Data Assimilation for 2-D Advection-Dispersion Equations

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Abstract. Data assimilation based on a variational principle for parameter estimation of 2-D advection-dispersion equations is considered. It is assumed that a priori estimations for the model parameters and the initial condition are available. Improvement of parameters for the radionuclide transport model is reduced to an optimization problem with quadratic cost functional. The cost functional comprises the measurement model and model errors, the initial condition uncertainty and parameter penalties. The existence of a unique solution for the state equations and the adjoint system is proved. Differential properties of the cost functional are investigated and a necessary condition for cost functional minimum is derived. Restrictions on the cost functional weights, which guarantee the existence of a unique stationary point, are derived.

1 Introduction

In this paper we concentrate on parameter estimation for the advection-dispersion equations, which, for example, can be used to describe radionuclide transport by surface water flow. The radionuclide transport in the aqueous phase and on suspended sediments by surface water flow is governed by the equations with the sink-source term describing physical-chemical interactions and erosion-deposition exchange processes [1-2]

$$\begin{aligned} \frac{\partial(hc_l)}{\partial t} + \frac{\partial}{\partial x_i}(v_i hc_l) = \frac{\partial}{\partial x_i} \left(h e_i \frac{\partial c_l}{\partial x_i} \right) - \lambda h c_l - \alpha_s h S \left(k_d^s \rho^{-l} c_l - c_s \right) - \\ -(1-\phi) z_* \alpha_b \left(k_d^b \rho_b \rho^{-l} c_l - c_b \right) \end{aligned} \quad (1)$$

$$\begin{aligned} \frac{\partial(hSc_s)}{\partial t} + \frac{\partial}{\partial x_i}(v_i hSc_s) = \frac{\partial}{\partial x_i} \left(h e_i \frac{\partial Sc_s}{\partial x_i} \right) - \lambda h Sc_s + \alpha_s h S \left(k_d^s \rho^{-l} c_l - c_s \right) + \\ + \rho_b^{-l} q_b c_b - q_s c_s \end{aligned} \quad (2)$$

where $h(x,t)$ is the surface water depth; $v_i(x,t)$ are the surface water velocity components; $\phi(x)$ is the porosity of upper soil layer; ρ is the density of water; $\rho_b(x)$ is the density of soil matrix; $S(x,t)$ is the suspended sediment concentration; $c_i(x,t)$ is the

volumetric radionuclide activity in aqueous phase; $c_s(x,t)$ is the radionuclide activity on suspended sediment; $c_b(x,t)$ is the volumetric radionuclide activity in upper soil layer; $z_*(x,t)$ is the thickness of active upper soil layer; λ is the radionuclide decay constant; $q_s(x,t)$ and $q_b(x,t)$ are the deposition and erosion rates; $e_i(x,t)$ – the diffusion coefficients; k_d^s , k_d^b and a_s , a_b are the partition coefficients and the exchange rates, respectively; $i=1,2$.

Contamination of the active upper soil layer is described by the equations

$$\begin{aligned} \frac{\partial}{\partial t}((1-\phi)z_*c_b) &= \frac{\partial}{\partial x_i} \left((1-\phi)z_*e_i^b \frac{\partial c_b}{\partial x_i} \right) + \\ &+ (1-\phi) \left[\alpha_b z_* \left(k_d^b \rho_b \rho^{-1} c_l - c_b \right) - \lambda z_* c_b \right] - \rho_b^{-1} q_b c_b + q_s c_s \end{aligned} \quad (3)$$

Values of the partition coefficients $k_d^s(x)$, $k_d^b(x)$ and exchange rates $\alpha_s(x)$, $\alpha_b(x)$ are determined by the soil physical-chemical properties and forms of radionuclide contamination. These coefficients characterize the interchange between the various radionuclide forms. So a forecast quality of radionuclide contamination of surface reservoirs depends on accuracy determination of their values. Experience of the Chernobyl accident has shown that exact values of the partition coefficient and exchange rates are unknown just after accident and at the best their estimations are only available.

Nowadays data assimilation methods used for parameter estimation is based on estimation theory or control theory [3]. Estimation theory usually involves a sequential estimations of both model and data errors by using a statistical approach. Control theory methods are generally based on variational principles.

In this paper, we consider variational assimilation approach [4] for parameter estimation of the model of radionuclide transport by surface water flow. In this case, parameter estimation problem reduces to minimization of a quadratic cost functional on a set of admissible values of the model parameters in neighborhood of their a priori estimations. On the set of admissible values of the model parameters the differential properties of the cost functional are investigated, a necessary condition for a minimum of the cost functional is derived, and a sufficient condition for existence of a unique stationary point is obtained.

2 Problem Statement

Rewrite the model equations (1)-(3) in the vector form

$$\frac{\partial}{\partial t}(A_0 c) + \frac{\partial}{\partial x_i}(A_i c) = \frac{\partial}{\partial x_i} \left(D_i \frac{\partial c}{\partial x_i} \right) - G(\mu, \nu) c + r, \quad (x, t) \in Q = \Omega \times (0, T) \quad (4)$$

where $c(x, t) = (c_1, c_2, c_3)^T = (c_l, Sc_s, c_b)^T$ is the state vector; $r(x, t) = (r_1, r_2, r_3)^T$ is the function of the model error; $\mu = (\mu_1, \mu_2)^T = (\alpha_s k_d^s / \rho, \alpha_b k_d^b \rho_b / \rho)^T$ and $\nu =$

$(v_1, v_2)^T = (\alpha_s, \alpha_b)^T$ is the parameter vector; Ω is a connected bounded set in E^2 with twice boundedly differentiable boundary $\partial\Omega$; E^n is the n -dimensional Euclidean space. The function of model errors $r(x, t)$ we shall consider as an auxiliary variable, which is needed to minimize.

Matrices A_0, A_i, D_i are diagonal matrices

$$A_0 = \text{diag} \{a_0^{11}, a_0^{22}, a_0^{33}\} = \text{diag} \{h, h, z\};$$

$$A_i = \text{diag} \{a_i^{11}, a_i^{22}, a_i^{33}\} = \text{diag} \{v_i h, v_i h, 0\};$$

$$D_i = \text{diag} \{d_i^{11}, d_i^{22}, d_i^{33}\} = \text{diag} \{he_i, he_i, ze_i^b\}.$$

Matrix $G(\mu, v)$ is represented as

$$G(\mu, v) = \begin{pmatrix} \lambda h + \tilde{\mu}_1 h S + \tilde{\mu}_2 z & -\tilde{v}_1 h & -\tilde{v}_2 z \\ -\tilde{\mu}_1 h S & \lambda h + \tilde{v}_1 h + q_1 & -q_2 \\ -\tilde{\mu}_2 z & -q_1 & \lambda z + \tilde{v}_2 z + q_2 \end{pmatrix},$$

where $z = (1 - \phi) z_*$; $q_1 = q_s / S$; $q_2 = q_b / \rho_b$; $\mu_i, v_i \in E^m$ and $\tilde{\mu}_i = \mu_i^T \psi(x)$, $\tilde{v}_i = v_i^T \psi(x)$; the function $\psi(x) = (\psi_1, \dots, \psi_m)^T$ satisfies to relations

$$\psi_k(x) = \begin{cases} 1, & x \in \Omega_k; \\ 0, & x \notin \Omega_k \end{cases}; \quad \Omega = \bigcup_{k=1}^m \Omega_k; \quad \Omega_i \cap \Omega_j = \emptyset, \quad i \neq j.$$

Let elements of the matrices A_0, A_i, D_i and G are bounded measurable functions on Q . The matrices A_0, A_i and D_i are differentiable with respect to t and x and the following inequalities are valid

$$v \leq d_i^{kk} \leq \pi, \quad v_l \leq a_0^{kk} \leq \pi_l, \quad v, v_l > 0, \quad k = \overline{1, 3}; \quad i = \overline{1, 2}$$

$$\begin{aligned} & \text{vrai} \max_{(x, t) \in Q} \left(\left\| \frac{\partial A_0}{\partial t} \right\|_E^2, \sum_{i=1}^2 \left\| \frac{\partial D_i}{\partial t} \right\|_E^2, \sum_{i=1}^2 \left\| \frac{\partial A_i}{\partial t} \right\|_E^2 \right) \leq \pi_2 \\ & \text{vrai} \max_{(x, t) \in Q} \left(\sum_{i=1}^2 \left\| \frac{\partial A_0}{\partial x_i} \right\|_E^2, \sum_{i=1}^2 \left\| \frac{\partial D_i}{\partial x_k} \right\|_E^2, \sum_{i=1}^2 \left\| \frac{\partial A_i}{\partial x_i} \right\|_E^2 \right) \leq \pi_3 \end{aligned} \quad (5)$$

$$\text{vrai} \max_{\substack{(x,t) \in Q \\ u \in U_{ad}}} \left(\sum_{i=1}^2 \|A_i\|_E^2, \|G\|_E \right) \leq \pi_4,$$

where $\|A\|_E^2 = \sum_{i,j=1}^n (a^{ij})^2$ is the Euclidean norm of a $n \times n$ -matrix $A = \{a^{ij}\}_{j=1}^i$.

For the equation (4), let's consider the first boundary value problem with homogeneous boundary condition

$$c(x, 0) = c^0(x), \quad x \in \Omega \quad (6)$$

$$c(x, t) = 0, \quad (x, t) \in \Gamma = \partial\Omega \times [0, T] \quad (7)$$

The measurement model is described by equation

$$c^d(x) = H(x)c(x, T) + \vartheta(x) \quad (8)$$

where $c^d(x)$ is the observation data; ϑ is the measurement error; $H(x)$ is the observation matrix, elements of which are bounded and measurable on Ω and have bounded derivatives with respect to x .

We shall assume that exact values of the model parameters and the initial condition are unknown and their a priori estimations are only available

$$\mu_i = \mu_i^a + \vartheta_i^\mu, \quad v_i = v_i^a + \vartheta_i^v, \quad c^0(x) = c_a^0(x) + \vartheta_c^0(x),$$

where μ_i^a and v_i^a are the given a priori estimations of the model parameters; c_a^0 is the known a priori estimation of the initial state; ϑ_i^μ and ϑ_i^v are the errors of the model parameters; ϑ_c^0 is the error of the initial state.

Denote by U the space $E^{2 \times m} \times E^{2 \times m} \times L_2(Q) \times \dot{W}_2^1(\Omega)$ with elements $u = (u_1, u_2, u_3, u_4)^T = (\mu, v, r, c^0)^T$. Introduce in the space U the following scalar product

$$\langle u, w \rangle_U = \langle u_1, w_1 \rangle_{E^{2 \times m}} + \langle u_2, w_2 \rangle_{E^{2 \times m}} + \langle u_3, w_3 \rangle_{L_2(Q)} + \langle u_4, w_4 \rangle_{W_2^1(\Omega)}$$

for $\forall u, w \in U$, where $\langle \xi, \eta \rangle_{E^{n \times k}} = \sum_{i=1}^n \sum_{j=1}^k \xi_{ij} \eta_{ij}$ is the scalar product in $E^{n \times k}$ (further

we shall omit dimension of the Euclidean space in scalar product when it can be done without ambiguity); $L_2(Q)$ is the Hilbert space of measurable functions on Q with finite scalar product

$$\langle f, g \rangle_{L_2(Q)} = \int_0^T \int_\Omega \langle f, g \rangle_E dx dt.$$

$\dot{W}_2^I(\Omega)$ is the subspace of the Hilbert space $W_2^I(\Omega)$, dense set in which is set of all infinitely differentiable finite functions on Ω . The scalar product in $W_2^I(\Omega)$ is defined by

$$\langle f, g \rangle_{W_2^I(\Omega)} = \int_{\Omega} \left\{ \langle f, g \rangle_E + \sum_{i=1}^2 \langle f_{x_i}, g_{x_i} \rangle_E \right\} dx.$$

Let U_{ad} is a closed convex bounded set in U , defining admissible values of the model parameters (4), the initial state (6) and the model error. Further, the set U_{ad} is called as set of admissible model parameters. Then, we shall consider the problem of improvement of the model parameters $u=(\mu, \nu, r, c^0)^T$ for the equation (4) by using the observations (8) as a problem of minimization the following cost functional on U_{ad}

$$\begin{aligned} \mathfrak{J}(u, c(x, t; u)) = & \int_{\Omega} \left\{ c^d(x) - H(x) c(x, T; u) \right\}^T R_0 \left\{ c^d(x) - H(x) c(x, T; u) \right\} dx + \\ & + \int_Q r^T R_I r dx dt + \int_{\Omega} \left(c^0(x) - c_a^0(x) \right)^T R_2 \left(c^0(x) - c_a^0(x) \right) dx + \\ & + \sum_{i=1}^2 \left\{ \left(\mu_i - \mu_i^a \right)^T R_{\mu_i} \left(\mu_i - \mu_i^a \right) + \left(\nu_i - \nu_i^a \right)^T R_{\nu_i} \left(\nu_i - \nu_i^a \right) \right\}, \end{aligned} \quad (9)$$

where $R_0(x)$, $R_I(x, t)$, $R_2(x)$, R_{μ_i} , R_{ν_i} are a positive-definite symmetric weight matrices. We shall assume that elements of the matrices $R_0(x)$, $R_2(x)$, $R_I(x, t)$ are a bounded measurable functions on Ω and Q ; the functions $c^d(x)$, $c_a^0(x) \in \dot{W}_2^I(\Omega)$. Moreover, the matrix $R_0(x)$ have bounded derivatives with respect to x on Ω . We can consider the weight matrices as parameters of data assimilation and their choice depends on users.

Using the method of the Lagrange multipliers, we get the following adjoint system

$$A_0 \frac{\partial c^*}{\partial t} + A_i \frac{\partial c^*}{\partial x_i} + \frac{\partial}{\partial x_i} \left(D_i \frac{\partial c^*}{\partial x_i} \right) - G^T(\mu, \nu) c^* = 0 \quad (10)$$

$$c^*(x, T) = A_0^{-1} R_0 H (c^d - Hc), \quad x \in \Omega \quad (11)$$

$$c^*(x, t) = 0, \quad (x, t) \in \Gamma \quad (12)$$

3 Existence of Solution of the State and Adjoint Problems

Consider a system of equations

$$B_0(x,t) \frac{\partial w}{\partial t} - \frac{\partial}{\partial x_i} \left(B_{ij}(x,t) \frac{\partial w}{\partial x_j} + B_i(x,t) w \right) + C_i(x,t) \frac{\partial w}{\partial x_i} + C(x,t) w = -f(x,t) \quad (13)$$

where $w(x,t)$ and $f(x,t)$ are a m -dimensional vector-functions; B_0 , B_{ij} , B_i , C_i and C are $m \times m$ -matrices (B_0 , B_{ij} are the diagonal matrices and $B_{ij} = B_{ji}$) with elements $b_0^{kk}(x,t)$, $b_{ij}^{kk}(x,t)$, $b_i^{kl}(x,t)$, $c_i^{kl}(x,t)$ and $c^{kl}(x,t)$, respectively; $x = (x_1, x_2)$.

We shall assume that the following relationships are valid

$$\sigma \zeta^T \zeta \leq \sum_{i,j=1}^2 b_{ij}^{kk} \zeta_i \zeta_j \leq \gamma \zeta^T \zeta, \quad \sigma > 0, \quad k = \overline{1, m}$$

$$\sigma_l \xi^T \xi \leq \xi^T B_0 \xi \leq \gamma_l \xi^T \xi, \quad \sigma_l > 0 \quad (14)$$

for any real $\xi = (\xi_1, \dots, \xi_m)^T$ and $\zeta = (\zeta_1, \zeta_2)^T$. The matrices B_0 , B_i , B_{ij} are differentiable with respect to t and x and

$$\text{vrai max}_{(x,t) \in Q} \left(\left\| \frac{\partial B_0}{\partial t} \right\|_E^2, \sum_{i,j} \left\| \frac{\partial B_{ij}}{\partial t} \right\|_E^2, \sum_i \left\| \frac{\partial B_i}{\partial t} \right\|_E^2 \right) \leq \gamma_2$$

$$\text{vrai max}_{(x,t) \in Q} \left(\sum_i \left\| \frac{\partial B_0}{\partial x_i} \right\|_E^2, \sum_{i,j} \left\| \frac{\partial B_{ij}}{\partial x_k} \right\|_E^2, \sum_i \left\| \frac{\partial B_i}{\partial x_i} \right\|_E^2 \right) \leq \gamma_3 \quad (15)$$

$$\text{vrai max}_{(x,t) \in Q} \left(\sum_{i=1}^2 \|B_i\|_E^2, \sum_{i=1}^2 \|C_i\|_E^2, \|C\|_E \right) \leq \gamma_4.$$

Consider the first initial-boundary value problem for the equation (13) with the following initial and boundary conditions

$$w(x, 0) = \phi_0(x), \quad x \in \Omega; \quad (16)$$

$$w(x, t) = 0, \quad (x, t) \in \Gamma. \quad (17)$$

Definition. The function $w(x, t) \in W_{2,0}^{2,1}(Q)$ is called a generalized solution of (13), (16)-(17) if for all t from $[0, T]$ and any vector-function $\eta(x, t) \in L_2(Q)$ the following identity is fulfilled

$$\int_0^t \int_{\Omega} \eta^T \left\{ B_0 w_t - \left(B_{ij} w_{x_j} + B_i w \right)_{x_i} + \left(C_i w_{x_i} + C w + f \right) \right\} dx dt = 0 \quad (18)$$

and

$$\int_{\Omega} [w(x, \Delta t) - \phi_0(x)]^2 dx \rightarrow 0 \quad \text{as } \Delta t \rightarrow +0. \quad (19)$$

$W_{2,0}^{2,l}(Q)$ is the Hilbert space of functions with zero-value at Γ , and the scalar product is defined by

$$(w, v)_{W_{2,0}^{2,l}(Q)} = \int_Q \sum_{k=1}^m \left[w_k v_k + \frac{\partial w_k}{\partial t} \frac{\partial v_k}{\partial t} + \sum_{i=1}^2 \frac{\partial w_k}{\partial x_i} \frac{\partial v_k}{\partial x_i} + \sum_{i,j=1}^2 \frac{\partial^2 w_k}{\partial x_i \partial x_j} \frac{\partial^2 v_k}{\partial x_i \partial x_j} \right] dx dt$$

Theorem 1. *Let the coefficients and free terms in the equation (13) satisfy to restrictions (14)-(15). Ω is a open connected bounded domain in E^2 with boundary $\partial\Omega$, having second bounded derivatives.*

Then, for an arbitrary function $\phi_0(x)$ from $\dot{W}_2^1(\Omega)$ and for an arbitrary function $f(x, t) \in L_2(Q)$, there is a unique solution of the problem (13), (16)-(17) in $W_{2,0}^{2,l}(Q)$ such that

$$\|w(x, t)\|_{W_{2,0}^{2,l}(Q)}^2 \leq M \left(\|\phi_0(x)\|_{W_2^1(\Omega)}^2 + \|f\|_{L_2(Q)}^2 \right)$$

and for all $t \in [0, T]$

$$\|w(x, t)\|_{L_2(\Omega)}^2 \leq \sigma_I^{-1} \exp\{\gamma_5 t / \sigma_I\} \left(\gamma_I \|\phi_0(x)\|_{L_2(\Omega)}^2 + \|f\|_{L_2(Q)}^2 \right),$$

where the constant M depends only on $\sigma, \sigma_I, \gamma, \gamma_I, \gamma_2, \gamma_3, \gamma_4, T, \partial\Omega$ and $\gamma_5 = 1 + \gamma_2 + 2\gamma_4 + 2\gamma_4 \sigma^{-1}$.

The solvability of the initial-boundary value problem (4), (6)-(7) can be proved by using the Galerkin method in similar way as in [5].

Corollary. *Let the coefficients of the equation (4) satisfy the restrictions (5) on U_{ad} . The matrices $H(x)$, $R_0(x)$ are bounded and measurable on Ω and have bounded derivatives with respect to x , and $c^d(x) \in \dot{W}_2^1(\Omega)$.*

Then, for each $u = (\mu, v, r, c^0)$ from U_{ad} , the problems (4), (6)-(7) and (10)-(12) admit a unique solution in $W_{2,0}^{2,l}(Q)$.

4 Existence of Cost Functional Minimum

Theorem 2. *Let state vector $c(x, t; u)$ is governed by the first initial-boundary value problem (4), (6)-(7), the coefficients of which satisfy to the restrictions (5). Let the set of admissible model parameters U_{ad} is a closed convex bounded set in U . Cost functional is defined by the relationship (9).*

Then $U^* = \left\{ u = (\mu, \nu, r, c^0)^T \in U_{ad} : \mathfrak{J}(u, c(x, t; u)) = \inf_{v \in U_{ad}} \mathfrak{J}(v, c(x, t; v)) \right\}$ is non-empty and weakly compact set. Any minimizing sequence $\{u^k\} \in U_{ad}$ converges weakly to U^* .

Proof. Let $\{u^k\} \in U_{ad}$ is a minimizing sequence, i.e.

$$\mathfrak{J}(u^k, c(x, t; u^k)) \rightarrow \inf_{u \in U_{ad}} \mathfrak{J}(u, c(x, t; u)) \quad \text{as } k \rightarrow \infty. \quad (20)$$

According to the Theorem 1, the problem (4), (6)-(7) admits a unique solution on U_{ad} such that $\|c(x, t; u)\|_{W_{2,0}^{2,l}(Q)} \leq M_I$, where the constant M_I does not depend on u .

Due to boundedness of the solutions $c(x, t; u)$ on U_{ad} and boundedness of the set U_{ad} there is a subsequence $\{u^N\}$ of the sequence $\{u^k\}$ that

- $c(x, t; u^N) \rightarrow \tilde{c}(x, t)$ weakly in $W_{2,0}^{2,l}(Q)$,
- $\mu^N \rightarrow \tilde{\mu}$ and $\nu^N \rightarrow \tilde{\nu}$ in $E^{2 \times m}$,
- $c^{0N} \rightarrow \tilde{c}^0$ weakly in $W_2^l(\Omega)$,
- $r^N \rightarrow \tilde{r}$ weakly in $L_2(Q)$.

Moreover, from the imbedding theorems [6, pp.35-36], we have that c^{0N} converges to $\tilde{c}^0$ in $L_2(\Omega)$ and $\|c(x, t; u^N) - \tilde{c}(x, t)\|_{L_2(\Omega)} \rightarrow 0$ as $N \rightarrow \infty$ uniformly with regard to $t \in [0, T]$. Since U_{ad} is a closed convex set, the set U_{ad} is weakly closed and $\tilde{u} = (\tilde{\mu}, \tilde{\nu}, \tilde{r}, \tilde{c}^0)^T \in U_{ad}$.

It is easy to show that $\tilde{c}(x, t)$ coincides with $c(x, t; \tilde{u})$. To show this, it is sufficiently in (18)-(19) written for the $c(x, t; u^N)$ to pass to the limit as $N \rightarrow \infty$. Hence, the function $\tilde{c}(x, t)$ is a solution of the problem (4), (6)-(7) for $u = \tilde{u}$.

The functional $\mathfrak{J}(u, c(x, t; u))$ is a convex continuous functional of the arguments, so it is weakly lower semicontinuous and

$$\liminf_{N \rightarrow \infty} \mathfrak{J}(u^N, c(x, t; u^N)) \geq \mathfrak{J}(\tilde{u}, \tilde{c}(x, t))$$

Therefore from (20) follows

$$\mathfrak{J}(\tilde{u}, \tilde{c}(x, t)) \leq \inf_{u \in U_{ad}} \mathfrak{J}(u, c(x, t; u)).$$

Thus $\mathfrak{J}(\tilde{u}, \tilde{c}(x, t)) = \inf_{u \in U_{ad}} \mathfrak{J}(u, c(x, t; u))$ and $\tilde{u} \in U^*$.

It remains for us to show that the set U^* is weakly compact. Let's take an arbitrary sequence $\{u^k\} \in U^*$. Then $\{u^k\} \in U_{ad}$ and there is a subsequence $\{u^N\}$ which converges weakly to some point $\tilde{u} \in U_{ad}$. But $\mathfrak{J}(u^N, c(x, t; u^N)) = \inf_{u \in U_{ad}} \mathfrak{J}(u, c(x, t; u))$,

$N=1,2,\dots$, so $\{u^N\}$ is a minimizing sequence. As shown above, the $\{u^N\}$ converges weakly to U^* , therefore $\tilde{u} \in U^*$. Hence, the set U^* is weakly compact that completes the proof.

Let's remark that the set of solutions of the problem (4), (6)-(7) is non-convex, therefore a minimum of the cost functional can be non-unique.

Theorem 3. *Let the assumptions of Theorem 2 are fulfilled.*

Then the cost functional (9) is continuously differentiated on U_{ad} and its gradient

$$\begin{aligned} \mathfrak{S}'(u) &= \left(\frac{\partial \mathfrak{S}}{\partial \mu}, \frac{\partial \mathfrak{S}}{\partial v}, \frac{\partial \mathfrak{S}}{\partial r}, \frac{\partial \mathfrak{S}}{\partial c^0} \right)^T \text{ is represented by} \\ \frac{1}{2} \frac{\partial \mathfrak{S}}{\partial \mu_i}(u, c(x, t; u)) &= R_{\mu_i} (\mu_i - \mu_i^a) + \chi^{\mu_i}, \\ \frac{1}{2} \frac{\partial \mathfrak{S}}{\partial v_i}(u, c(x, t; u)) &= R_{v_i} (v_i - v_i^a) + \chi^{v_i}, \\ \frac{1}{2} \frac{\partial \mathfrak{S}}{\partial r}(u, c(x, t; u)) &= R_I r(x, t) - c^*(x, t; u), \\ \frac{1}{2} \frac{\partial \mathfrak{S}}{\partial c^0}(u, c(x, t; u)) &= R_2 [c^0(x) - c_a^0(x)] - A_0 c^*(x, 0; u), \end{aligned} \quad (21)$$

where $c^*(x, t; u)$ is the solution of the adjoint problem (10)-(12), $\chi^{\mu_i}, \chi^{v_i} \in E^m$ and

$$\begin{aligned} \chi_k^{\mu_i}(u) &= \int_0^T \int_{\Omega_k} c^{*T}(x, t; u) \frac{\partial G}{\partial \mu_i} c(x, t; u) dx dt, \\ \chi_k^{v_i}(u) &= \int_0^T \int_{\Omega_k} c^{*T}(x, t; u) \frac{\partial G}{\partial v_i} c(x, t; u) dx dt. \end{aligned} \quad (22)$$

For any point $u^* \in U^*$, it is necessary the following inequality is fulfilled

$$\left\langle \mathfrak{S}'(u^*), u - u^* \right\rangle_U \geq 0 \quad \text{for all } u \in U_{ad}.$$

5 Sufficient Condition of Existence of Stationary Points

In the previous section has been shown that the set of minimum of the cost functional (9) on U_{ad} is non-empty. But the point of cost functional minimum can be both interior, and boundary point of U_{ad} . It is clear that an interior point of cost functional minimum is the stationary point.

Theorem 4. *Let state function $c(x, t; u)$ is governed by the first initial-boundary value problem (4), (6)-(7), the coefficients of which satisfy to restrictions (5). Let the set of admissible model parameters U_{ad} is a convex closed bounded set and the following*

inequalities are valid for all $u = (\mu, v, r, c^0)^T \in U_{ad}$

$$\begin{aligned}\|\mu_i - \mu_i^a\|_{E^m} &\leq \delta_{\mu_i}, & \|v_i - v_i^a\|_{E^m} &\leq \delta_{v_i}, \\ \|r\|_{L_2(Q)} &\leq \delta_r, & \|c^0 - c_a^0\|_{W_2^1(\Omega)} &\leq \delta_c.\end{aligned}$$

Then it is sufficient for existence of a unique stationary point on U_{ad} that the weight functions $R_0, R_1, R_2, R_{\mu_i}, R_{v_i}$ satisfied to the following inequalities for all $u, w \in U_{ad}$ and $q \in (0, 1)$

$$\begin{aligned}\|R_I^{-1} c^*(x, t; u)\|_{L_2(Q)} &\leq \delta_r, & \|R_2^{-1} A_0 c^*(x, 0; u)\|_{W_2^1(\Omega)} &\leq \delta_c, \\ \|R_{\mu_i}^{-1} \chi^{\mu_i}(u)\|_{E^m} &\leq \delta_{\mu_i}, & \|R_{v_i}^{-1} \chi^{v_i}(u)\|_{E^m} &\leq \delta_{v_i}, \\ \|R_I^{-1} [c^*(x, t; u) - c^*(x, t; w)]\|_{L_2(Q)}^2 &+ \|R_2^{-1} A_0 [c^*(x, 0; u) - c^*(x, 0; w)]\|_{W_2^1(\Omega)}^2 + \\ &+ \|R_{\mu_i}^{-1} (\chi^{\mu_i}(u) - \chi^{\mu_i}(w))\|_{E^m}^2 + \|R_{v_i}^{-1} (\chi^{v_i}(u) - \chi^{v_i}(w))\|_{E^m}^2 \leq q^2 \|u - w\|_U^2,\end{aligned}$$

where $c^*(x, t; u)$ is the solution of the adjoint problem (10)-(12), and $\chi^{\mu_i}(u), \chi^{v_i}(u) \in E^m$ are defined by (22).

Really, we can rewrite the stationarity conditions (21) as the following operator equation $u = F(u)$. It is obviously that under assumptions of Theorem 4, the operator F is contracting and mapping the set U_{ad} into itself.

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