

Management of Contamination Risks and Identification of Contamination Sources*

A. Kryazhimskii^a and V. Maksimov^b

^aV.A. Steklov Institute of Mathematics, Russian Academy of Sciences,
117966 Moscow, Russia (kryazhim@ihp.ru)

^bInstitute of Mathematics and Mechanics, URAS,
620219 Ekaterinburg, Russia (maksimov@imm.uran.ru)

Abstract: Some aspects of management of contamination risks based on monitoring contamination sources are under consideration. The case when direct measurements are impossible and the values of the contamination inputs should be estimated through observations of indirect indicators is studied. Standard mathematical models describing the diffusion of a contaminant in the form of partial differential equations of the parabolic type are used. A model-based technique for the reconstruction of the evolution of the intensities of point-concentrated contamination sources through observations of the concentration of the contaminant is presented. Results of numerical experiments are discussed.

Keywords: Contamination Risks; Identification; Uncertainty.

1 INTRODUCTION

Management of contamination risks is based on monitoring contamination sources. The most reliable monitoring strategy is direct measurements. However, sometimes direct measurements may not be possible due to the location of the contamination sources. In such situations the values of the contamination inputs should be estimated through observations of indirect indicators. A typical indirect indicator is the concentration of the contaminant in an observation area. If the observation area is small enough, a deficit in data may lead to strong uncertainties in the resulting estimates. The nonstationarity of the contamination sources whose intensities may change over time in a poorly predictable manner, often discontinuously, increases the uncertainty.

The uncertainty can be minimised if the estimation technique invokes the structure of the input-observation map given by an adequate mathematical model. Standard mathematical models describing the diffusion of a contaminant have the form of partial differential equations of the parabolic type. In our report we present a model-based technique

for the reconstruction of the evolution of the intensities of point-concentrated contamination sources through indirect observations. The technique (originating from the mathematical theory of control of uncertain systems) allows to estimate the highest and/or lowest bounds for the “power” of the intensities compatible with a given observation record.

We conclude with a discussion of numerical experiments.

2 CONTAMINATION MODEL

Let us imagine a water reservoir occupying an area Ω and n contamination sources located in subareas $\Omega_1, \dots, \Omega_n$ of Ω . Our modelling approach assumes that the input concentration rate of the contaminant at every point ξ in the source area Ω_j is modeled as $u_j(t)\omega_j(\xi)$ where t is the current time. The positive value $u_j(t)$ is a measure of the time-varying intensity of the source located in Ω_j . If $\omega_j(\xi)$ is normalised so that $\int_{\Omega_j} \omega_j(\xi) d\xi = 1$, then $u_j(t)$ represents the current rate of the contamination inflow in Ω_j . We assume that the contamination intensities

*This work was partially supported by the International Institute for Applied Systems Analysis, Laxenburg, Austria, and the Russian Foundation for Basic Research, project # 00-01-00682.

do not exceed some values estimated in advance:

$$0 \leq u_j(t) \leq u_j^*, \quad j = 1, \dots, n. \quad (1)$$

In what follows, $x(t, \xi)$ is the current concentration of the contaminant at a point ξ in Ω . Some information on the distribution of $x(t, \xi)$ in Ω is registered by m sensors. The sensors are either travelling across Ω or stationary. The travelling sensors register the concentration at points $y_1(t), \dots, y_m(t)$ changing their locations in Ω ; the currently registered signals are, therefore,

$$z_k(t) = x(t, y_k(t)). \quad (k = 1, \dots, m) \quad (2)$$

The stationary sensors register weighted average concentrations $z_1(t), \dots, z_m(t)$ in fixed subareas $\Theta_1, \dots, \Theta_m$ of Ω :

$$z_k(t) = \int_{\Theta_k} p_k(\xi) x(t, \xi) d\xi \quad (k = 1, \dots, m); \quad (3)$$

the positive weight coefficients $p_k(\xi)$ are supposed to be given and can always be normalised so that $\int_{\Theta_k} p_k(\xi) d\xi = 1$.

We are concerned with the following Travelling-Sensor Intensity Reconstruction (TSIR) Problem, and Stationary-Sensor Intensity Reconstruction (SSIR) Problem.

TSIR Problem: Observing the concentrations $z_1(t), \dots, z_m(t)$ (2) of the contaminant at the travelling points $y_1(t), \dots, y_m(t)$, reconstruct the intensities of the contamination sources, $u_1(t), \dots, u_n(t)$, in the source areas $\Omega_1, \dots, \Omega_m$.

SSIR Problem: Observing the weighted average concentrations $z_1(t), \dots, z_m(t)$ (3) of the contaminant in the areas $\Theta_1, \dots, \Theta_m$, reconstruct the intensities of the contamination sources, $u_1(t), \dots, u_n(t)$, in the source areas $\Omega_1, \dots, \Omega_m$.

To solve the TSIR and SSIR Problems, we use the following parabolic equation describing diffusion of the contaminant in Ω [Marchuk, 1982]:

$$\frac{\partial x(t, \xi)}{\partial t} + a_1 \frac{\partial x(t, \xi)}{\partial \xi_1} + a_2 \frac{\partial x(t, \xi)}{\partial \xi_2} - \Delta x(t, \xi) = (4)$$

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

Here ξ_1 and ξ_2 are the coordinates of a point ξ in Ω , $\Delta = \partial^2 / \partial \xi_1^2 + \partial^2 / \partial \xi_2^2$ is the Laplace operator responsible for diffusion, and a_1 and a_2 are constant transition coefficients. The concentration $x(t, \xi)$ at the boundary, Γ , of Ω is zero:

$$x(t, \xi) = 0 \quad (\xi \in \Gamma). \quad (5)$$

We assume that the sensor data cover a bounded time interval, $[0 \leq t \leq \vartheta]$, and the initial distribution of the contaminant is given:

$$x(0, \xi) = x_0(\xi). \quad (6)$$

In order to ensure the existence of a solution of (4) – (6), we assume that the boundary Γ of the plain area Ω is smooth, the functions $u_j(t)$ ($j = 1, \dots, n$) are piecewise continuous and the function $x_0(\xi)$ is continuous [Marchuk, 1982].

3 SPECIFICATION OF PROBLEMS

If the number of sensors, m , is small compared to the number of contamination source areas, n , the data provided by the sensors may be insufficient for reconstructing all the contamination intensities, $u_1(t), \dots, u_n(t)$, and the TSIR and SSIR Problems may not be solvable. However, some significant – although partial – information on the input $u = (u_1(t), \dots, u_n(t))$ can be delivered even by poor sensor networks. In this section we specify the statements of the SSIR and TSIR Problems by pointing out the reconstructable information on the input u .

We assume that the sought information on u is the *input performance index*

$$J(u) = \int_0^{\vartheta} (q_1(t)u_1(t) + \dots + q_n(t)u_n(t)) dt. \quad (7)$$

Here $q_1(t), \dots, q_n(t)$ are fixed time-dependent output weight coefficients. This form of the output covers a broad scope of substantial information on u . For example, if we want $J(u)$ to give us the average intensity of the source located in a selected area, say, Ω_k , on the time interval marked by t_1 and t_2 , we set $q_j(t) = 0$ for $j \neq k$, $q_k(t) = 1$ for $t_1 \leq t \leq t_2$, and $q_k(t) = 0$ for $t < t_1$ and $t > t_2$, thus, getting $J(u) = \int_{t_1}^{t_2} u_k(t) dt$. If we want $J(u)$ to give us the total average contamination inflow intensity on the

time interval marked by t_1 and t_2 , we set $q_j(t) = 1$ for $t_1 \leq t \leq t_2$ and $q_j(t) = 0$ for $t < t_1$ and $t > t_2$ ($j = 1, \dots, n$). A more detailed information on the input can be gained through using several input performance indecies of the form (7).

Now let us come back to the TSIR and SSIR Problems.

An observed collection of sensor data, $z = (z_1(t), \dots, z_m(t))$, selects a set of (virtually admissible) inputs u compatible with z . A (virtually admissible) input $u = (u_1(t), \dots, u_n(t))$ is *compatible* with z if the solution $x(t, \xi)$ of (4) – (6) associated with this particular input u satisfies (3) for all t , $0 \leq t \leq \vartheta$. Thus, any input u compatible with z is able to produce the sensor data z along the diffusion process modeled by (4) – (6). If the model (4) – (6) is adequate, the actual input is necessarily compatible with the sensor data z ; conversely, every input compatible with z is a real candidate for being the actual one.

Let $J_{\min}(z)$ and $J_{\max}(z)$ be, respectively, the minimum and maximum values of $J(u)$ across all inputs u compatible with z . The interval between $J_{\min}(z)$ and $J_{\max}(z)$ represents a measure of the uncertainty in identifying the actual value of the input performance index subject to the given sensor data z .

Therefore, we specify the TSIR an SSIR Problems as follows.

TSIR Problem: Observing the collection $z = (z_1(t), \dots, z_m(t))$ (2) of concentrations of the contaminant at the travelling points $y_1(t), \dots, y_m(t)$, find $J_{\min}(z)$ and $J_{\max}(z)$.

SSIR Problem: Observing the collection $z = (z_1(t), \dots, z_m(t))$ (3) of weighted average concentrations of the contaminant in the areas $\Theta_1, \dots, \Theta_m$, find $J_{\min}(z)$ and $J_{\max}(z)$.

Note that $J_{\max}(z) = -J_{\min}^*$ where $J_{\min}^*(z)$ is the minimum value of

$$J^*(u) = \int_0^{\vartheta} (-q_1(t)u_1(t) - \dots - q_n(t)u_n(t))dt.$$

across the set of all inputs u compatible with the sensor data z . This simple observation reduces the problem of finding $J_{\max}(z)$ to a problem identical to that of finding $J_{\min}(z)$. Therefore, considering the TSIR and SSIR Problems, we may focus on a methodology of finding $J_{\min}(z)$ only.

4 TSIR PROBLEM: PRELIMINARIES

Here we describe the input-output transformation in the TSIR Problem, which lies in the basis of our solution algorithm.

Let $X_0(t, \xi)$ designate the solution of the equation

$$\frac{\partial x(t, \xi)}{\partial t} + a_1 \frac{\partial x(t, \xi)}{\partial \xi_1} + a_2 \frac{\partial x(t, \xi)}{\partial \xi_2} - \quad (8)$$

$$\Delta x(t, \xi) = 0$$

with the boundary condition (5) and initial state (6), and $X_j(t, \xi)$ ($j = 1, \dots, n$) designate the solution of (8) with the boundary condition (5) and initial state $x(0, \xi) = \omega_j(\xi)$; here and in what follows, we set $\omega_j(\xi) = 0$ for ξ not belonging to the source area Ω_j . Then the solution of (4) – (6) has the form

$$x(t, \xi) =$$

$$X_0(t, \xi; x_0) + \int_0^t \sum_{j=1}^n u_j(\tau) X_j(t - \tau, \xi) d\tau$$

[Marchuk, 1982], which, together with (2), implies

$$z_k(t) = X_0(t, y_k(t)) + \quad (9)$$

$$\int_0^t \sum_{j=1}^n X_j(t - \tau, y_k(t)) u_j(\tau) d\tau.$$

Introducing the matrix function

$$C(t, \tau) = (X_j(t - \tau, y_k(t)),$$

$$(j = 1, \dots, n, k = 1, \dots, m),$$

we rewrite (9) as

$$z_k(t) = X_0(t, y_k(t)) + \int_0^t C(t, \tau) u(\tau) d\tau;$$

here and in what follows we treat $(u_1(\tau), \dots, u_n(\tau))$ as a column vector; the latter formula gives us an analytic representation of the input-output transformation in the TSIR Problem.

5 TSIR PROBLEM: SOLUTION ALGORITHM

Introduce the vector $g(t) = (g_1(t), \dots, g_m(t))$:

$$g_k(t) = z_k(t) - X_0(t, y_k(t)), \quad k = 1, \dots, m.$$

Let us describe the algorithm solving the TSIR Problem.

Algorithm.

Parameters: N, l_N — natural, $\alpha_N > 0$.

Output: $J_N^{(\min)}, J_N^{(\max)}$ — real.

Variables: $y_i^{(\min)}(\cdot), y_i^{(\max)}(\cdot) \in L^2(T, R^n)$.

Initial step:

Let $y_0(\cdot) = y_0^{(\max)}(\cdot) = y_0^{(\min)}(\cdot)$.

i -th step ($0 \leq i \leq l_N - 1$): Compute

$$(r_i^{(\min)}(t))_j =$$

$$\begin{cases} u_j^*, & (\beta_i^{(\min)}(t))_j + \alpha_N q_j(t)/2 \leq 0 \\ 0, & (\beta_i^{(\min)}(t))_j + \alpha_N q_j(t)/2 > 0 \end{cases},$$

$$(r_i^{(\max)}(t))_j =$$

$$\begin{cases} u_j^*, & (\beta_i^{(\max)}(t))_j + \alpha_N q_j(t)/2 \leq 0 \\ 0, & (\beta_i^{(\max)}(t))_j + \alpha_N q_j(t)/2 > 0 \end{cases},$$

$$(j = 1, \dots, n),$$

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

$$\beta_i^{(\min)}(t) = \int_0^\vartheta \psi_i^{(\min)}(\sigma)' C(t, \sigma) r(t) d\sigma dt,$$

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

Analogously we compute $(\beta_i^{(\max)}(t))_j$.

Let

$$y_{i+1}^{(\min)}(\cdot) = y_i^{(\min)}(\cdot) + r_i^{(\min)}(\cdot)/l_N,$$

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

Final step:

Assume that $v_N^{(\min)}(\cdot) = y_{l_N}^{(\min)}(\cdot)$, $v_N^{(\max)}(\cdot) = y_{l_N}^{(\max)}(\cdot)$.

Proposition 1 Let functional $J(\cdot)$ be defined by (7) and J_{\min}, J_{\max} be, respectively, its minimum and maximum values on $U(z(\cdot))$. Let

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

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

$$J_N^{(\min)} \rightarrow J_{\min}, \quad J_N^{(\max)} \rightarrow J_{\max} \quad (N \rightarrow \infty).$$

6 SSIR PROBLEM: SOLUTION ALGORITHM

The algorithm solving the SSIR Problem is similar to the one described above. However, here we assume that

$$g_k(t) = z_k(t) - \int_{\Omega} \xi_k(t, \xi) x_0(s) ds,$$

a k -th row of the matrix $C(t, \sigma)$ is an n -dimensional vector $c_k(t, \sigma)$ with the coordinates

$$c_{kj}(t, \sigma) = c_{kj}(s - t) = \int_{\Omega_j} \zeta_k(\sigma - t, \xi) \omega_j(\xi) d\xi,$$

($\sigma \geq t$). Here $\zeta_k(\cdot, \cdot)$ is a solution of the problem

$$\frac{\partial \zeta(t, \xi)}{\partial t} - a_1 \frac{\partial \zeta(t, \xi)}{\partial \xi_1} - a_2 \frac{\partial \zeta(t, \xi)}{\partial \xi_2} -$$

$$\Delta \zeta(t, \xi) = 0,$$

$$\zeta(0, \xi) = p_k(\xi)$$

on T with the boundary condition

$$\zeta(t, \xi) = 0 \quad (\xi \in \Gamma).$$

See [Kryazhinskii et al., 1995; Maksimov, 2000] for other algorithms solving the SSIR Problem.

7 RESULTS OF NUMERICAL EXPERIMENTS

The SSIR Problem has been simulated on a personal computer. The algorithm has been tested for various values of the regularisation parameter α .

Other parameters have been chosen as follows:

- time interval: $[0, 1]$;
- domain Ω : square 53×53 ;
- sizes of spatial grid ω_h : 53×53 ;
- step of time grid: $1/40$;
- transition coefficients: $a_1 = a_2 = 18.33$;
- parameters t_1 and t_2 : $t_1 = 0.1$, $t_2 = 0.5$.

Figures 1–3 show the results of calculation of (J_N^{min}, J_N^{max}) for various values of the parameter α . The bold line represents the exact value $J_N^{min} = J_N^{max} = 0.275437$ for the function $z(t) = \sin(t)$.

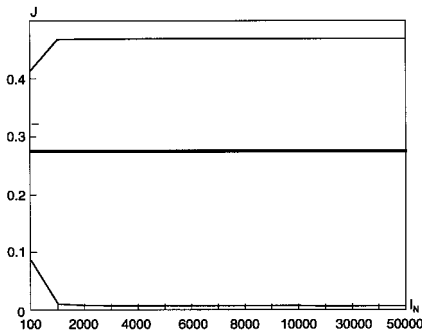


Figure 1. $\alpha = e^{-8}$

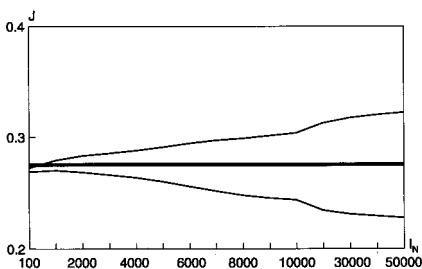


Figure 2. $\alpha = e^{-10}$

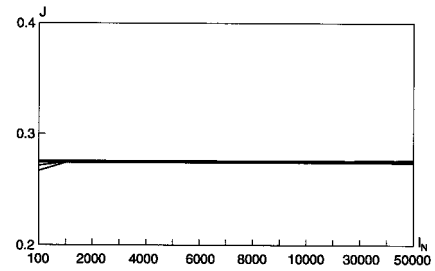


Figure 3. $\alpha = e^{-12}$

8 REFERENCES

- Linnerooth-Bayer, J., R.E. Löfstedt, and G. Sjöstedt (Eds.), *Transboundary Risk Management*, International Institute for Applied Systems Analysis, 2001.
- Beck, M.B., and E. Halfon, Uncertainty, identifiability and the propagation of prediction errors: a case study of lake Ontario, *Journal of Forecasting*, 10, 135–161, 1991.
- Beck, M.B., A.J. Jakeman, and M.J. McAleer (Eds.), *Construction and Evaluation of Models of Environmental Systems*, *Modelling Change in Environmental Systems*, John Wiley & Sons Ltd., 1993.
- Marchuk, G.I., *Mathematical Modelling in Environmental Problems*. Moscow: Nauka, 1982.
- Curtain, R.F., and H. Zwart, *An Introduction to Infinite-Dimensional Linear Systems Theory*, Springer-Verlag, 1996.
- Kryazhinskii, A.V., V.I. Maksimov, and E.A. Samarskaia, On Estimation of Forcing Functions in Parabolic Systems, IIASA Working Paper (WP-95-75), International Institute for Applied Systems Analysis, 1995.
- Maksimov, V.I., The problems of dynamical reconstruction of inputs of infinite-dimensional systems, Ekaterinburg, 2000.