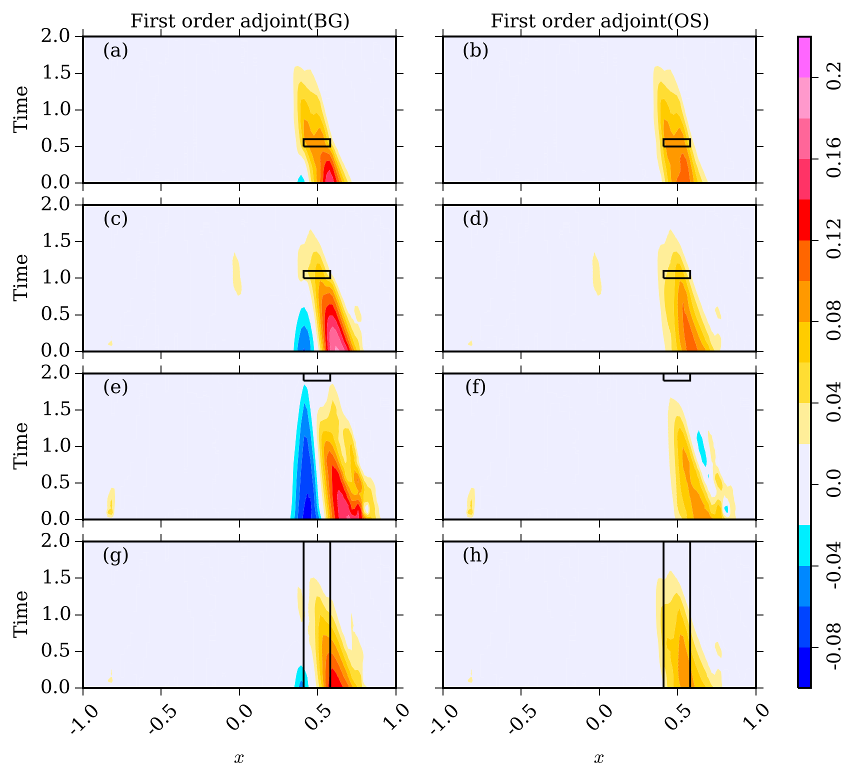

Figure 5. Difference between and the optimality system sensitivity and the direct model sensitivity using the background initial condition (left column) and the optimal initial condition (right column).

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The sensitivity to the future, the negative sensitivity and the difference in intensity show that the direct model sensitivity can be strongly misleading. The sensitivity, mathematically defined as the gradient of the response function with respect to the source, shows what happens if the source changes including the errors in the source function. Because any change in the source induces a change in the solution of the data assimilation problem, the sensitivity to the future and the negative sensitivity are especially important because they are the direct consequence of the data assimilation process as mentioned earlier. The sensitivity to the future and the negative sensitivity also give additional diagnosis tools: they show the space-time region where the error in the source function must be minimized to avoid errors in the computed sensitivity. Although the effect of the data assimilation process is highlighted only by the sensitivity to the future and the negative sensitivity, that effect is actually present everywhere. The reason being that, when the source changes, the solution of the optimality system can locally change the initial concentration of the pollutant and/or the transport velocity in order to match the observation, which results in the variation of the number of particles reaching the response region from a specific region. It means that the higher sensitivity is also a direct consequence on deriving the sensitivity from the optimality system. The sensitivity to the future, the negative sensitivity and the higher sensitivity show the indirect effects of the source onto the target region.

5. CONCLUSION

The direct model sensitivity and the optimality system sensitivity of a response function to a source function in a problem of pollution are studied. The theoretical analysis shows that the optimality system sensitivity includes components that are not present in the direct model sensitivity. Numerical experiments show that the optimality system sensitivity detects higher sensitivity than the direct model sensitivity for the test problem. It was also shown that if the sensitivity window intersects the assimilation window, the sensitivity can be negative even for a passive tracer, which is not possible in the direct model sensitivity. Moreover, if the upper bound of the response window is lower than the upper bound of the assimilation window, then the response region can be sensitive to the future. The sensitivity to the future and the negative sensitivity are especially important because they highlight the effect of the data assimilation process in the computed sensitivity. In addition, they show the space-time region where the error in the source function must be minimized to avoid errors in the computed sensitivity. The sensitivity with respect to the source on a data assimilation problem must be derived on the optimality system, because it is the only method that actually shows the direct and indirect effects of the source function onto the response region. The direct model sensitivity shows only the direct effects of the source function onto the response region and totally ignored the effect of the data assimilation.

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