Working Paper

On Estimation of Forcing Functions in Parabolic Systems

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WP-95-75
December 1995

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Preface

The present paper is an outcome of a research carried out at the Dynamic Systems project and the project on Advanced Computer Applications in 1994/95. The research is motivated by a problem of reconstruction of time-varying intensities of pollution sources in a water reservoir via measuring pollutant concentrations in accessible domains. We start with convergent input estimation algorithms for a system described by a general parabolic equation. One of the algorithms is specified for a particular diffusion-type groundwater contamination model, and tested numerically.

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Introduction

The management of environmental systems rests on available data on systems states. Data on pollution regimes are typically of special importance. If there is no direct access to the pollution sources, the data are gained through observations of pollutant concentrations in accessible domains. Normally such indirect observations carry not enough information, and the pollution regimes (forcing functions) cannot be entirely reconstructed. Some signals on these regimes can however be reconstructed precisely, and for other signals the admissible diapasones can be estimated.

In section 1 we give a classification of fully reconstructible linear signals, provide algorithms to find admissible diapasones for given linear signals, and point out situations where input regimes are reconstructible precisely. Our analysis is restricted to models represented by abstract parabolic systems (see Lions, 1971).

Methodologically, the problems under consideration belong to the category of inverse problems for parabolic systems (see, e.g., Lavrentyev, et. al., 1980; Banks and Kunisch, 1982; Kurzhanski and Khapalov, 1989; Kunisch and White, 1989; Barbu, 1991; Osipov, et. al., 1991; Ainsemba, et. al., 1994). The innovation of the proposed approach consists in employing the technique of adjoint equations of Lions, 1971, and Marchuk, 1982, for the estimation of time varying inputs. In this part, the paper develops the technique suggested in Kryazhimskii and Osipov, 1993. The method is based on a reduction of an input reconstruction problem to a linear finite-dimensional integral equation whose solutions form a subspace in a functional space of all admissible inputs. The subspace is "flat" in some functional "directions". These "directions" characterize all fully reconstructible linear signals. The reconstructibility analysis is carried out in subsections 1.3 – 1.5.

In subsections 1.6, 1.7 an important special case where the integral equation has a single solution, and therefore the input regimes are entirely reconstructible, is described. A finite-dimensional step-by-step input reconstruction algorithm based on the method of dynamical regularization (see Osipov and Kryazhimskii, 1995) is described.

For a general case where the integral equation has many sulutions, we fix a linear signal on forcing regimes and estimate the interval of signal values compatible with an observation result (subsections 1.8, 1.9). This setting is well coordinated with the notion of normal solutions widely used in theory of ill-posed problems (see Tikhonov and Arsenin,

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For this author, the research was supported partly by International Science Foundation Grant No NMD000 and Grant No 93-011-16129 of the Fund for Fundamental Research of the Russian Academy of Sciences.

1979). It is also close to a problem of estimation of support functionals of informational sets (theory of observation; see Kurzhanskii, 1977). We provide two estimation algorithms employing a special convex optimization technique suggested in Kryazhimskii and Osipov, 1987 (and later developed in Kryazhimskii, 1994, and Ermoliev, et. al., 1995).

In section 2 the above estimation algorithms are specified for a model of a contamination process described by a partial differential equation of the parabolic type (see, e.g., Marchuk, 1982). The fact that instead of the initial partial differential equation one deals with a finite-dimensional integral equation results in a considerable reduction of complexity. Namely, in contrast with traditional regularization techniques, the method requires a single integration of the (adjoint) parabolic system (on the stage of defining the integral equation).

In section 3 we apply the estimation methodology of section 2 to a groundwater contamination transport model integrated in *XGW: A Prototype Expert System User Interface for Interactive Modeling of Groundwater Contamination*, an information system developed at IIASA's project on Advanced Computer Applications.

1 The Abstract Parabolic System

1.1 System equation

Let $(V, \|\cdot\|)$ be a separable and reflexive Banach space, $(H, |\cdot|_H)$ be a real Hilbert space, $H = H^*$, $(\cdot,\cdot)$ stand for the scalar product in H, and V be imbedded in H densly and continuously. Consider the parabolic system

$$\dot{x}(t) + Ax(t) = Bu(t) + f(t), \tag{1.1}$$

$$t \in T = [0, \vartheta], \qquad x(0) = x_0 \in H.$$

Here $A : V \to V^*$ is a linear continuous operator satisfying, with some $c > 0$ and $\lambda \in \mathbf{R}$, the condition

$$\langle Ay, y\rangle + \lambda |y|_H^2 \geq c\|y\|^2 \qquad \forall y \in V;$$

$\langle\cdot,\cdot\rangle$ is the duality between V and V^*; $x(t)$ is a system's state at time t; $u(t)$ is the n-dimensional value of a time-varying input to the system; $f(\cdot) \in \mathbf{L}_2(T; H)$ is a given disturbance; $B : U = \mathbf{R}^n \to V$,

$$Bu = \sum_{j=1}^{n} \omega_j u_j, \quad \omega_j \in V, \quad u_j \in \mathbf{R}.$$

We fix an initial state x_0.

Definition 1.1. A function $x(\cdot) = x(\cdot; x_0, u(\cdot))$ is called a *solution* of (1.1) on T if

a) $x(\cdot) \in W(T; V) = \{y(\cdot) \in \mathbf{L}_2(T; V) : \dot{y}(\cdot) \in \mathbf{L}_2(T; V^*)\}$;

b) for a. a. $t \in T$ the equality (1.1) is true, i.e.

$$< \dot{x}(t), v > + < Ax(t), v >= (Bu(t) + f(t), v) \quad \forall v \in V$$

holds.

By Theorem 1.2 of Lions, 1971 (p. 110) for every $u(\cdot) \in \mathbf{L}_2(T; U)$ there exists a unique solution of (1.1). In what follows, for simplicity it is assumed that $f(t) = 0$.

1.2 Observation and reconstruction

Let the above system be observed. The Observer knows the system equation (1.1) and, at every time t the vector

$$z(t) = Px(t), \qquad P \in \mathbf{L}(H; \mathbf{R}^m), \tag{1.2}$$

carrying information on system's state $x(t)$. Input values $u(t)$ are unknown to the Observer. The Observer's task is to reconstruct $u(t)$ on the basis of all available data, i. e. the system equation (1.1), the initial state, the observation operator P and the observation results (1.2).

1.3 Reconstructible functionals

Denote $\mathbf{L}^2_{s,\xi} = \mathbf{L}^2([s,\xi], \mathbf{R}^n)$. An *input on* $[0,s]$ $(s \geq 0)$ is identified with a function $u(\cdot)$ from $\mathbf{L}^2_{0,s}$. The set of all $u(\cdot)$ compatible with $z(\cdot)$, i. e. satisfying (1.2) where $x(\cdot)$ is a solution to (1.1) will be denoted by $U_s(z(\cdot))$. For the set of all observation results on $[0,s]$ we shall use the notation Z_s. The symbol $x(\cdot)$ is used for a function with the value $x(t)$ at a point t; the restriction of $x(\cdot)$ to an interval $[s,\xi]$ (belonging to the set of definition of $x(\cdot)$) is denoted $x(\cdot)_{s,\xi}$.

A continuous linear functional l on the space $\mathbf{L}^2_{0,s}$ of all inputs on $[0,s]$ will be as usual identified with an element

$$l(\cdot) \in \mathbf{L}^2_{0,s} \tag{1.3}$$

determined by

$$l(u(\cdot)) = \int_0^s (l(t), u(t))_{\mathbf{R}^n} dt.$$

For every above $l(\cdot)$ and every observation result $z(\cdot)$ on $[0,s]$, introduce the image of the set $U_s(z(\cdot))$ under $l(\cdot)$:

$$R_s(l(\cdot), z(\cdot)) = \left\{ \int_0^s (l(t), u(t))_{\mathbf{R}^n} dt \ : \ u(\cdot) \in U_s(z(\cdot)) \right\}. \tag{1.4}$$

Introduce the following definitions.

Definition 1.2. A functional (1.3) will be called *reconstructible at* $z(\cdot) \in Z_s$ if the set (1.4) is one-element, and *non-reconstructable at* $z(\cdot)$ if this set coincides with the whole real line.

Definition 1.3. A functional (1.3) reconstructible (respectively, non-reconstructable) at every $z(\cdot) \in Z_s$ will be called *reconstructible* (respectively, *non-reconstructable*) *on* $[0,s]$.

Definition 1.4. We shall say that *an input is reconstructible at* $z(\cdot) \in Z_s$ if every functional (1.4) is reconstructible at $z(\cdot)$.

Definition 1.5. If the latter holds for every $z(\cdot) \in Z_s$, we shall say that *the input is reconstructible on* $[0,s]$.

Let us study the following problem: given an observation result $z(\cdot)$ on $[0,s]$, find all functionals (1.3) reconstructible at $z(\cdot)$ and all functionals (1.3) non-reconstructible at $z(\cdot)$.

1.4 Compatibility criterion

We assume $Px = \{(p_1, x), ..., (p_m, x)\}$ where $\{p_1, \dots, p_m\} \in \prod_{j=1}^{m} H$. For any $k \in [1:m]$ and $\sigma \geq 0$, define $w_k(\cdot, \sigma)$ to be the solution of the Cauchy problem

$$\dot{w}(t) = A^* w(t) \tag{1.5}$$

$$w(\sigma) = p_k \tag{1.6}$$

on $]-\infty, \sigma]$ and zero on $]\sigma, \infty[$. Set

$$(\phi_k(t;\sigma))_j = (w_k(t,\sigma), \omega_j), \quad j \in [1:n], \tag{1.7}$$

where $(\cdot,\cdot)$ stands for the scalar product in H; let also

$$\phi_k(\cdot;\sigma) = \{(\phi_k(\cdot,\sigma))_1, (\phi_k(\cdot,\sigma))_2, \dots, (\phi_k(\cdot,\sigma))_n\},$$

$$g_k(a,\sigma) = a_k - (w_k(0,\sigma), x_0), \quad (a = \{a_1, a_2, \dots, a_m\} \in \mathbf{R}^m). \tag{1.8}$$

Here A^* is the operator adjoint to A. By Theorem 1.2 of Lions, 1971 (p. 110, 121) there exists a unique solution of system (1.5), (1.6) such that $w(\cdot,\sigma) \in \mathbf{W}([-r,\sigma]; V)$ for any $r \in (\sigma, +\infty)$.

Theorem 1.1 *An input $u(\cdot)$ is compatible with an observation result $z(\cdot)$ on $[0,s]$ (or, equivalently, $u(\cdot) \in U_s(z(\cdot))$ if and only if*

$$\int_0^\sigma (\phi_k(t,\sigma)_{0,s}, u(t))_{\mathbf{R}^n} dt = g_k(z(\sigma),\sigma) \tag{1.9}$$

for all $\sigma \in [0,s]$ and $k \in [1:m]$.

Proof. Let $u(\cdot)$ be compatible with $z(\cdot)$, and $x(\cdot)$ be the trajectory corresponding to $u(\cdot)$. Then for all $t \in [0,s]$ we have (1.2) or, equivalently,

$$z^{(k)}(t) = (p_k, x(t)) \tag{1.10}$$

for every $k \in [1:m]$. Take arbitrary $\sigma \in [0,s]$ and $k \in [1:m]$. Let

$$w(\cdot) = w_k(\cdot,\sigma). \tag{1.11}$$

Multiply scalarly (1.1) by $w(t)$ and (1.5) by $x(t)$, distract and integrate from 0 to σ. We get

$$\int_0^\sigma [(w(t), \dot{x}(t)) + (\dot{w}(t), x(t))]\, dt =$$

$$-\int_0^\sigma [\langle w(t), A(t)x(t)\rangle - \langle A^*(t)w(t), x(t)\rangle]\, dt + \int_0^\sigma (w(t), Bu(t))\, dt\ .$$

The left hand side is integrated explicitly, and the first integrand in the right hand side is zero. Therefore the above equality can be rewritten as

$$\int_0^\sigma (\phi_k(t,\sigma), u(t))_{\mathbf{R}^n} dt = (w(\sigma), x(\sigma)) - (w(0), x(0))\ .$$

This equality is equivalent to (1.9) (see (1.11) and (1.7) to compare the left hand sides, and (1.6), (1.10), (1.11), and (1.8), to compare the right hand sides).

Conversely, let $u(\cdot)$ satisfy (1.9) for all $\sigma \in [0, s]$ and $k \in [1 : m]$. Suppose that $u(\cdot)$ is not compatible with $z(\cdot)$. Then there exist $\sigma \in [0, s]$ and $i \in [1 : m]$ such that

$$z^{(i)}(\sigma) \neq (p_i, x(\sigma)) \tag{1.12}$$

where $x(\cdot)$ is the trajectory corresponding to $u(\cdot)$. As above, we come to the equality analogous to (1.9) with $z(\sigma)$ replaced by $Px(\sigma)$. Distract this equality from (1.9). The result contradicts to (1.12). The theorem is proved.

1.5 Reconstructibility alternative

From Theorem 1.1 follows that for $l(\cdot) = \phi_k(\cdot, \sigma)_{0,s}$ where $\sigma \in [0, s]$ and $k \in [1 : m]$, the value $\int_0^s (l(t), u(t))_{\mathbf{R}^n} dt$ does not depend on $u(\cdot) \in U_s(z(\cdot))$; therefore the above $l(\cdot)$ is reconstructible at $z(\cdot)$. Note that this is so for an arbitrary $z(\cdot) \in Z_s$ meaning that $l(\cdot)$ is reconstructible on $[0, s]$. The next theorem states that this holds for every functional from the linear hull of all above $l(\cdot)$, and all other functionals are non-reconstructible on $[0, s]$.

Let

$$K_s = \{\phi_k(\cdot, \sigma)_{0,s} \ : \ \sigma \in [0, s], \ k \in [1 : m]\},$$

$$L_s = \mathrm{Lin} K_s.$$

By Lin$E$ we denote the linear hull of a set E in the space $\mathbf{L}^2([s, \xi]; \mathbf{R}^n)$.

Theorem 1.2 *Every $l(\cdot) \in L_s$ is reconstructible on $[0, s]$, and every $l(\cdot) \in \mathbf{L}^2_{0,s} \setminus L_s$ is non-reconstructable on $[0, s]$.*

From Theorem 1.2 and the definition of input reconstructibility the next Corollary follows.

Corollary 1.1 *The following assertions are equivalent:*
(i) an input is reconstructible on $[0, s]$,
(ii) an input is reconstructible at a certain $z(\cdot)$,
(iii) $L_s = \mathbf{L}^2_{0,s}$.

1.6 Input reconstructibility conditions

Let us provide a sufficient input reconstructibility condition. We assume $n = m$. Introduce the $n \times n$-dimensional matrices

$$D(p) = \{(\omega_j, p_k)\}_{j,k=1}^n,$$

$$K(s, t) = \{a_{k,j}(s, t)\}_{j,k=1}^n,$$

where k is a row number and j is a column number,

$$a_{k,j}(s, t) = \begin{cases} (A\omega_j, z_k(s - t, 0)), & t \geq s \\ 0, & t < s \end{cases}$$

and $z_k(t, 0)$ is the unique solution of the equation

$$\dot{z}(t) + A^* z(t) = 0, \quad t \in [0, \vartheta]$$

$$z(0) = p_k$$

in the sense of Definition 1.1.

Let the following condition be fulfilled.

Condition 1.1 $\omega_j \in \{x \in V : Ax \in H\} \quad \forall j \in [1:n]$.

Then the next theorem is true.

Theorem 1.3 *Let* $\{((\omega_1, p_j), \ldots, (\omega_n, p_j)) \ : \ j \in [1:n]\}$, *be a basis in* $\mathbf{R}^n$. *Then an input is reconstructible on* $[0, s]$.

Proof. Differentiate (1.9) for $\sigma = s$ at an s. We get

$$(B^* p_k, u(s))_{\mathbf{R}^n} + \int_0^s \frac{d}{ds}(\phi_k(t,s), u(t))_{\mathbf{R}^n} dt = \frac{d}{ds} g_k(z(s), s). \tag{1.13}$$

It is easily seen that equation (1.5) implies the equality

$$\frac{d}{ds}(\phi_k(t,s))_j = \frac{d}{ds}(\omega_j, w_k(t,s)) = \frac{d}{ds}(\omega_j, w_k(t-s, 0)) =$$
$$= -\frac{d}{d\xi}(\omega_j, w_k(\xi, 0)) = -\langle \frac{d}{d\xi} w_k(\xi, 0), \omega_j \rangle = \tag{1.14}$$
$$= \langle A^* w_k(\xi, 0), \omega_j \rangle = (A\omega_j, w_k(t-s, 0)) = (A\omega_j, z_k(s-t, 0)) \qquad \forall j \in [1:n].$$

Here $\xi = t - s$. From (1.13), (1.14) we have

$$D(p)u(s) + \int_0^s K(s,t)u(t)dt = \dot{g}(s, z), \tag{1.15}$$

$$\dot{g}(s, z) = \{\dot{g}_1(z(s), s), \ldots, \dot{g}_n(z(s), s)\}.$$

Note that the integral equation (1.15) has the unique solution

$$u(\cdot) \in \mathbf{L}_2(T; \mathbf{R}^n).$$

The theorem is proved.

In the case where an input is reconstructible on $[0, \vartheta]$ we shall assume $u(\cdot)$ to be the unique element of the set $U_\vartheta(z(\cdot))$.

1.7 Dynamical input reconstruction

Let us describe a dynamical algorithm to approach $u(\cdot)$ assuming Condition 1.1 and conditions of Theorem 1.3 to be fulfilled. Here we suppose that $z(t)$ is measured inaccurately; namely, measurements results

$$z_h^*(t) = (z_{1,h}^*(t), z_{2,h}^*(t), \ldots, z_{n,h}^*(t)) \in \mathbf{R}^n$$

satisfy

$$|z_h^*(t) - z(t)| \le h \tag{1.16}$$

where h is a (small) upper bound for measurement errors, and $|\cdot|$ stands for the eucledean norm in $\mathbf{R}^n$.

Fix a family Δ_h of partitions of the interval T with diameters $\delta(h)$,

$$\Delta_h = \{\tau_{h,i}\}_{i=0}^{m_h}, \quad \tau_{h,0} = 0, \quad \tau_{h,m_h} = \vartheta, \quad \tau_{h,i+1} - \tau_{h,i} = \delta(h).$$

Introduce the discrete time control system

$$\begin{aligned} w^{(1)}(\tau_{i+1}) &= w^{(1)}(\tau_i) + \delta D(p) v_i^h, \quad w^{(1)}(0) = 0, \\ w^{(2)}(\tau_{i+1}) &= \delta^2 \sum_{k=1}^{i+1} \sum_{j=1}^{k} K(\tau_k, \tau_{j-1}) v_{j-1}^h, \quad \tau_i = \tau_{h,i}, \\ w^{(3)}(\tau_{i+1}) &= \delta \sum_{j=1}^{i+1} K(\tau_{i+2}, \tau_{j-1}) v_{j-1}^h, \quad w^{(j)} \in \mathbf{R}^n, \quad j \in [1:3]. \end{aligned} \tag{1.17}$$

Algorithm 1.1
Parameters:
$h \in (0,1)$,
partition $\Delta = \Delta_h = \{\tau_{h,i}\}_{i=0}^{m_h}$, $m = m_h$.
Output:
$v^h(\cdot) \in \mathbf{L}^2_{0,\vartheta}$.
Variables:
$v_i \in \mathbf{R}^n$,
$w(\tau_{h,i}) = \{w^{(1)}(\tau_{h,i}), w^{(2)}(\tau_{h,i}), w^{(3)}(\tau_{h,i})\} \in \mathbf{R}^{3n}$.
Initial Step:
Put $w(\tau_{h,0}) = 0$.
***i*-th Step** $(1 \le i \le m_h - 1)$ **:**
The step is performed during the time interval $\delta_{h,i} = [\tau_{h,i}, \tau_{h,i+1})$.
Compute

$$\nu_i = (g^*(\tau_{i+1}) - g^*(\tau_i))/\delta - w^{(3)}(\tau_i),$$

$$g^*(\tau_i) = \{g_1^*(\tau_i), g_2^*(\tau_i), \ldots, g_n^*(\tau_i)\},$$

$$g_k^*(\tau_i) = z_{k,h}^*(\tau_i) - (w_k(0,\tau_i), x_0) = z_{k,h}^*(\tau_i) - (z_k(\tau_i, 0), x_0), \quad k \in [1:n].$$

$$v_i^h = \begin{cases} |\nu_i| D^{-1}(p)\, s_i \,/\, |s_i|, & |s_i| \neq 0 \\ 0, & |s_i| = 0; \end{cases}$$

$$s_i = g^*(\tau_i) - g^*(0) - w^{(1)}(\tau_i) - w^{(2)}(\tau_i).$$

Set

$$v^h(t) = v_{i-1}^h \qquad (t \in \delta_{h,i}).$$

Perform transformation (1.17).

Theorem 1.4 *Let* $h/\delta(h) \to 0$, $\delta(h) \to 0$ *as* $h \to 0$. *Then*

$$v^h(\cdot) \to u(\cdot)$$

weakly in $\mathbf{L}^2(T; \mathbf{R}^n)$.

The proof of the Theorem is similar to those of the corresponding assertions of Maksimov, 1992a, 1992b. The following technical lemma is used.

Lemma 1.1 *The bounds*

$$\varepsilon(\tau_i) = |g(\tau_i) - g(0) - w^{(1)}(\tau_i) - w^{(2)}(\tau_i)|^2 \le c(h/\delta + \delta) \quad \forall i \in [1 : m_h - 1],$$

$$\sum_{j=1}^{m_h-1} \delta |v_{j-1}^h|^2 \le c_*, \quad g(t) = g(z(t), t)$$

hold uniformly with respect to all $h \in (0,1)$, $\{\Delta_h\}$ *with diameter* $\delta = \delta(h)$, $h/\delta(h) \le 1$ *and* $z^*(\cdot)$ *satisfying (1.16).*

Proof. Let us estimate the evolution of

$$\varepsilon(\tau_i) = |g(\tau_i) - g(0) - w^{(1)}(\tau_i) - w^{(2)}(\tau_i)|^2 =$$

$$= |g(\tau_i) - g(0) - \sum_{k=1}^{i} D(p) v_{k-1}^h - \sum_{k=1}^{i} \delta (\sum_{j=1}^{k} \delta K(\tau_k, \tau_{j-1}) v_{j-1}^h)|^2 \tag{1.18}$$

$$(i \in [1 : m_h]).$$

Note that for $t \in [\tau_k, \tau_{k+1}]$ due to the equality

$$v^h(t) = v_j^h, \quad t \in [\tau_j, \tau_{j+1})$$

we have

$$|\int_0^s K(s,\tau) v^h(\tau) d\tau - \sum_{j=1}^{k} \delta K(\tau_k, \tau_{j-1}) v_{j-1}^h| \le$$

$$\le 2\omega_k(\delta)\delta \sum_{j=1}^{k} |v_{j-1}^h| + k_0 \delta |v_k^h|,$$

$$|K(t,\tau)|_n \le k_0 \quad (t, \tau \in T),$$

where $|\cdot|_n$ is the $n \times n$-matrice norm. Consequently

$$\begin{aligned} \varepsilon_1(\tau_i) \quad &\equiv \quad |\int_0^{\tau_i} \{\dot{g}(s) - D(p) v^h(s) - \int_0^s K(s,\tau) v^h(\tau) d\tau\} ds| \le \\ &\le \quad \varepsilon^{1/2}(\tau_i) + |\int_0^{\tau_i}\int_0^s K(s,\tau) v^h(\tau) d\tau ds - \sum_{k=1}^{i}\sum_{j=1}^{k} \delta^2 K(\tau_k, \tau_{j-1}) v_{j-1}^h| \le \\ &\le \quad \varepsilon^{1/2}(\tau_i) + \delta\{2\vartheta + \omega_k(\delta) + k_0\delta\} \sum_{j=1}^{i} |v_{j-1}^h|, \end{aligned} \tag{1.19}$$

where $\omega_k(\cdot)$ is a modulo of continuity of the function $K(t,\tau) = K(t-\tau)$, $0 \le \tau \le t \le \vartheta$. Further on, we have

$$\sum_{k=1}^{i+1}\sum_{j=1}^{k} \delta^2 K(\tau_k, \tau_{j-1}) v_{j-1}^h = \sum_{j=1}^{i+1} \{\sum_{k=j}^{i+1} \delta^2 K(\tau_k, \tau_{j-1}) v_{j-1}^h\}, \tag{1.20}$$

$$\sum_{j=1}^{i+1}\sum_{k=j}^{i+1} \delta^2 K(\tau_k, \tau_{j-1}) v_{j-1}^h = \sum_{j=1}^{i}\sum_{k=j}^{i} \delta^2 K(\tau_k, \tau_{j-1}) v_{j-1}^h +$$

$$+\sum_{j=1}^{i}\delta^2 K(\tau_{i+1},\tau_{j-1})v_{j-1}^h+\sum_{k=j}^{i+1}\delta^2 K(\tau_k,\tau_i)v_i^h. \tag{1.21}$$

Therefore it follows from (1.18) – (1.21) that

$$\varepsilon(\tau_{i+1})=\varepsilon(\tau_i)+2r_i'\mu_i+|\mu_i|^2, \tag{1.22}$$

where

$$r_i=g(\tau_i)-g(0)-w^{(1)}(\tau_i)-w^{(2)}(\tau_i),$$

$$\mu_i=g(\tau_{i+1})-g(\tau_i)-\delta^2\{2K(\tau_{i+1},\tau_i)+K(\tau_i,\tau_i)\}v_i^h-$$

$$-\delta^2\sum_{j=1}^{i}K(\tau_{i+1},\tau_{j-1})v_{j-1}^h-\delta D(p)v_i^h.$$

One can easily get the inequalities

$$|r_i|\le C_1+C_2\delta\sum_{j=1}^{i}|v_{j-1}^h|,\quad i\ge 1 \tag{1.23}$$

$$|\mu_i|^2\le C_3\delta\{\int_{\tau_i}^{\tau_{i+1}}|\dot g(s)|^2ds+\sum_{j=1}^{i+1}\delta^2|v_{j-1}^h|^2+\delta|v_i^h|^2\}, \tag{1.24}$$

where the constants $C_j,\ j\in[1:3]$ do not depend on i,δ. Hence, taking into account the definition of v_i^h we deduce from (1.22) that

$$\varepsilon(\tau_{i+1})\le\varepsilon(\tau_i)+4h|\mu_i|+C_4(1+|r_i|)\delta^2|v_i^h|+|\mu_i|^2+C_5h(|r_i|+h). \tag{1.25}$$

Note that

$$d_i\equiv\delta_i|v_{i-1}^h|^2\le a_i+C_6\delta\sum_{j=1}^{i-1}d_j,$$

$$\sum_{j=1}^{m_h-1}a_j<+\infty.$$

Consequently,

$$\sum_{j=1}^{m_h-1}\delta|v_{j-1}^h|^2\equiv|v^h(\cdot)|^2_{\mathbf{L}_2(T;U)}\le C_7<+\infty. \tag{1.26}$$

Thus, by (1.23) – (1.26) we have

$$\varepsilon(\tau_{i+1})\le\varepsilon(\tau_i)+C_8(h/\delta+\delta),\quad i\in[0:m_h-1].$$

Lemma is proved.

Remark 1.1. The auxilliary discrete time control system (1.17) can be replaced by the following continuous time one:

$$\dot w^{(1)}(t)=D(p)v^h(t),$$

$$\dot w^{(2)}(t)=w^{(3)}(t),\quad t\in T,$$

$$w^{(1)}(0)=w^{(2)}(0)=0,$$

where

$$w^{(3)}(t) = \int_0^t K(t,\tau)v^h(t)d\tau.$$

In this case an analogue of Theorem 1.4. holds true.

Remark 1.2. If the solution $z(\cdot)$ of the adjoint equation is sufficiently smooth, for instance, $\dot{z}(\cdot) \in \mathbf{L}_2(T;H)$, then Condition 1.1 can be replaced by the weaker condition $\omega_j \in H$. In this case Theorems 1.3 and 1.4 remain true if one puts

$$a_{k,j}(s,t) = \left\{ \begin{array}{ll} -(\omega_j, \dot{z}_k(s-t,0)), & t \geq s \\ 0 & t < s \end{array} \right\}.$$

1.8 Approximations to extremal inputs

Let us now consider the general case where the input reconstructibility condition of Theorem 1.3 does not hold.

Fix an observation result $z(\cdot) \in Z_\vartheta$. Here we suppose that upon all inputs $u(\cdot)$ the constraint

$$u(\cdot) \in G \tag{1.27}$$

is imposed; G is a given convex bounded set in $\mathbf{L}^2_{0,\vartheta}$. Therefore, we will be interested in finding inputs from the set $U_\vartheta(z(\cdot);G) = U_\vartheta(z(\cdot) \cap G$.

We shall point out a method to approach either the minimum value of a certain convex functional on $U_\vartheta(z(\cdot;G)$, or its minimizer. The norm and the scalar product in $\mathbf{L}^2_{0,\vartheta}$ will in what follows be denoted $\|\cdot\|_\vartheta$ and $(\cdot,\cdot)_\vartheta$, respectively. The proposed method is intended to solve the system of integral equations (1.9) under the constraint (1.27). We rewrite (1.9) as

$$\Phi u(\cdot) = g(\cdot). \tag{1.28}$$

Here $g(\sigma)$ is the vector with coordinates $g_k(z(\sigma),\sigma)$ $(k = 1,...,m)$, and Φ is the linear operator from $\mathbf{L}^2(T,\mathbf{R}^n)$ to $\mathbf{L}^2(T,\mathbf{R}^m)$ of the form

$$\Phi u(\cdot) = \int_0^\sigma C(t,\sigma)u(t)dt; \tag{1.29}$$

$C(t,\sigma)$ is the $m \times n$-matrix whose k-th row $(k \leq m)$ is the vector $\phi_k(t,\sigma)$.

We shall use a modification of the Tikhonov's regularization method to approach a solution of the equation (1.28) (equivalent to (1.9)) under the constraint (1.27). Let $J(\cdot)$ be a convex functional on $\mathbf{L}^2_{0,\vartheta}$, bounded on G, and J^0 be its minimum value on $U_\vartheta(z(\cdot);G)$. It is known that if $J(\cdot)$ is strictly convex (in particular, $J(\cdot) = \|\cdot\|^2_\vartheta$), then there exists a unique (in the sense of $\mathbf{L}^2_{0,\vartheta}$) element providing the minimum of $J(\cdot)$ over $U_\vartheta(z(\cdot;G)$; we shall denote this element by $u^0(\cdot)$.

Theorem 1.5 *Let* $v_N \in G$,

$$\| \Phi v_N(\cdot) - g(\cdot) \|^2_\vartheta + \alpha_N J(v_N(\cdot)) - \alpha_N J^0 \leq \epsilon_N \ (N = 1,2,...), \tag{1.30}$$

$$\epsilon_N \to 0+, \quad \alpha_N \to 0+, \quad \epsilon_N/\alpha_N \to 0+ \ (N \to \infty).$$

Then

$$J(v_N(\cdot)) \to J^0 \ (N \to \infty) \tag{1.31}$$

and, if $J(\cdot)$ *is strictly convex,*

$$\| v_N(\cdot) - u^0(\cdot) \|_\vartheta \to 0. \ (N \to \infty) \tag{1.32}$$

A standard proof pattern see, e.g., in Vasilyev, 1981 (p. 182).

The following finite-step algorithm to calculate $v_N(\cdot)$ satisfying (1.30) with appropriate ϵ_N and α_N was given in Kryazhimskii and Osipov, 1987.

Algorithm 1.2.
Parameters:
$N,\ l_N$ – natural,
$\alpha_N > 0$.
Output:
$v_N(\cdot) \in G$.
Variable:
$y_i(\cdot) \in \mathbf{L}^2(T, \mathbf{R^n})$.
Initial Step:
Put $y_0(\cdot) = 0$.
***i*-th Step** $(0 \le i \le l_N - 1)$:
Find a solution $r_i(\cdot)$ of the problem

$$2(\Phi y_i(\cdot) - ig(\cdot)/l_N, \Phi r(\cdot))_\vartheta + \alpha J(r(\cdot)) \to \min,\ r(\cdot) \in G. \tag{1.33}$$

Put

$$y_{i+1}(\cdot) = y_i(\cdot) + r_i(\cdot)/l_N. \tag{1.34}$$

Final Step:
Put $v_N(\cdot) = y_{l_N}(\cdot)$.

Lemma 1.2 (Kryazhimskii and Osipov, 1987, Lemma 1.1). *Let $v_N(\cdot)$ be the output of Algorithm 1.2. Then (1.30) holds with $\epsilon_N = c^2/m$ where c is such that $\| \Phi u(\cdot) - g(\cdot) \|_\vartheta \le c$ for all $u(\cdot) \in G$.*

Lemma 1.2 and Theorem 1.5 yield the following.

Theorem 1.6 *Let*

$$\alpha_N \to 0+, \quad 1/\alpha_N l_N \to 0+ \quad (N \to \infty)$$

and $v_N(\cdot)$ be the output of Algorithm 1.2 for $N = 1, 2, \ldots$. Then (1.31) holds, and if $J(\cdot)$ is strictly convex, (1.32) is true.

1.9 Uncertain initial state

In this subsection we modify Algorithm 1.2 for the case where the initial state x_0 is unknown. Namely, suppose that we are given the constraint

$$x_0 \in X_0 \tag{1.35}$$

where X_0 is a convex and bounded set in H. The constraint (1.27) is kept. Now $U_\vartheta(z(\cdot))$ will stand for the set of all inputs compatible with $z(\cdot)$ for some x_0 satisfying (1.35). Let, as above $U_\vartheta(z(\cdot); G) = U_\vartheta(z(\cdot)) \cap G$.

For a certain x_0, write out the right hand side of (1.28) as (see (1.7))

$$g(\cdot) = z(\cdot) - \Xi x_0(\cdot); \tag{1.36}$$

here

$$\Xi x_0(\sigma) = ((w_1(0,\sigma), x_0), \ldots (w_m(0,\sigma), x_0). \tag{1.37}$$

Define the operator Ψ from $\mathbf{L}^2(T, \mathbf{R}^m) \times H$ into $\mathbf{L}^2(T, \mathbf{R}^m)$ by

$$\Psi(u(\cdot), x_0) = \Phi u(\cdot) + \Xi x_0(\cdot). \tag{1.38}$$

Then (1.28) can be rewrirren as

$$\Psi(u(\cdot), x_0) = z(\cdot). \tag{1.39}$$

For solving this equation under the constraints (1.27), (1.35), the following modification of Algorithm 1.2 is suggested:

Algorithm 1.3.
Parameters:
N, l_N – natural,
$\alpha_N > 0$.
Output:
$v_N(\cdot) \in G$.
Variables:
$y_i(\cdot) \in \mathbf{L}^2(T, \mathbf{R}^n)$,
$\nu_i \in H$.
Initial Step:
Put $y_0(\cdot) = 0$,
$\nu_0 = 0$.
i-**th Step** $(0 \leq i \leq l_N - 1)$ **:**
Find a solution $(r_i(\cdot), \mu_i)$ of the problem

$$2(\Psi(y_i(\cdot), \nu_i) - iz(\cdot)/m, \Psi(r(\cdot), \mu) + \alpha J(r(\cdot)) \to \min, \ r(\cdot) \in G, \ \mu \in X_0. \tag{1.40}$$

Put

$$y_{i+1}(\cdot) = y_i(\cdot) + r_i(\cdot)/l_N \quad \nu_{i+1} = \nu_i + \mu_i/l_N. \tag{1.41}$$

Final Step:
Put $v_N(\cdot) = y_{l_N}(\cdot)$.

Keeping the notations J^0 and $u^0(\cdot)$ of the previous subsection, we obtain, in a similar manner, the following theorem.

Theorem 1.7 *Let*

$$\alpha_N \to 0+, \quad 1/\alpha_N l_N \to 0+ \quad (N \to \infty)$$

and $v_N(\cdot)$ be the output of Algorithm 1.3 for $N = 1, 2, \ldots$. Then (1.31) holds, and if $J(\cdot)$ is strictly convex, (1.32) is true.

2 Application: Reconstruction of Pollution Intensities

2.1 Informal problem setting

In this section we apply some previous results to a standard model of pollution diffusion. Informal problem setting is as follows. Given a water reservoir covering a domain Ω. Several pollution sources are concentrated in subdomains $\Omega_1, \ldots, \Omega_n$ of Ω. In other subdomains $\Theta_1, \ldots, \Theta_m$ concentration of the pollutant is measured. It is required to reconstruct unknown time-varying intensities $u_1(t), \ldots, u_n(t)$ of the pollution sources via measurement results $z_1(t), \ldots, z_m(t)$.

2.2 Models for sources and observation results

In our model, we assume Ω to be a two-dimensional bounded region; ξ will stand for a varying point of Ω. We suppose that the pollutant's input concentration rate at every point $\xi \in \Omega_j$ is given by $u_j(t)\omega_j(\xi)$ where

$$\omega_j(\xi) > 0 \ (\xi \in \Omega_j), \quad \omega_j(\xi) = 0 \ (\xi \notin \Omega_j). \tag{2.1}$$

Thus, $u_j(t)$ serves for a measure of the intensity of the source distributed over Ω_j. It is reasonable to assume the calibration condition

$$\int_{\Omega_j} \omega_j(\xi) d\xi = 1. \tag{2.2}$$

Then $u_j(t)$ represents the rate of the total pollutant's inflow from the domain Ω_j. In what follows, $x(t,\xi)$ stands for a current concentration of the pollutant at point ξ. A result of current measurements of $x(t,\xi)$ in the observation domain Θ_k is modeled as

$$z_k(t) = \int_{\Theta_k} p_k(\xi) x(t,\xi) d\xi. \tag{2.3}$$

Here

$$p_k(\xi) > 0 \ (\xi \in \Theta_k), \quad p_k(\xi) = 0 \ (\xi \notin \Theta_k), \tag{2.4}$$

$$\int_{\Theta_k} p_k(\xi) d\xi = 1. \tag{2.5}$$

Thus, $z_k(t)$ is the average pollutant's concentration in Θ_k with the weight function $p_k(\cdot)$.

2.3 Parabolic model

Following the traditional approach (see, e.g., Marchuk, 1982), we model the pollutant's diffusion process in the domain Ω by the parabolic equation

$$\frac{\partial x(t,\xi)}{\partial t} + a_1 \frac{\partial x(t,\xi)}{\partial \xi_1} + a_2 \frac{\partial x(t,\xi)}{\partial \xi_2} - \Delta x(t,\xi) = Bu(t)(\xi) \tag{2.6}$$

with the boundary condition

$$x(t,\xi) = 0 \ (\xi \in \Gamma) \ . \tag{2.7}$$

Here Δ is the Laplace operator, a_1, a_2 are constant transition coefficients, Γ is the boundary of Ω, $u(t) = (u_1(t), ..., u_n(t))$ is the vector of source intensities, and

$$Bu(t)(\xi) = \sum_{j=1}^{n} u_j(t)\omega_j(\xi) \ . \tag{2.8}$$

Time t varies over $T = [0, \vartheta]$; the initial concentration is fixed,

$$x(0,\xi) = x_0(\xi). \tag{2.9}$$

We suppose that the functions $\omega_j(\cdot)$ $(j = 1, ..., n)$ and $p_k(\xi)(\cdot)$ $(k = 1, ..., m)$ are twice continuously differentiable and satisfy (2.1) – (2.5), and the boundary Γ of the area Ω is sufficiently smooth.

According to Lions, 1971, (2.6) is a particular case of (1.1), and all conditions of subsection 1.1 are fulfilled with $V = H_0^1(\Omega)$ and $H = \mathbf{L}^2(\Omega, \mathbf{R})$. Thus all the results of section 1 are valid.

Remark 2.1 One can easily verify that $w_k(t,\sigma) = w_k(t,\sigma,\cdot)$ (see subsection 1.4, (1.5), (1.6)) has the form

$$w_k(t,\sigma,\cdot) = 0 \ (t > \sigma), \quad w_k(t,\sigma,\cdot) = \zeta_k(\sigma - t,\cdot) \ (t \leq \sigma) \tag{2.10}$$

where $\zeta_k(\cdot,\cdot)$ is the solution of the Cauchy problem

$$\frac{\partial \zeta(t,\xi)}{\partial t} - a_1 \frac{\partial \zeta(t,\xi)}{\partial \xi_1} - a_2 \frac{\partial \zeta(t,\xi)}{\partial \xi_2} - \Delta \zeta(t,\xi) = 0, \ \zeta(0,\xi) = p_k(\xi) \tag{2.11}$$

on $[0,\infty)$ with the boundary condition

$$\zeta(t,\xi) = 0 \ (\xi \in \Gamma) \ . \tag{2.12}$$

2.4 Problem specification: approximations to extremal inputs

Specify the problem sketched out in subsection 2.1. Note that the inputs (pollution intensities) $u_j(t)$ are nonnegative and bounded; we shall also assume that finite upper bounds u_j^* for them are given. Therefore we come to the constraint (1.27) having the special form

$$0 \leq u_j(t) \leq u_j^* \quad (j = 1,2,...) \ . \tag{2.13}$$

Fix an observation result $z(\cdot)$ (of the form (2.3)). The set $U_\vartheta(z(\cdot);G)$ is now undersyood as the collection of all inputs $u(\cdot)$ satisfying (2.13) and compatible with the observation result $z(\cdot)$, i.e. such that (2.3) holds for the solution $x(\cdot,\cdot)$ of the problem (2.6), (2.7), (2.9).

Consider a linear functional $J^*(\cdot)$ on $\mathbf{L}^2_{0,\vartheta}$ determined by a function $q(\cdot) \in \mathbf{L}^2_{0,\vartheta}$,

$$J^*(u(\cdot)) = \int_0^\vartheta q(t)' u(t) dt \ . \tag{2.14}$$

The first problem we will be interested in is finding the minimum and maximum values for $J^*(\cdot)$ over $U_\vartheta(z(\cdot);G)$; we shall denote these values respectively $J^*_{\min}$ and $J^*_{\max}$. A reasonable form for $q(\cdot)$ is

$$q_j(t) = 0 \ (j \neq j^*), \quad q_{j^*}(t) = 1 \ (t \in [\tau_1,\tau_2] \subset [0,\vartheta]), \quad q_{j^*}(t) = 0 \ (t \notin [\tau_1,\tau_2]) \ . \tag{2.15}$$

In this case $J^*(u(\cdot))$ is the avarege intensity of the j^*-th source (concentrated on Ω_{j^*}) over the time interval $[\tau_1,\tau_2] \subset [0,\vartheta]$, and $J^*_{\min}$, $J^*_{\max}$ are, respectively, its minimum and maximum values that do not contradict to the observation result $z(\cdot)$. Having these values, one can claim that the actual average intensity of the j^*-th source over the time interval $[\tau_1,\tau_2]$ is locked between them. If one puts

$$q_j(t) = 1 \ (t \in [\tau_1,\tau_2]), \quad q_j(t) = 0 \ (t \notin [\tau_1,\tau_2]) \quad (j = 1,...,n), \tag{2.16}$$

then $J^*(u(\cdot))$ turns into the total avarege intensity of all sources over the time interval $[\tau_1,\tau_2]$, and $J^*_{\min}$, $J^*_{\max}$ stand, respectively, for its admissible minimum and maximum values.

Our second problem will be to find the minimum value $J^{**}_{\min}$ of the quadratic functional

$$J^{**}(u(\cdot)) = \int_0^\vartheta \sum_{j=1}^n u_j^2(t) dt = \| u(\cdot) \|^2_\vartheta \tag{2.17}$$

and the input $u^{**}(\cdot)$ minimizing $J^{**}(\cdot)$ over $U_\vartheta(z(\cdot);G)$.

2.5 Pre-solver

For solving the above problems, we use Algorithm 1.2. Considering the first problem, we take

$$J(u(\cdot)) = J^*(u(\cdot)) = \int_0^\vartheta q(t)'u(t)dt \tag{2.18}$$

and

$$J(u(\cdot)) = -J^*(u(\cdot)) = \int_0^\vartheta (-q(t))'u(t)dt \; . \tag{2.19}$$

Clearly, $J^*_{\min} = J^0$ for $J(\cdot)$ defined by (2.18), and $J^*_{\max} = -J^0$ for $J(\cdot)$ defined by (2.19). Dealing with the second problem, we use Algorithm 1.2 with

$$J(u(\cdot)) = J^{**}(u(\cdot)) \; . \tag{2.20}$$

We need to specify once more the structure of the function $g(\cdot)$ (see (1.28)) and the operator Φ (1.29).

By definition, for every $\sigma \geq 0$, a k-th coordinate of the m-vector $g(\sigma)$ is given by

$$g_k(\sigma) = g_k(z_k(\sigma), \sigma) = z_k(\sigma) - \int_\Omega \zeta_k(\sigma, \xi)x^0(\xi)d\xi \; ; \tag{2.21}$$

here (1.8) and Remark 2.1 have been taken into account. Also by definition, a k-th row of the matrix $C(t,\sigma)$ is the n-vector $\phi_k(t,\sigma)$ with coordinates (1.7). Hence (1.7) is the element $c_{kj}(t,\sigma)$ of the matrix $C(t,\sigma)$. Using Remark 2.1, we can write

$$c_{kj}(t,\sigma) = c_{kj}(\sigma - t) = \int_{\Omega_j} \zeta_k(\sigma - t, \xi)\omega_j(\xi)d\xi \quad (\sigma \geq t) \; . \tag{2.22}$$

Thus

$$C(t,\sigma) = C(\sigma - t) = (c_{kj}(\sigma - t)), \quad (k = 1,...,m, \; j = 1,...,n) \quad (\sigma \geq t) \; . \tag{2.23}$$

Let us now specify the form of a solution $r_i(\cdot)$ to the extremal problem (1.33) (which is the single nontrivial part of Algorithm 1.2). Consider the first term in the minimized functional,

$$Q_i(r(\cdot)) = 2(\Phi y_i(\cdot) - ig(\cdot)/l_N, \Phi r(\cdot))_\vartheta \; . \tag{2.24}$$

According to (1.29) we have

$$Q_i(r(\cdot)) = 2\int_0^\vartheta \psi_i(\sigma)' \int_0^\sigma C(t,\sigma)r(t)dtd\sigma$$

where

$$\psi_i(\sigma) = \int_0^\sigma C(\tau,\sigma)y_i(\tau)d\tau - ig(\sigma)/l_N. \tag{2.25}$$

Using the Fubini's theorem, continue as follows:

$$\begin{aligned} Q_i(r(\cdot)) &= 2\int_0^\vartheta \int_0^\sigma \psi_i(\sigma)'C(t,\sigma)r(t)dtd\sigma = \\ & 2\int_0^\vartheta \int_t^\vartheta \psi_i(\sigma)'C(t,\sigma)r(t)d\sigma dt = \\ & 2\int_0^\vartheta \sum_{j=1}^n (\beta_i(t))_j r_j(t)dt \end{aligned}$$

where $(\beta_i(t))_j$ is the j-th coordinate of the vector

$$\beta_i(t) = \int_t^{\vartheta} \psi_i(\sigma)' C(t,\sigma) d\sigma \ . \tag{2.26}$$

Now, for the functional (2.18), the problem (1.33) takes the form

$$2\int_0^{\vartheta} \sum_{j=1}^{n} ((\beta_i(t))_j + \alpha_N q_j(t)/2)(r(t))_j dt \to \min, \quad 0 \le (r(t))_j \le u_j^* \ (j=1,...,n) \ . \tag{2.27}$$

It is solved by

$$(r_i^{(\min)}(t))_j = \begin{cases} u_j^*, & (\beta_i(t))_j + \alpha_N q_j/2 \le 0 \\ 0, & (\beta_i(t))_j + \alpha_N q_j/2 > 0 \end{cases} \quad (j=1,...,n) \ . \tag{2.28}$$

Similarly, for the functional (2.19), the problem (1.33) is solved by

$$(r_i^{(\max)}(t))_j = \begin{cases} u_j^*, & (\beta_i(t))_j - \alpha_N q_j/2 \le 0 \\ 0, & (\beta_i(t))_j - \alpha_N q_j/2 > 0 \end{cases} \quad (j=1,...,n) \ . \tag{2.29}$$

For the functional (2.20), the problem (1.33) takes the form

$$2\int_0^{\vartheta} \sum_{j=1}^{n} (\beta_i(t))_j (r(t))_j + \alpha_N (r(t))_j^2/2 dt \to \min, \quad 0 \le (r(t))_j \le u_j^* \ (j=1,...,n)$$

and is solved by

$$(r_i(t))_j = \begin{cases} -(\beta_i(t))_j/\alpha_N, & -(\beta_i(t))_j/\alpha_N \in [0,u_j^*] \\ 0, & -(\beta_i(t))_j/\alpha_N < 0 \\ u_j^*, & -(\beta_i(t))_j/\alpha_N > u_j^* \end{cases} \quad (j=1,...,n) \ . \tag{2.30}$$

2.6 Approximation algorithms

Consider the first problem indicated in subsection 2.4. Combining the pre-solving costruction of the previous subsection and Algorithm 1.2, we specify the latter as follows.

Algorithm 2.1.
Parameters:
N, l_N – natural,
$\alpha_N > 0$.
Output:
$J_N^{(\min)}, J_N^{(\max)}$ – real.
Variables:
$y_i^{(\min)}(\cdot)$, $y_i^{(\max)}(\cdot) \in \mathbf{L}^2(T,\mathbf{R}^n)$.
Pre-Solver:
For $k = 1,...,m$ compute $\zeta_k(t,\xi)$ $(t \in [0,\vartheta],\ \xi \in \Omega)$, a solution to (2.11), (2.12).
For $k = 1,...,m$ compute (2.21) $(\sigma \in [0,\vartheta])$.
Compute matrixes (2.22), (2.23) $(\sigma \in [0,\vartheta],\ t \in [0,\sigma])$.
Initial Step:
Put
$y_0^{(\min)}(t) = 0$, $y_0^{(\max)}(t) = 0$ $(t \in [0,\vartheta])$.
i-th Step $(0 \le i \le l_N - 1)$ **:**

Put
$y_i(t) = y_i^{(\max)}(t)$, $y_i(t) = y_i(t)^{(\min)}$.
Compute
$\psi_i(t) = \psi_i^{(\max)}(t)$, $\psi_i(t) = \psi_i(t)^{(\min)}$ (2.25),
$\beta_i(t) = \beta_i^{(\max)}(t)$, $\beta_i(t) = \beta_i(t)^{(\min)}$ (2.26),
$r_i^{(\min)}(t)$ (2.28), $r_i^{(\max)}(t)$ (2.29) $(t \in [0, \vartheta])$.
Put

$$y_{i+1}^{(\min)}(t) = y_i^{(\min)}(t) + r_i^{(\min)}(t)/l_N \quad y_{i+1}^{(\max)}(t) = y_i^{(\max)}(t) + r_i^{(\max)}(t)/l_N \quad (t \in [0, \vartheta]).$$

Final Step:
Put

$$J_N^{(\min)} = \int_0^{\vartheta} q(t)' y_N^{(\min)}(t) dt, \quad J_N^{(\max)} = \int_0^{\vartheta} q(t)' y_N^{(\max)}(t) dt.$$

Theorem 1.6 yields the following.

Theorem 2.1 *Let functional $J^*(\cdot)$ be defined by (2.14), and $J^*_{\min}$, $J^*_{\max}$ be, respectively, its minimum and maximum values on $U_\vartheta(z(\cdot; G))$. Let*

$$\alpha_N \to 0+, \quad 1/\alpha_N l_N \to 0+ \quad (N \to \infty)$$

and $(J_N^{(\min)}, J_N^{(\max)})$ be the output of Algorithm 2.1 for $N = 1, 2, \ldots$. Then

$$J_N^{(\min)} \to J^*_{\min}, \quad J_N^{(\max)} \to J^*_{\max} \quad (N \to \infty).$$

Consider the second problem of subsection 2.4. Algorithm 1.2 solving this problem, takes the following form.

Algorithm 2.2.
Parameters:
N, l_N – natural,
$\alpha_N > 0$.
Output:
$v_N(\cdot) \in G$.
Variable:
$y_i(\cdot), \mathbf{L}^2(T, \mathbf{R^n})$.
Pre-Solver:
Same as in Algorithm 2.1
Initial Step:
Put
$y_0(t) = 0$, $(t \in [0, \vartheta])$.
i**-th Step** $(0 \le i \le l_N - 1)$ **:**
Compute
$\psi_i(t)$ (2.25), $\beta_i(t)$ (2.26), $r_i(t)$ (2.30) $(t \in [0, \vartheta])$.
Put

$$y_{i+1}(t) = y_i(t) + r_i(t)/l_N \quad (t \in [0, \vartheta]).$$

Final Step:
Put

$$v_N(t) = y_{l_N}(t) \ (t \in [0, \vartheta]).$$

Theorem 1.6 yields the following.

Theorem 2.2 *Let functional $J^{**}(\cdot)$ be defined by (2.17), and $J^{**}_{\min}$ and $u^{**}(\cdot)$ be, respectively, its minimum value and its minimizer on $U_\vartheta(z(\cdot;G))$. Let*

$$\alpha_N \to 0+, \quad 1/\alpha_N l_N \to 0+ \quad (N \to \infty)$$

and $v_N(\cdot)$ be the output of Algorithm 2.2 for $N = 1, 2, \ldots$. Then

$$J^{**}(v_N(\cdot)) \to J^{**}_{\min} \quad (N \to \infty)$$

and

$$\| v_N(\cdot) - u^{**}(\cdot) \|_\vartheta \to 0 \quad (N \to \infty) .$$

2.7 Uncertain initial state: pre-solver

In the next subsection we shall modify Algorithms 2.1 and 2.2 for the case where the initial state x_0 is not given precisely. Thus we shall suppose that the inclusion (1.35) is satisfied, where X_0 is a convex bounded set in $H = \mathbf{L}^2(\Omega, \mathbf{R})$.

We follow the method of subsection 1.9. The set $U_\vartheta(z(\cdot); G)$ is now the collection of all inputs $u(\cdot)$ satisfying (2.13) and such that (2.3) holds for the solution $x(\cdot, \cdot)$ of the problem (2.6), (2.7), (2.9) for a certain x_0 satisfying (1.35). We keep the functionals (2.14) and (2.17) introduced in subsection 2.4, as well as the notations $J^*_{\min}$, $J^*_{\max}$, $J^{**}_{\min}$, and $u^{**}(\cdot)$.

For simplicity we specify the form of the set X_0; namely we assume it to be a convex hull of a finite number of admissible initial distributions $x_p^0(\cdot) \in H$ of concentrations $(p = 1, \ldots, I)$. Thus we put

$$X_0 = \{x_0(\cdot) = \sum_{p=1}^{I} \lambda_p x_p^0(\cdot) \ : \ \lambda \in S\} \tag{2.31}$$

where

$$S = \{\lambda \in \mathbf{R}^I \ : \ \lambda_p \geq 0 \ (p = 1, \ldots, I), \ \sum_{p=1}^{I} \lambda_p = 1\} . \tag{2.32}$$

Specify the form of a solution $(r_i(\cdot), \mu_i(\cdot))$ to the extremal problem (1.40) (Algorithm 1.2) for the functional (2.14). Since $\mu_i(\cdot) \in X_0$ and (2.31) holds, we shall consider in (1.40), instead of $\mu(\cdot)$, coefficient vectors $\lambda_i \in S$:

$$\mu_i(\cdot) = \sum_{p=1}^{I} (\lambda_i)_p x_p^0(\cdot) .$$

Then

$$\nu_i(\cdot) = \sum_{p=1}^{I} (\Lambda_i)_p x_p^0(\cdot) \tag{2.33}$$

and the first term in the minimized functional in (1.40) has the form (see (1.38)

$$Q_i(r(\cdot), \lambda) = 2(\Phi y_i(\cdot) + \Xi \nu_i(\cdot) - iz(\cdot)/l_N, \Phi r(\cdot) + \Xi \sum_{p=1}^{I} \lambda_p x_p^0(\cdot) . \tag{2.34}$$

Introduce the m-vector function

$$\zeta(\sigma, \xi) = (\zeta_1(\sigma, \xi), \ldots, \zeta_m(\sigma, \xi)) . \tag{2.35}$$

In view of (1.37), (2.33) we have

$$\Xi\nu(\sigma) = \int_{\Omega} \zeta(\sigma,\xi)\nu(\xi)d\xi = \sum_{p+1}^{I} \gamma_p(\sigma)(\Lambda_i)_p \tag{2.36}$$

where

$$\gamma_p(\sigma) = \int_{\Omega} \zeta(\sigma,\xi)x_p^0(\xi)d\xi \ . \tag{2.37}$$

Hence (see also (1.29)) (2.34) takes the form

$$Q_i(r(\cdot),\lambda) = 2\int_0^{\vartheta} \psi_i(\sigma)' \int_0^{\sigma} C(t,\sigma)r(t)dtd\sigma) + 2\int_0^{\vartheta} \psi_i(\sigma)' \sum_{p=1}^{I} \gamma_p(\sigma)\lambda_p$$

where (see (2.36))

$$\psi_i(\sigma) = \int_0^{\sigma} C(\tau,\sigma)y_i(\tau)d\tau + \sum_{p+1}^{I} \gamma_p(\sigma)(\Lambda_i)_p - iz(\sigma)/l_N \ . \tag{2.38}$$

Using, like in subsection 2.5, the Fubini's theorem and introducing the function $\beta_i(\cdot)$ (2.26), we easily see that the problem (1.40) is reduced to the problems (2.27) and

$$\Gamma_i'\lambda \to \min, \ \lambda \in S, \tag{2.39}$$

where

$$(\Gamma_i)_p = \int_0^{\vartheta} \int_{\Omega} \psi_i(\sigma)'\zeta(\sigma,\xi)x_p^0(\xi)d\xi d\sigma \ (p = 1,...,I) \ . \tag{2.40}$$

The problem (2.27) is solved, like in subsection 2.5, by (2.28), and the problem (2.39) is solved by

$$(\lambda_i)_p = 0 \ (1 \le p \le I, \ p \ne p_i^*) \quad (\lambda_i)_{p_i^*} = 1 \tag{2.41}$$

where p^* minimizes $(\Gamma_i)_p$:

$$(\Gamma_i)_{p_i^*} = \min\{(\Gamma_i)_1, ..., (\Gamma_i)_I\} \ . \tag{2.42}$$

For the functional (2.19), the solution of the problem (2.27) is given by (2.29).

Finally, considering the second problem of subsection 2.4 where the functional (2.17) is minimized, we conclude (like in subsection 2.5) that the problem (2.27) is solved by (2.30).

2.8 Uncertain initial state: approximation algorithms

Consider the first problem indicated in subsection 2.4. Due to the costructions of subsection 2.7, Algorithm 1.3 (subsection 1.9) solving this problem, takes the following form.

Algorithm 2.3.
Parameters:
$N, \ l_N$ – natural,
$\alpha_N > 0$.
Output:
$J_N^{(\min)}, J_N^{(\max)}$ – real.
Variables:
$y_i^{(\min)}(\cdot), \ y_i^{(\max)}(\cdot) \in \mathbf{L}^2(T, \mathbf{R}^n)$,

$\Lambda_i \in \mathbf{R}^I$.

Pre-Solver:

For $k = 1, ..., m$ compute

$\zeta_k(t,\xi) \quad (t \in [0,\vartheta],\ \xi \in \Omega)$, a solution to (2.11), (2.12).

Compute vectors (2.35).

For $p = 1, ..., I$ compute (2.37) $(\sigma \in [0,\vartheta])$.

Compute matrixes (2.23) $(\sigma \in [0,\vartheta],\ t \in [0,\sigma])$.

Initial Step:

Put

$y_0^{(\min)}(t) = 0,\ y_0^{(\max)}(t) = 0\ (t \in [0,\vartheta])$,

$\Lambda_0 = 0$.

***i*-th Step** $(0 \le i \le l_N - 1)$ **:**

Put

$y_i(t) = y_i^{(\max)}(t),\ y_i(t) = y_i(t)^{(\min)}$.

Compute

$\psi_i(t) = \psi_i^{(\max)}(t),\ \psi_i(t) = \psi_i(t)^{(\min)}$ (2.25),

$\beta_i(t) = \beta_i^{(\max)}(t),\ \beta_i(t) = \beta_i(t)^{(\min)}$ (2.26),

$r_i^{(\min)}(t)$ (2.28), $r_i^{(\max)}(t)$ (2.29) $(t \in [0,\vartheta])$,

Γ_i (2.40),

p_i^* (2.42),

λ_i (2.41).

Put

$$y_{i+1}^{(\min)}(t) = y_i^{(\min)}(t) + r_i^{(\min)}(t)/l_N, \quad y_{i+1}^{(\max)}(t) = y_i^{(\max)}(t) + r_i^{(\max)}(t)/l_N \quad (t \in [0,\vartheta]),$$

$$\Lambda_{i+1} = \Lambda_i + \lambda_i/l_N.$$

Final Step:

Put

$$J_N^{(\min)} = \int_0^\vartheta q(t)' y_N^{(\min)}(t)dt, \quad J_N^{(\max)} = \int_0^\vartheta q(t)' y_N^{(\max)}(t)dt.$$

Theorem 1.6 yields the following.

Theorem 2.3 *Let functional $J^*(\cdot)$ be defined by (2.14), and $J^*_{\min}$, $J^*_{\max}$ be, respectively, its minimum and maximum values on $U_\vartheta(z(\cdot;G))$. Let*

$$\alpha_N \to 0+, \quad 1/\alpha_N l_N \to 0+ \quad (N \to \infty)$$

and $(J_N^{(\min)}, J_N^{(\max)})$ be the output of Algorithm 2.3 for $N = 1, 2, ...$ Then

$$J_N^{(\min)} \to J^*_{\min}, \quad J_N^{(\max)} \to J^*_{\max} \quad (N \to \infty)\ .$$

Consider the second problem of subsection 2.4. Algorithm 1.2 solving this problem, takes the following form.

Algorithm 2.4.

Parameters:

$N,\ l_N$ – natural,

$\alpha_N > 0$.

Output:

$v_N(\cdot) \in G$.

Variable:
$y_i(\cdot), \mathbf{L}^2(T, \mathbf{R^n})$.
Pre-Solver:
Same as in Algorithm 2.1.
Initial Step:
Put
$y_0(t) = 0 \ (t \in [0, \vartheta]), \ \Lambda_0 = 0$.
i-th Step $(0 \le i \le l_N - 1)$ **:**
Compute
$\psi_i(t)$ (2.38),
$\beta_i(t)$ (2.26),
$r_i(t)$ (2.30) $(t \in [0, \vartheta])$,
Γ_i (2.40),
p_i^* (2.42),
λ_i (2.41).
Put

$$y_{i+1}^{(\min)}(t) = y_i^{(\min)}(t) + r_i(t)/l_N, \quad (t \in [0, \vartheta]),$$

$$\Lambda_{i+1} = \Lambda_i + \lambda_i/l_N.$$

Final Step:
Put

$$v_N(t) = y_{l_N}(t) \ (t \in [0, \vartheta]).$$

Theorem 1.6 yields the following.

Theorem 2.4 *Let functional $J^{**}(\cdot)$ be defined by (2.17), and $J^{**}_{\min}$ and $u^{**}(\cdot)$ be, respectively, its minimum value and its minimizer on $U_\vartheta(z(\cdot; G))$. Let*

$$\alpha_N \to 0+, \quad 1/\alpha_N l_N \to 0+ \quad (N \to \infty)$$

and $v_N(\cdot)$ be the output of Algorithm 2.4 for $N = 1, 2, \ldots$. Then

$$J^{**}(v_N(\cdot)) \to J^{**}_{\min} \ (N \to \infty)$$

and

$$\| v_N(\cdot) - u^{**}(\cdot) \|_\vartheta \to 0 \ (N \to \infty) \ .$$

3 Groundwater Contamination Modeling and Source Estimation

3.1 Model

In this section we apply the estimation methodology of section 2 to a groundwater contamination transport model integrated in *XGW: A Prototype Expert System User Interface for Interactive Modeling of Groundwater Contamination*, an information system developed at IIASA's project on Advanced Computer Applications. A general contamination model expolited in XGW takes into account the fluid motion and the contaminant transport in an unconfined aquifer; it is represented by the next system of two-dimensional (2D) partial differential equations (see Bear and Verruijt, 1987; Kaden, Diersch, and Fedra, 1990; Kriksin, Samarskaia, and Tishkin 1993; Samarskaia, 1994),

$$\frac{\partial(\epsilon_0 \cdot H)}{\partial t} + \operatorname{div}(\epsilon \cdot (H - h_b) \cdot U) = Q_H, \tag{3.43}$$

$$\bar{U} = -K \cdot \operatorname{grad}(H), \tag{3.44}$$

$$\begin{aligned} \frac{\partial(\Theta \cdot (H - h_b) \cdot C)}{\partial t} &+ \operatorname{div}(\epsilon \cdot (H - h_b) \cdot U \cdot C) + \Theta \cdot (H - h_b) \cdot \sigma \cdot C \\ &= \operatorname{div}(\epsilon \cdot (H - h_b) \cdot D \cdot \operatorname{grad} C) + Q_C, \end{aligned} \tag{3.45}$$

here

t	=	time,
x, y	=	horisontal Cartesian space coordinates,
$\bar{U} = (\bar{u}, \bar{v}) = (\bar{u}(x,y,t), \bar{v}(x,y,t))$	=	components of fluid velocities in the horisontal x- and y-directions,
$H = H(x,y,t)$	=	head elevation of the free surface of an aquifer,
$h_b = h_b(x,y)$	=	a profile of an impermeable bedrock,
$C = C(x,y,t)$	=	pollutant concentration,
$K = K(x,y)$	=	a tensor of conductivity,
$D = D(x,y,t)$	=	a tensor of hydrodynamic dispersion,
$\epsilon_0 = \epsilon_0(x,y,t)$	=	a drainable porosity,
$\epsilon = \epsilon(x,y,t)$	=	a kinematic porosity,
$\Theta_0 = \Theta_0(x,y,t)$	=	a sorption coefficient,
σ	=	a concentration decay rate,
$\Theta = \Theta(x,y,t) = \epsilon + (1-\epsilon) \cdot \Theta_0$	=	a specific retardation factor.

The right-hand sides $Q_C = Q_C(x,y,t)$ and $Q_H = Q_H(x,y,t)$ represent, respectively, sources and sinks,

$$Q_H = Q_H^r + Q_H^{pi} - Q_H^{po} + Q_H^s, \quad Q_C = Q_H^r\, C^r + Q_H^s\, C^s - Q_H^{po}\, C, \tag{3.46}$$

where

Q_H^r	=	a volumetric recharge rate,
Q_H^{pi}	=	a volumetric injection rate of non-contaminated water at point (x,y),
Q_H^{po}	=	a volumetric discharge rate at point (x,y),
Q_H^s	=	a volumetric flow rate of a contamination source at point (x,y),
C^s	=	concentration of pumped fluid at a contamination source located as above,
C^r	=	concentration of recharged/infiltrated fluid.

This 2D model is obtained through averaging 3D space equations over the vertical space coordinate, which is justified by the assumption that a pressure distribution is hydrostatic. The model ignores Coriolis accelerations (the Dupuit's assumption). Thus the velocities in a water table aquifer are assumed to be horizontal and invariant to vertical shifts. A physical basis for the model is the mass conservation law for the fluid and contaminant.

The 2D nonlinear equations (3.43)-(3.45) govern time-varying distributions of horizontal fluid velocities $\bar{u}(x,y,t)$, $\bar{v}(x,y,t)$, the water table $H(x,y,t)$ and the pollutant concentration $C(x,y,t)$ over a planar groundwater domain Ω.

We shall assume that the water table $H(x,y,t)$ is given. Then the fluid velocities $\bar{u}(x,y,t)$ and $\bar{v}(x,y,t)$ are expressed through equation (3.44), and the model is reduced to the convection-dispersion mass transport equation (3.45). Note that the equation is general enough; it captures convection and dispersion effects, sources and sinks, and can serve for modelling various transport and distribution processes. A specification of initial and boundary conditions depends on a nature of a process under investigation.

3.2 Modeling algorithm

Let the domain Ω be a quadrangle,

$$\Omega = [0, a_x] \times [0, a_y].$$

For a numerical solution of equation (3.45), a time grid w_τ and a space grid w_h are introduced,

$$\begin{aligned} w_\tau &= \{t_n = n\tau,\ \ n = 0,1,2,...,N_\tau, \tau = T/N_\tau\}, \\ w_h &= \{(x_i, y_j) \in \Omega,\ \ x_i = i\Delta x,\ \ y_j = j\Delta y, \\ &\quad \Delta x = a_x/N_x,\ \ \Delta y = a_y/N_y,\ \ i = 0,1,2,...,N_x,\ \ j = 0,1,2,...,N_y\}. \end{aligned}$$

In the XGW model the following finite-difference algorithmic schemes are incorporated (see Peaceman and Rachford, 1955):

- a finite-difference scheme based on an implicit alternating-direction procedure (ADIP-type scheme);
- a fully implicit finite-difference scheme with an ADI iteration technique, based on Douglas-Rachford stabilising correction method.

In a finite-difference scheme, values of spatial variables at time step $n+1$ (t_{n+1}) are computed through a spatial distribution at time step n. The zero time step (t_0) corresponds to the initial condition.

The ADIP-based difference approximation for the transport equation (3.45) has the form

$$\begin{aligned} \frac{\Theta_{i,j}(HC)^{n+1/2}_{i,j} - \Theta_{i,j}(HC)^{n}_{i,j}}{0,5\,\Delta t} &+ \frac{WC^{n+1/2}_{i+1/2,j} - WC^{n+1/2}_{i-1/2,j}}{\Delta x} \\ &- \frac{WD^{n+1/2}_{i+1/2,j} - WD^{n+1/2}_{i-1/2,j}}{\Delta x} + \sigma \cdot \Theta_{i,j}(HC)^{n+1/2}_{i,j} \\ &= \frac{WD^{n}_{i,j+1/2} - WD^{n}_{i,j-1/2}}{\Delta y} - \frac{WC^{n}_{i,j+1/2} - WC^{n}_{i,j-1/2}}{\Delta y} \\ &+ (Q^n_C)_{i,j}, \end{aligned} \tag{3.47}$$

$$\frac{\Theta_{i,j}(HC)^{n+1}_{i,j} - \Theta_{i,j}(HC)^{n+1/2}_{i,j}}{0,5\,\Delta t} + \frac{WC^{n+1}_{i,j+1/2} - WC^{n+1}_{i,j-1/2}}{\Delta y}$$

$$
\begin{aligned}
- & \frac{WD^{n+1}_{i,j+1/2} - WD^{n+1}_{i,j-1/2}}{\Delta y} + \sigma \cdot \Theta_{i,j}(HC)^{n+1}_{i,j} \qquad (3.48)\\
= & \frac{WD^{n+1/2}_{i+1/2,j} - WD^{n+1/2}_{i-1/2,j}}{\Delta x} - \frac{WC^{n+1/2}_{i+1/2,j} - WC^{n+1/2}_{i-1/2,j}}{\Delta x}\\
+ & (Q_C^{n+1/2})_{i,j},
\end{aligned}
$$

where

$$
\begin{aligned}
WC^{n+1/2}_{i+1/2,j} &= \frac{\epsilon_{i+1,j} + \epsilon_{i,j}}{2} \cdot \frac{(H^{n+1}_{i+1,j} - h_{b\,i+1,j}) + (H^{n+1}_{i,j} - h_{b\,i,j})}{2} \times \\
& [\ u^{n+1/2}_{i+1/2,j} \frac{C^{n+1/2}_{i+1,j} + C^{n+1/2}_{i,j}}{2} - |u^{n+1/2}_{i+1/2,j}| \frac{C^{n+1/2}_{i+1,j} - C^{n+1/2}_{i,j}}{2}\ ],\\
WC^{n+1}_{i,j+1/2} &= \frac{\epsilon_{i,j+1} + \epsilon_{i,j}}{2} \cdot \frac{(H^{n+1}_{i,j+1} - h_{b\,i,j+1}) + (H^{n+1}_{i,j} - h_{b\,i,j})}{2} \times \\
& [\ v^{n+1}_{i,j+1/2} \frac{C^{n+1}_{i,j+1} + C^{n+1}_{i,j}}{2} - |v^{n+1}_{i,j+1/2}| \frac{C^{n+1}_{i,j+1} - C^{n+1}_{i,j}}{2}\ ],\\
WC^{n}_{i,j+1/2} &= \frac{\epsilon_{i,j+1} + \epsilon_{i,j}}{2} \cdot \frac{H^{n}_{i,j+1} + H^{n}_{i,j}}{2} \times \qquad (3.49)\\
& [\ v^{n}_{i,j+1/2} \frac{C^{n}_{i,j+1} + C^{n}_{i,j}}{2} - |v^{n}_{i,j+1/2}| \frac{C^{n}_{i,j+1} - C^{n}_{i,j}}{2}\ ],
\end{aligned}
$$

$$
\begin{aligned}
WD^{n+1/2}_{i+1/2,j} &= [\epsilon D_{xx}(H^{n+1/2}) - h_b)]_{i+1/2,j} \frac{C^{n+1/2}_{i+1,j} - C^{n+1/2}_{i,j}}{\Delta x},\\
WD^{n+1}_{i,j+1/2} &= [\epsilon D_{yy}(H^{n+1} - h_b)]_{i,j+1/2} \frac{C^{n+1}_{i,j+1} - C^{n+1}_{i,j}}{\Delta y}, \qquad (3.50)
\end{aligned}
$$

The difference equations (3.47), (3.48) are unconditionally stable and convergent (see Samarskii, 1971). Each of them has the three-point structure

$$
\mathcal{A}_i z_{i-1} - \mathcal{C}_i z_i + \mathcal{B}_i z_{i+1} = -\mathcal{F}_i, \qquad i = 1, ..., N-1 \qquad (3.51)
$$

and satisfies boundary conditions of the type

$$
\begin{aligned}
z_0 &= \alpha_1 z_1 + \beta_1, \qquad (3.52)\\
z_N &= \alpha_2 z_{N-1} + \beta_2,
\end{aligned}
$$

where coefficients $\alpha_1, \alpha_2, \beta_1, \beta_2$ are determined by the initial boundary condition.

In the considered model, equations (3.51) are solved via a simplified Gaussian elimination method (the so-called backward substitution algorithm, see Forsythe and Moler, 1967; Samarskii and Nikolaev 1989).

For brievity we do not present here the formulas for the fully implicit finite-difference scheme.

3.3 Estimation of forcing functions

Let in (3.45) the source intensity $Q_C(x, y, t)$ have the form

$$
Q_C(x, y, t) = u(t)\omega(x, y) \qquad (3.53)
$$

where $\omega(x,y)$ is a known smooth function and $u(t)$ is an unknown forcing function. We focus on the estimation of $u(t)$ for the following special case of the equation (3.45):

$$\frac{\partial C}{\partial t} + \bar{u}\,\frac{\partial C}{\partial x} + \bar{v}\,\frac{\partial C}{\partial y} + \gamma\,C - D\,\frac{\partial^2 C}{\partial x^2} - D\,\frac{\partial^2 C}{\partial y^2} = u(t)\,\omega(x,y), \tag{3.54}$$

$$C(t,x,y)\,|_\Gamma = 0,$$
$$C(0,x,y) = 0.$$

Here

$$\begin{aligned} \bar{u} &= const_0,\ \bar{v} = const_1,\ \gamma = const_2,\ D = const_3, \\ \Omega &= \{\ (x,y):\ 0 \le x \le a_x,\ \ 0 \le y \le a_y\ \}. \end{aligned}$$

We see that the above boundary problem has the form (2.6)-(2.9) (with $n = 1$) in slightly different notations (x is replaced by C and ξ by (x,y)). As in section 2, we assume that observation results are given by

$$z(t) = \int\int_\Omega C(t,x,y)\,p(x,y)\,dxdy \tag{3.55}$$

(so, $m = 1$). A nonnegative smooth function $p(x,y)$ defined on Ω determines a contaminant concentration observation domain,

$$\Theta = \{\ (x,y):\ (x,y) \in \Omega,\ \ p(x,y) \ge\ 0\ \}. \tag{3.56}$$

Below, basing on observation results $z(t)$, we estimate numerically the mean value of the forcing function $u(t)$ over an interval $[\tau_1,\tau_2]$,

$$J(u(\cdot)) = \int_{\tau_1}^{\tau_2} u(t)dt.$$

For modeling observation results $z(t)$ we compute $C(t,x,y)$ as an approximate solution of equation (3.54) using the numerical method described in subsection 3.2 (with Q_C given in (3.53)); values $z(t)$ are calculated through (3.55). Next, a finite-difference equation corresponding to the conjugate problem,

$$\frac{\partial \zeta}{\partial t} - u\,\frac{\partial \zeta}{\partial x} - v\,\frac{\partial \zeta}{\partial y} + \gamma\,\zeta - D\,\frac{\partial^2 \zeta}{\partial x^2} - D\,\frac{\partial^2 \zeta}{\partial y^2} = 0, \tag{3.57}$$

$$\begin{aligned} \zeta(t,x,y)\,|_\Gamma &= 0, \\ \zeta(0,x,y) &= p(x,y), \end{aligned} \tag{3.58}$$

is solved numerically; each of the finite-difference schemes described in subsection 3.2 has been employed.

Using the modeled observation results $z(t)$ and the obtained approximate solution of (3.57), (3.59), we implement Algorithm 2.1 (see subsection 2.6) for the estimation of the value $J(u(\cdot))$.

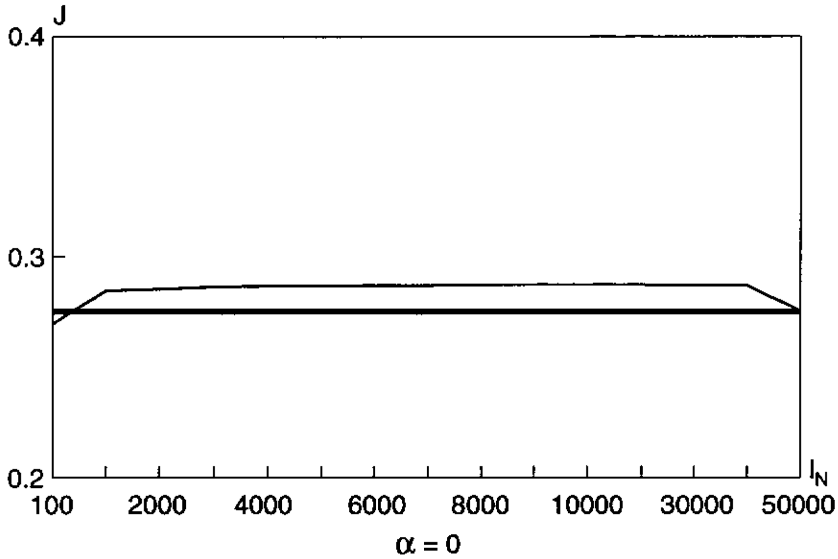


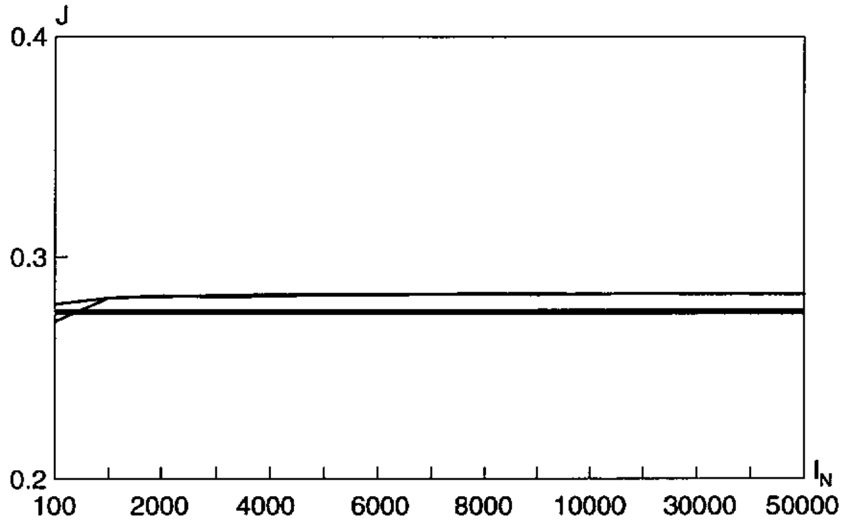
Figure 1

3.4 Test results

Algorithm 2.1 has been tested for various regularization parameters α, and numbers of iterations l_N. Other parameters have been chosen as follows:

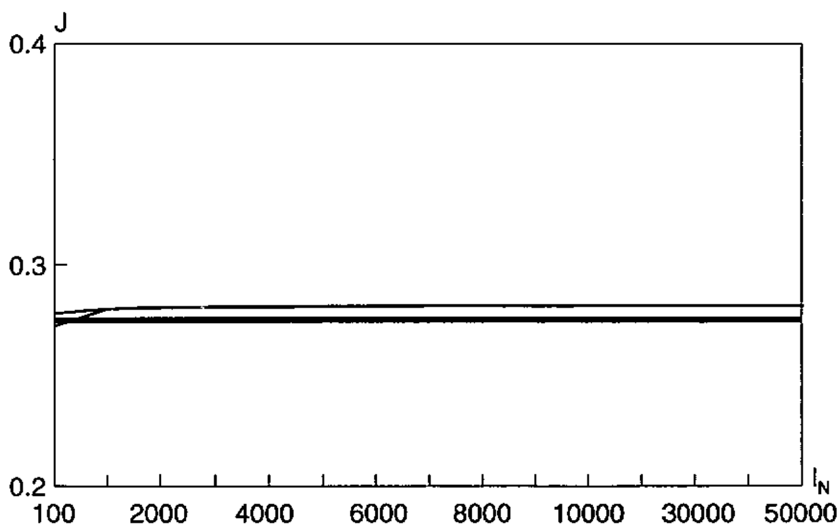
- time interval: $[0, 1]$;
- sizes of domain Ω: $a_x = a_y = 53$;
- sizes of space grid w_h: $N_x = N_y = 53$ $(\Delta x = \Delta y = 1)$;
- size of time grid w_t: $N_\tau = 40$, $(\tau = 1/40)$;
- dispersion coefficient: $D = 18.33$;
- source weight: a smooth function $\omega(x, y)$ close to 1/9 for $31 \leq x \leq 34$, $26 \leq y \leq 29$ and zero otherwise;
- observation weight: a smooth function $p(x, y)$ close to 1/9 for $24 \leq x \leq 27$, $26 \leq y \leq 29$ and zero otherwise;
- objective function's time parameters (see (2.15)): $\tau_1 = 0.1$, $\tau_2 = 0.5$;
- forcing function: $u(t) = \sin(t)$.

Figures 1–12 show the results of numerical approximations to the minimum and maximum values J_N^{min} and J_N^{max}, which, in the considered example, coincide with the exact value $J(u(\cdot))$. The bold line represents the exact value $J(u(\cdot)) = 0.275437$. Figures 1–6 correspond to the ADIP finite-difference scheme. Figures 7-12 correspond to the fully implicit scheme.



$\alpha = e^{-18}$

Figure 2



$\alpha = e^{-14}$

Figure 3

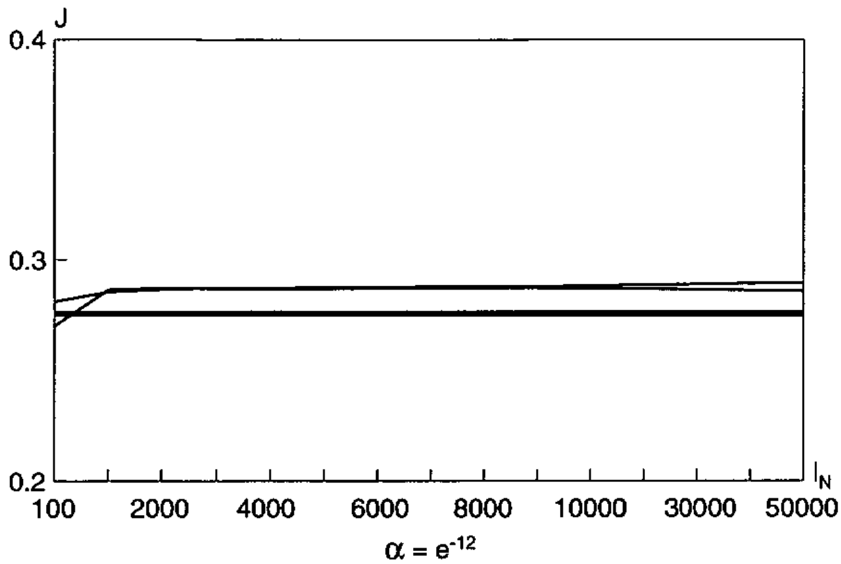


Figure 4

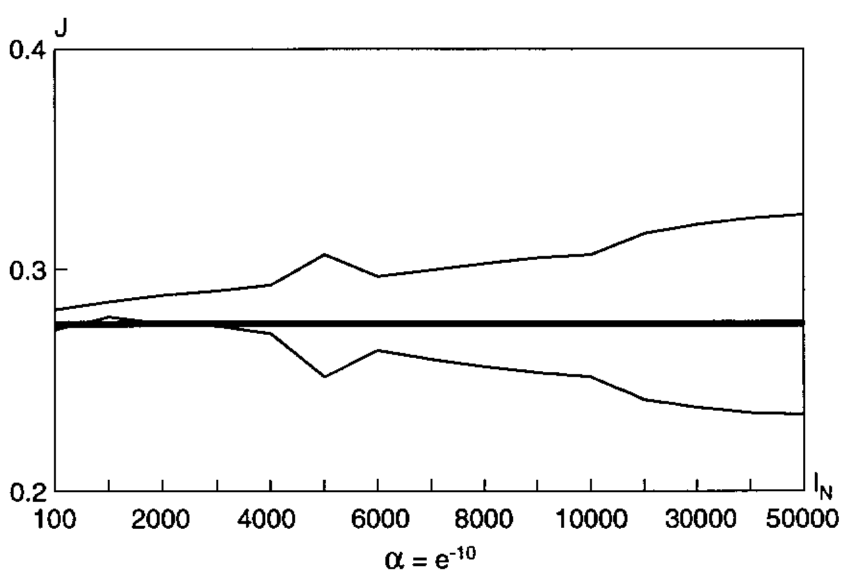


Figure 5

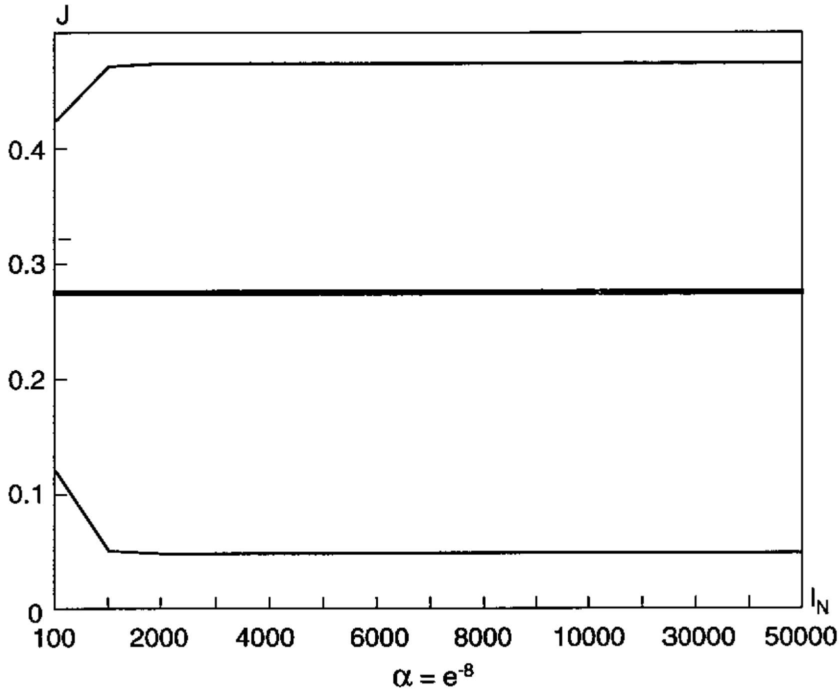


Figure 6

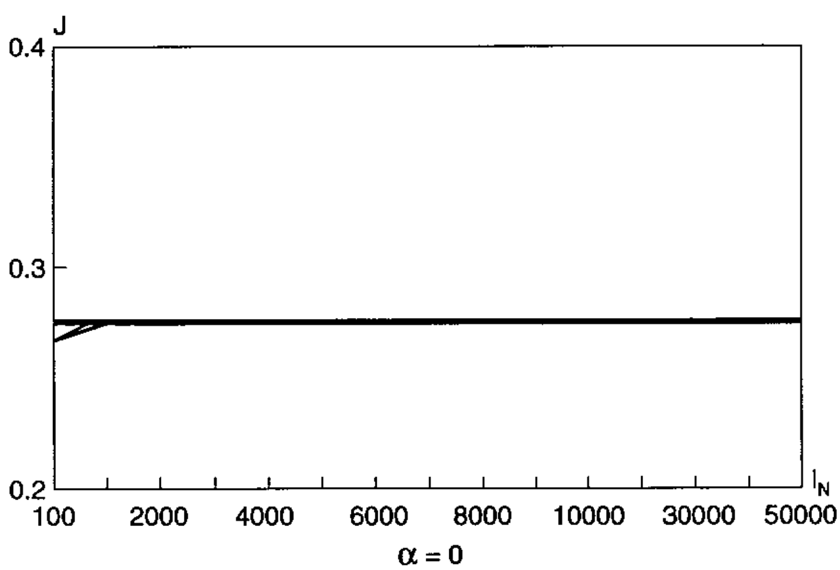


Figure 7

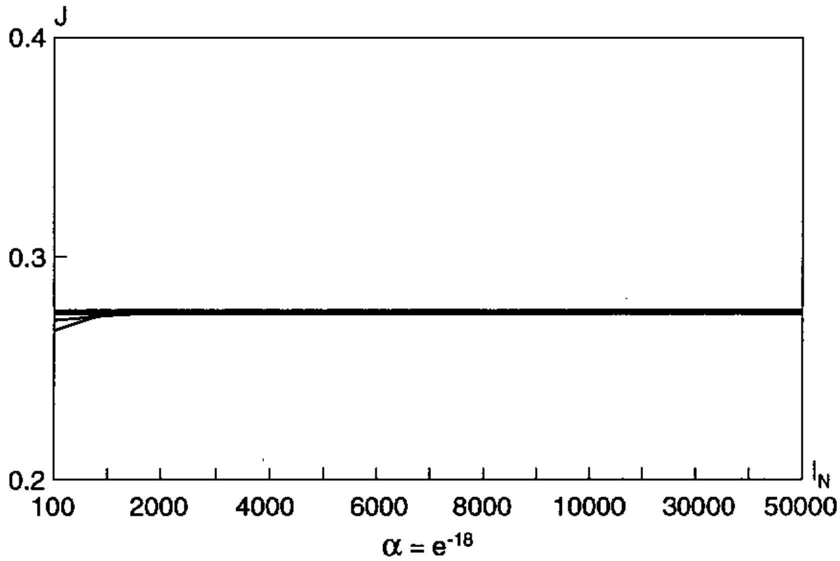


Figure 8

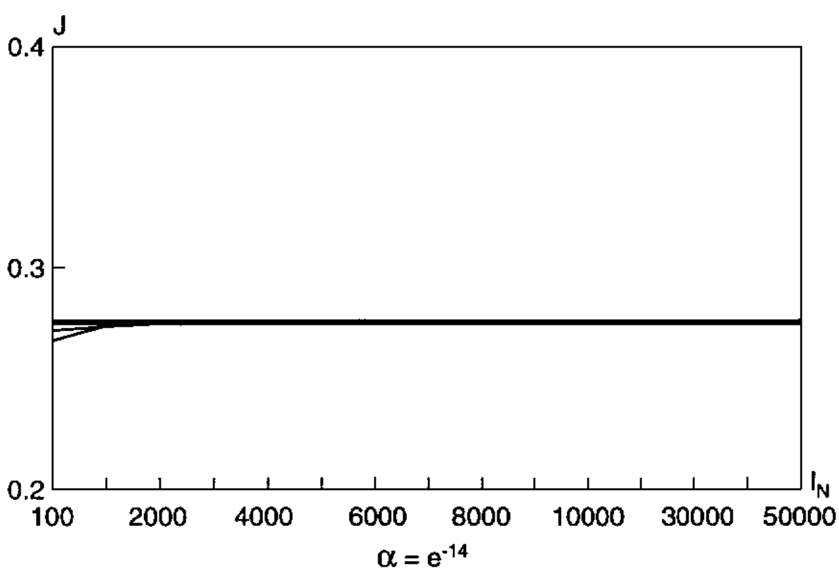


Figure 9

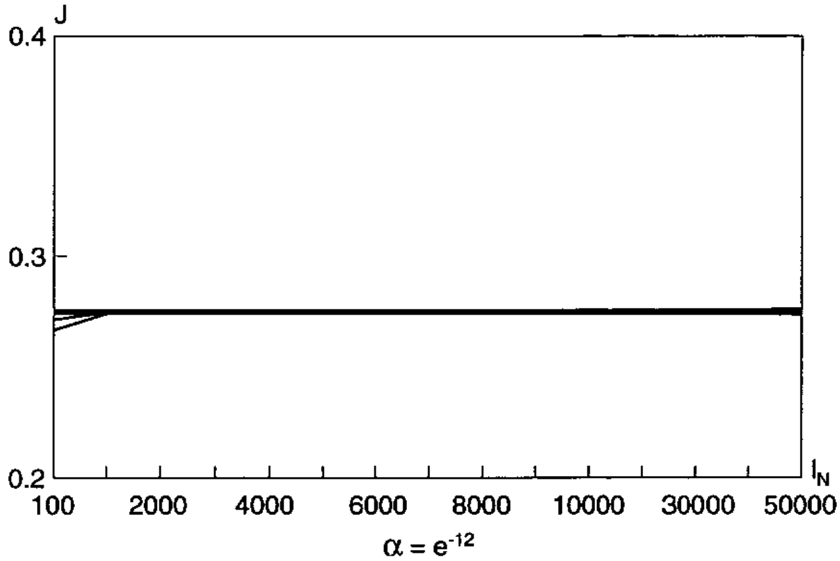


Figure 10

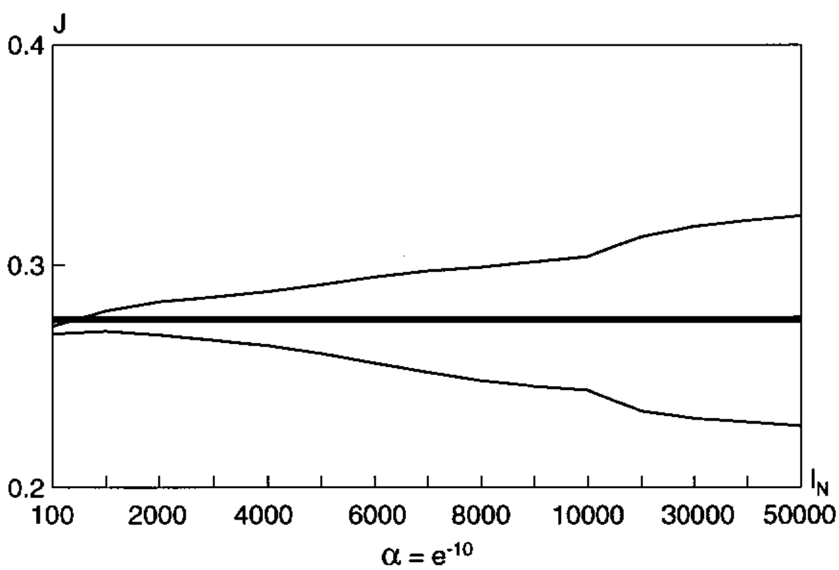


Figure 11

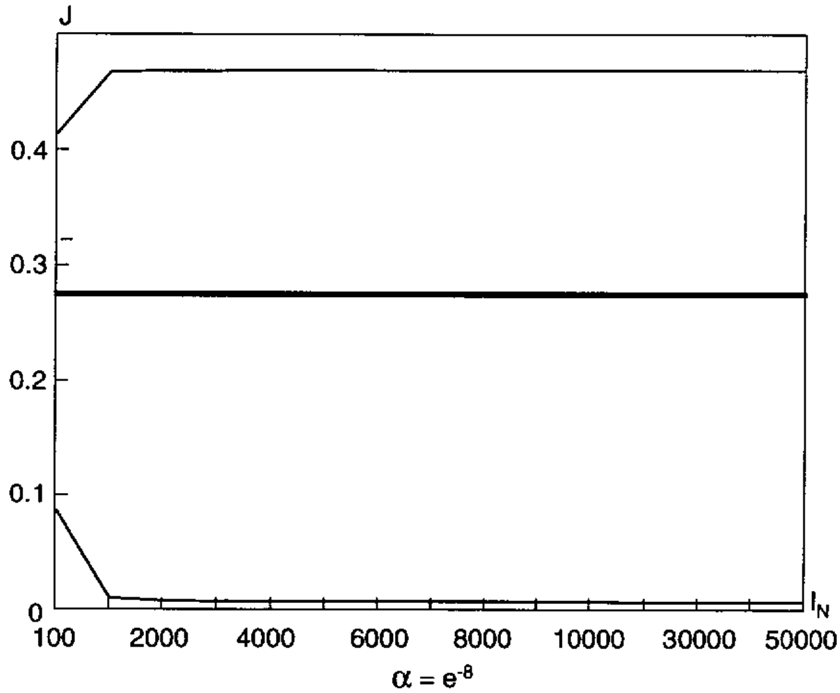


Figure 12

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