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NUMERICAL IDENTIFICATION OF A COEFFICIENT IN A PARABOLIC QUASILINEAR EQUATION

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INTRODUCTION

Let T, b and $l \in \mathbb{R}^+$; $\varphi, \xi \in L_\infty(0, T)$ be given. Our aim is to solve the following optimal control problem: to determine the function ψ in some reasonable class of functions in such a way that the generalised solution $u = u_\psi(t, x)$ of the problem

$$\frac{\partial u}{\partial t} + \frac{\partial \psi(u)}{\partial x} = b \frac{\partial^2 u}{\partial x^2} \quad \text{on} \quad (0, T) \times (0, \infty)\,, \tag{I.1}$$

$$u(t, 0) = \varphi(t) \quad \text{on} \quad \langle 0, T\rangle\,, \tag{I.2}$$

$$u(0, x) = 0 \quad \text{on} \quad \langle 0, \infty\rangle\,, \tag{I.3}$$

$$\lim_{x\to\infty} \sup_{t\in\langle 0,T\rangle} |u(t, x)| = 0 \tag{I.4}$$

may minimise the functional

$$\int_0^T [u_\psi(t, l) - \xi(t)]^2 \, \mathrm{d}t\,. \tag{I.5}$$

The exact definition of the generalised solution is given in Appendix.

In Section 1 we specify among other the class in which we shall look for the function ψ, keeping in view the requirement of its numerical realization. The methods of numerical solution of the problem are described in Section 2. Finally, in Section 3, a numerical example is given. Some auxiliary theoretical results are summarized in Appendix.

This problem appeared in connection with mathematical modelling of gas chromatography. I should like to dedicate my article to the memory of its inspirer and my adviser, Dr. Karel Boček, from the Institute of Hygiene and Epidemiology in Prague. My thanks are due also to Dr. Oldřich John, from the Faculty of Mathematics and Physics of Charles University in Prague, for very valuable suggestions and remarks.

1. PARAMETRISATION OF THE PROBLEM

Let K be a compact subset of $\mathbb{R}^p$ and for all $a \in K$ let a function $\psi_a \in C^2(\mathbb{R}^1)$ be defined so that ψ_a' and ψ_a'' are bounded functions and ψ_a'' is Lipschitz continuous. Let T, b, l be positive numbers; let φ and ξ be fixed elements of the space $L_\infty(0, T)$. Let us write u_a for the generalised solution of the boundary value problem (I.1), (I.2), (I.3) and (I.4) for $\psi = \psi_a$. We want to determine $\alpha \in K$ so that

$$\int_0^T (u_\alpha(t, l) - \xi(t))^2 \, dt \leqq \int_0^T (u_a(t, l) - \xi(t))^2 \, dt \tag{1.1}$$

for all $a \in K$.

Let us remark that $\varphi \in L_\infty(0, T)$ implies $u_a(\cdot, x) \in L_\infty(0, T)$ for all $x \in \langle 0, \infty)$. Conditions for the existence of a solution of this problem are formulated in Appendix.

The coefficient ψ_a in the equation (I.1) is closely connected with the distribution coefficient of two substances in the chromatographics column, which is to be established from the chromatogram $\xi(t)$ ($\xi(t)$ describes the time distribution of the concentration of the investigated matter in the gas substance at the end of the column).

2. METHOD OF NUMERICAL SOLUTION

To obtain the numerical solution of the problem, the following steps are to be executed:

1. To find an adequate method for the numerical solution of the "direct" problem (I.1), (I.2), (I.3) and (I.4). Let us write $\tilde{u}_a$ for the approximate solution of this problem for $a \in K$ and $\psi = \psi_a$.

2. To define an adequate approximation of the functional

$$\Phi(u) = \int_0^T (u(t, l) - \xi(t))^2 \, dt$$

(by means of a quadrature formula). Let us write $\tilde{\Phi}$ for this approximative functional.

3. To give a method for the minimisation of the function $\tilde{I}(a) = \tilde{\Phi}(\tilde{u}_a)$ on the set K.

Ad 1. Since the problem is defined on a rectangular domain, the finite difference method will do the job.

Let N, M be positive integers and let $L > 0$, $L \gg l$. Put $\tau = TN^{-1}$, $h = LM^{-1}$. Denote by u_m^n the value of a numerical solution at the point $(n\tau, mh)$. The boundary conditions (I.2), (I.3) and (I.4) are approximated in a natural way:

$$u_0^n = \varphi(n\tau) \quad \text{for} \quad n = 0, 1, \ldots, N\,, \tag{2.1}$$

$$u_m^0 = 0 \quad \text{for} \quad m = 1, 2, \ldots, M - 1\,, \tag{2.2}$$

$$u_M^n = 0 \quad \text{for} \quad n = 0, 1, \ldots, N\,. \tag{2.3}$$

The discrete approximation of the equation (I.1) is of the form

$$(2.4)\qquad (1 + 2b\eta\tau h^{-2})\, u_m^{n+1} - b\eta\tau h^{-2} u_{m+1}^{n+1} - b\eta\tau h^{-2} u_{m-1}^{n+1} =$$
$$= [1 - 2b(1-\eta)\,\tau h^{-2}]\, u_m^n + [b(1-\eta)\,\tau h^{-2} - \tfrac{1}{2}\psi'(u_m^n)\,\tau h^{-1}]\, u_{m+1}^n +$$
$$+ [b(1-\eta)\,\tau h^{-2} + \tfrac{1}{2}\psi'(u_m^n)\,\tau h^{-1}]\, u_{m-1}^n$$

for $\quad n = 0, 1, \ldots, N-1, \quad m = 1, 2, \ldots, M-1$

where $\eta \in \langle 0, 1 \rangle$. Changing the parameter η we get the spectrum of different schemes ($\eta = 0$ gives the explicit method, $\eta = \frac{1}{2}$ the Crank-Nicholson method, $\eta = 1$ the implicit method). Passing from the n-th to the $(n+1)$-st time step we solve the system of linear equations. The matrix of this system does not change.

The situation when the practical calculations are performed, is characterized by an additional condition

$$(2.5)\qquad \inf\{\psi'(x),\, x \in \mathbb{R}^1\} \geqq \delta > 0\,.$$

In this case it is easy to see that the explicit finite difference scheme (which is the one exclusively used) is stable if $\tau h^{-2} \leqq 1/(2b)$ and $h \leqq 2b\delta^{-1}$. The methods introduced are modifications of standard methods used for the numerical solution of linear parabolic problems (see for example [1]).

Ad. 2. In order to approximate our functional Φ we use the simplest formula:

$$(2.6)\qquad \tilde{\Phi}(w) = \tau \,.\, \sum_{n=1}^{N} (w_R^n - \xi(n\tau))^2\,, \quad w = \{w_m^n\}_{\substack{m=1,2,\ldots M-1\\ n=1,2,\ldots,N}}$$
$$\Phi(u) \approx \tilde{\Phi}(\{u(n\tau, mh)\}) \approx \Phi(\{u_m^n\})$$
$$R\tau = l\,, \quad R \in \mathbb{N}\,.$$

Ad 3. To minimise the function $\tilde{I}$ we use a certain modification of the conjugate gradient method. In every iteration of this method we must know the values of the mappings $\tilde{I}$ and grad $\tilde{I}$. We shall study possible methods of calculation of the value grad $\tilde{I}$.

1. The direct method

Put

$$(2.7)\qquad v_m^n(a) = \operatorname{grad} u_m^n(a) \quad \text{for} \quad n = 0, 1, \ldots, N\,, \quad m = 0, 1, \ldots, M\,.$$

We can use the following recursive formulae for the calculation of these values. Let ψ_a be sufficiently smooth.

$$(2.8)\qquad v_0^n = v_M^n = 0 \quad \text{for} \quad n = 0, 1, \ldots, N\,,$$

$$(2.9)\qquad v_m^0 = 0 \qquad \text{for} \quad m = 1, 2, \ldots, M-1\,,$$

$$(2.10)\qquad v_m^{n+1} = (1 - 2b\tau h^{-2})\, v_m^n + \left(b\tau h^{-2} - \tfrac{1}{2}\psi_a'(u_m^n)\,\tau h^{-1}\right) v_{m+1}^n + \left(b\tau h^{-2} + \tfrac{1}{2}\psi_a'(u_m^n)\,\tau h^{-1}\right) v_{m-1}^n - \tfrac{1}{2}\tau h^{-1}\left(\operatorname{grad}_a \psi_a'(u_m^n) + \psi_a''(u_m^n)\, v_m^n\right)\left(u_{m+1}^n - u_{m-1}^n\right)$$

for $\quad n = 0, 1, \ldots, N - 1\,, \quad m = 1, 2, \ldots, M - 1\,.$

Further, it is evident that

$$(2.11)\qquad \operatorname{grad} \tilde{I}(a) = 2\tau \sum_{n=1}^{N} v_R^n (u_R^n - \xi(n\tau))$$

where $R\tau = l\,, \quad R \in \mathbb{N}$.

2. The dual method

Let us denote

$$(2.12)\qquad a = (a_1, a_2, \ldots, a_p)^{\mathsf{T}} \quad \text{for all} \quad a \in K\,,$$

$$(2.13)\qquad u^n = (u_1^n, u_2^n, \ldots, u_{M-1}^n)^{\mathsf{T}} \quad \text{for} \quad n = 0, 1, \ldots, N\,,$$

$$(2.14)\qquad \frac{\partial \tilde{\Phi}}{\partial u^n} = \left(\frac{\partial \tilde{\Phi}}{\partial u_1^n}, \ldots, \frac{\partial \tilde{\Phi}}{\partial u_{M-1}^n}\right) \quad \text{for} \quad n = 0, 1, \ldots, N\,, \quad \tilde{\Phi} = \tilde{\Phi}(\{u_m^n\})\,,$$

$$(2.15)\qquad \frac{\mathrm{d}u^k}{\mathrm{d}a} = \left(\frac{\partial u_i^k}{\partial a_j}\right)_{\substack{i=1,2,\ldots,M-1\\ j=1,2,\ldots,p}} \quad \text{for} \quad k = 0, 1, \ldots, N\,.$$

Let us remark that all calculations are performed with an arbitrary sufficiently smooth function $\tilde{\Phi}$ of $(M - 1)\,.\,(N + 1)$ variables. In our particular case

$$\frac{\partial \tilde{\Phi}}{\partial u_i^n} = 2\tau(u_R^n - \xi(n\tau))\,\delta_{Ri}\,.$$

Let us define the mapping:

$$(2.16)\qquad f : \mathbb{R}^{M-1} \times \mathbb{R}^p \times \mathbb{R}^1 \to \mathbb{R}^{M-1}\,, \quad f = (f_1, f_2, \ldots, f_{M-1})^{\mathsf{T}}\,,$$

$$f_1(v_1, \ldots, v_{M-1}, a_1, \ldots, a_p, c) = bh^{-2}(c - 2v_1 + v_2) - \tfrac{1}{2}\psi_a'(v_1)\,(v_2 - c)\, h^{-1}\,,$$

$$f_j(v_1, \ldots, v_{M-1}, a_1, \ldots, a_p, c) = bh^{-2}(v_{j-1} - 2v_j + v_{j+1}) - \tfrac{1}{2}\psi_a'(v_j)\,(v_{j+1} - v_{j-1})\, h^{-1}\,, \quad j = 2, 3, \ldots, M - 2\,,$$

$$f_{M-1}(v_1, \ldots, v_{M-1}, a_1, \ldots, a_p, c) = bh^{-2}(v_{M-2} - 2v_{M-1}) + \tfrac{1}{2}\psi_a'(v_{M-1})\, v_{M-2} h^{-1}\,.$$

Then the explicit finite difference method for our problem can be written in the form

$$(2.17)\qquad u^{n+1} = u^n + \tau f(u^n, a, \varphi(n\tau)) \quad \text{for} \quad n = 0, 1, \ldots, N - 1\,, \qquad u^0 = 0\,.$$

Hence we have

$$\text{(2.18)}\qquad \frac{du^{n+1}}{da} = \frac{du^n}{da} + \tau\left[\frac{\partial}{\partial u^n} f(u^n, a, \varphi(n\tau))\frac{du^n}{da} + \frac{\partial}{\partial a} f(u^n, a, \varphi(n\tau))\right]$$

for $n = 0, 1, \ldots, N - 1$; $du^0/da = 0$.

In this formula the standard notation is used. Further, it is evident that

$$\text{(2.19)}\qquad \operatorname{grad} \tilde{I}(a) = \sum_{i=1}^{N} \frac{\partial \tilde{\Phi}}{\partial u^i}\frac{du^i}{da} = \sum_{i=1}^{N}\sum_{j=1}^{M-1}\left(\frac{\partial \tilde{\Phi}}{\partial u_j^i}\frac{\partial u_j^i}{\partial a_1}, \ldots, \frac{\partial \tilde{\Phi}}{\partial u_j^i}\frac{\partial u_j^i}{\partial a_p}\right).$$

Let us define vectors $g_i^n \in \mathbb{R}^{M-1}$ for $n = 0, 1, \ldots, N + 1$; $i = 0, 1, \ldots, N$ so that

$$\text{(2.20)}\qquad g_i^n = 0, \quad n = i + 1, \ldots, N, N + 1,$$

$$\text{(2.21)}\qquad g_i^i = \left(\frac{\partial \tilde{\Phi}}{\partial u^i}\right)^{\mathsf{T}},$$

$$\text{(2.22)}\qquad g_i^n = g_i^{n+1} + \tau\left(\frac{\partial}{\partial u^n} f(u^n, a, \varphi(n\tau))\right)^{\mathsf{T}} g_i^{n+1}, \quad n = 0, 1, \ldots, i - 1.$$

Then

$$\text{(2.23)}\qquad \frac{\partial \tilde{\Phi}}{\partial u^i}\frac{du^i}{da} = (g_i^i)^{\mathsf{T}}\frac{du^i}{da} - (g_i^0)^{\mathsf{T}}\frac{du^0}{da} = \sum_{j=0}^{i-1}\left[(g_i^{j+1})^{\mathsf{T}}\frac{du^{j+1}}{da} - (g_i^j)^{\mathsf{T}}\frac{du^j}{da}\right] =$$

$$= \sum_{j=0}^{i-1}\left[(g_i^{j+1})^{\mathsf{T}}\left(\frac{du^{j+1}}{da} - \frac{du^j}{da}\right) + (g_i^{j+1} - g_i^j)^{\mathsf{T}}\frac{du^j}{da}\right].$$

Using (2.18), (2.20), (2.22) and the last formula we obtain the relation

$$\text{(2.24)}\qquad \frac{\partial \tilde{\Phi}}{\partial u^i}\cdot\frac{du^i}{da} = \tau\sum_{j=0}^{N}(g_i^{j+1})^{\mathsf{T}}\frac{\partial}{\partial a} f(u^j, a, \varphi(j\tau)).$$

Put

$$\text{(2.25)}\qquad g^n = \sum_{i=0}^{N} g_i^n, \quad n = 0, 1, \ldots, N + 1.$$

Using (2.19) we may write

$$\text{(2.26)}\qquad \operatorname{grad} \tilde{I}(a) = \tau\sum_{j=0}^{N}(g^{j+1})^{\mathsf{T}}\frac{\partial}{\partial a} f(u^j, a, \varphi(j\tau)).$$

The sequence of the vectors $\{g^n\}_{n=0}^{N+1}$ solves the difference equation

(2.27)

$$g^n = g^{n+1} + \tau\left(\frac{\partial}{\partial u^n} f(u^n, a, \varphi(n\tau))\right)^{\mathsf{T}} g^{n+1} + \left(\frac{\partial \tilde{\Phi}}{\partial u^n}\right)^{\mathsf{T}} \quad \text{for} \quad n = N, N - 1, \ldots 0$$

with the initial condition

(2.28) $$g^{N+1} = 0\,,$$

because

$$g^{n+1} + \tau\left(\frac{\partial}{\partial u^n} f(u^n, a, \varphi(n\tau))\right)^{\mathsf{T}} g^{n+1} + \left(\frac{\partial\tilde{\Phi}}{\partial u^n}\right)^{\mathsf{T}} =$$

$$= \sum_{i=n+1}^{N}\left[g_i^{n+1} + \tau\left(\frac{\partial}{\partial u^n} f(u^n, a, \varphi(n\tau))\right)^{\mathsf{T}} g_i^{n+1}\right] + g_n^n = \sum_{i=n+1}^{N} g_i^n + g_n^n = g^n\,.$$

Denote

(2.29) $$g^n = (p_1^n, \ldots, p_{M-1}^n)^{\mathsf{T}} \quad \text{for} \quad n = 0, 1, \ldots, N+1$$

and put $p_0^n = p_M^n = 0$, $n = 0, 1, \ldots, N+1$. Using (2.16), (2.27) and (2.28), we obtain

(2.30) $$p_i^n = (b\tau h^{-2} - \psi_a'(u_{i-1}^n)\, \tfrac{1}{2}\tau h^{-1})\, p_{i-1}^{n+1} +$$
$$+ (1 - 2b\tau h^{-2} - \psi_a''(u_i^n)\, \tfrac{1}{2}\tau h^{-1}(u_{i+1}^n - u_{i-1}^n))\, p_i^{n+1} +$$
$$+ (b\tau h^{-2} + \psi_a'(u_{i+1}^n)\, \tfrac{1}{2}\tau h^{-1})\, p_{i+1}^{n+1} + \frac{\partial\tilde{\Phi}}{\partial u_i^n}$$

for $$n = N, N-1, \ldots, 0\,, \quad i = 1, 2, \ldots, M-1\,;$$
$$p_i^{N+1} = 0 \quad \text{for} \quad i = 1, 2, \ldots, M-1\,.$$

Further, it is evident that

(2.31) $$\frac{\partial}{\partial a} f(u^n, a, \varphi(n\tau)) = -\left(\frac{\partial\psi_a'(u_i^n)}{\partial a_j}\, \frac{u_{i+1}^n - u_{i-1}^n}{2h}\right)_{\substack{i=1,\ldots,M-1\\ j=1,\ldots,p}}.$$

Hence we have

(2.32)
$$\frac{\partial}{\partial a_k} \tilde{I}((a_1, \ldots, a_p) = -\tau \sum_{j=0}^{N} \sum_{i=0}^{M-1} p_i^{j+1}\, \frac{\partial\psi_a'(u_i^n)}{\partial a_k}\, \frac{u_{i+1}^n - u_{i-1}^n}{2h}\,, \quad k = 1, 2, \ldots, p\,.$$

The algorithm for the calculation of grad $\tilde{I}(a)$ dy means of the dual method is now quite clear. It is apparent that the dual method is more advantagenous than the direct method, if p is sufficiently large. Evidently, the method introduced is closely connected with the known principle of Lagrarge multipliers. Its vatious generalizations are often used for the solution of optimal control problems of mathematical physics (see [2]).

Let us now give a sketch of our modification of the conjugate gradient method. Denote

a_0 ... the initial approximation of the solution,

l_1 ... the maximal number of iterations,

k_1 ... the number of iterations executed,

a_{opt} ... the approximation of the optimal solution obtained by our method.

Let K be a p-dimensional bounded interval $\langle d_1, h_1 \rangle \times \ldots \times \langle d_p, h_p \rangle$. The algorithm of the method can be described as follows:

1. We choose $a_0 \in K$ and put $k_1 = 0$.
2. $k_1 + 1 \to k_1$.
3. If $k_1 > l_1$ or grad $\tilde{I}(a_0) = 0$, we put $a_{opt} = a_0$. The calculation is finished.
4. We put $s_0 = -[\text{grad } \tilde{I}(a_0)]^T$.
5. We put $(s_0)_j = 0$ for all $j = 1, 2, \ldots, p$ satisfying $[(a_0)_j = h_j \,\&\, (s_0)_j > 0]$ or $[(a_0)_j = d_j \,\&\, (s_0)_j < 0]$.
6. If $s_0 = 0$, we put $a_{opt} = a_0$ and the calculation is finished.
7. We calculate $\alpha_0 \in M_0$ so that $\tilde{I}(a_0 + \alpha_0 s_0) \leqq \tilde{I}(a_0 + \alpha s_0)$ for all $\alpha \in M_0$, where $M_0 = \{\alpha \geqq 0; a_0 + \alpha s_0 \in K\}$.
8. We put $a_1 = a_0 + \alpha_0 s_0$.
9. If there exists j such that $(s_0)_j$ was replaced by zero in step 5 we put $a_0 = a_1$ and go back to step 2 of the algorithm.
10. For all $i = 1, 2, \ldots, p$ we execute

    a. $k_1 + 1 \to k_1$.

    b. If $k_1 > l_1$ or grad $\tilde{I}(a_i) = 0$, we put $a_{opt} = a_i$ and the calculation is finished.

    c. We put $m_i = \dfrac{\text{grad } \tilde{I}(a_i) \,.\, [\text{grad } \tilde{I}(a_i)]^T}{\text{grad } \tilde{I}(a_{i-1}) \, [\text{grad } \tilde{I}(a_{i-1})]^T}$,

    $$s_i = -[\text{grad } \tilde{I}(a_i)]^T + m_i s_{i-1}.$$

    d. We calculate $\alpha_i \in M_i$ such that $\tilde{I}(a_i + \alpha_i s_i) \leqq \tilde{I}(a_i + \alpha s_i)$ for all $\alpha \in M_i$, where $M_i = \{\alpha \geqq 0, a_i + \alpha s_i \in K\}$.

    e. We put $a_{i+1} = a_i + \alpha_i s_i$.
11. We put $a_0 = a_{p+1}$ and return to step 2.

The just described minimisation method is based on the Fletcher-Reeves algorithm, which is included in the standard user's library of the computers of series EC (subroutine FMCG). This algorithm serves to the determination of the local minimum of a nonconvex nonlinear function of many variables defined on $\mathbb{R}^n$, $n \in \mathbb{N}$. By a simple modification we obtain our method, which is suitable for the minimisation on multidimensional bounded closed interval. A survey of the methods, which are often used for numerical solution of optimal control problems, is given in [3].

If for example $K = \langle d_1, h_1 \rangle \times \langle d_2, h_2 \rangle \times \ldots \times \langle d_p, h_p \rangle \cap \{x; f(x) \geqq \chi\}$, f is a nonlinear continuous function, we may combine the method introduced above with the method of penal function (see Section 3).

The one-dimensional minimisation needed in steps 7 and 10d of the algorithm was taken over from subroutine FMCG. We shall not describe its algorithm here.

3. EXAMPLE

In this section we describe one numerical experiment, which can serve to the practical identification of the distribution coefficient. For a large concentration of the investigated matter in the gas substance the distribution coefficient k_1 is given by a known constant (K_1), for a small concentration by an unknown constant $(a_1 + K_1)$, which is greater than $K_1 (a_1 > 0)$. Our aim is to identify the value a_1 and the values a_2, a_3 that determine the interval in which the value of the distribution coefficient "passes" from $a_1 + K_1$ to K_1.

Putting

$$k_1(y, a_1, a_2, a_3) = \begin{cases} a_1 + K_1 \quad \text{for} \quad y \in (-\infty, a_2\rangle\,, \\ a_1 \dfrac{\int_y^{a_3} (t - a_2)^2 (a_3 - t)^2 \, \mathrm{d}t}{\int_{a_2}^{a_3} (t - a_2)^2 (a_3 - t)^2 \, \mathrm{d}t} + K_1 \\ \quad \text{for } y \in \langle a_2, a_3 \rangle\,, \\ K_1 \text{ for } y \in \langle a_3, \infty) \end{cases} \tag{3.1}$$

we obtain a reasonable expression for the distribution coefficient. $k_1(\cdot, a_1, a_2, a_3)$ is a piecewise polynomial nonincreasing function from $C^2(\mathbb{R}^1)$, $\tilde{k}_1 = k_1 / \langle a_2, a_3 \rangle$ is the unique polynomial of the fifth order which satisfies $\tilde{k}_1(a_2) = a_1 + K_1$, $\tilde{k}_1(a_3) = K_1$, $\tilde{k}_1'(a_i) = \tilde{k}_1''(a_i) = 0$, $i = 2, 3$. In every real situation the physicists are able to determine positive constants K_i, $i = 2, \ldots, 7$ so that $a_1 \in \langle K_2, K_3 \rangle$, $a_2 \in \langle K_4, K_5 \rangle$, $a_3 \in \langle K_6, K_7 \rangle$. Further $(\mathrm{d}/\mathrm{d}y)(y \, . \, k_1(y, a)) \geqq 0$. Hence we choose

$$R_1 = \{(a_1, a_2, a_3) \in \mathbb{R}^3; K_2 \leqq a_1 \leqq K_3, K_4 \leqq a_2 \leqq K_5 < K_6 \leqq a_3 \leqq K_7\}\,, \tag{3.2}$$

$$R_2 = \left\{(a_1, a_2, a_3) \in \mathbb{R}^3; h_1(y, a) = \frac{\mathrm{d}}{\mathrm{d}y}(y \, . \, k_1(y, a)) \geqq 0\right\},$$

$$K = R_1 \cap R_2\,; \quad a = (a_1, a_2, a_3)\,; \quad p = 3\,.$$

The function $\psi_a'(y)$ is given by

$$\psi_a'(y) = \frac{K_8}{1 + \frac{\mathrm{d}}{\mathrm{d}y}(y \,.\, k_1(y, a))} \tag{3.3}$$

where K_8 is a known positive constant. The problem of minimisation of the function $\tilde{I}$ on K can be replaced by the problem of minimisation of the function $\tilde{I} + K_9 \,.\, \hat{p}$ on the cartesian product of the intervals R_1, where K_9 is a sufficiently large positive real number and $\hat{p}$ a suitable penal function corresponding to the condition which defines the set R_2. We choose

$$(3.4) \qquad \hat{p}(a) = 0 \quad \text{for all} \quad a \in R_1 \quad \text{for which} \quad \min\{h_1(y, a), y \geqq 0\} \geqq 0\,,$$

$$\hat{p}(a) = [\min\{h_1(y, a), y \geqq 0\}]^2 = h_1^2((a_2 + a_3 + (a_2^2 + a_3^2 - a_2 a_3)^{1/2})/3, a)$$

in the other cases.

Possible numerical difficulties connected with the case when $1 + h_1(\cdot, a)$ is not a positive function can be removed with the help of the following adjustment of the function ψ_a' (which does not change the value of this function on K):

$$\psi_a'(y) = h_2\left(1 + \frac{\mathrm{d}}{\mathrm{d}y}(y \,.\, k_1(y, a))\right), \tag{3.5}$$

$$h_2(\eta) \begin{cases} \dfrac{K_8}{\eta}\,, & \eta \in \langle K_{10}, \infty)\,, \\ -\dfrac{K_8}{K_{10}^2}\eta + \dfrac{2K_8}{K_{10}}\,, & \eta \in (-\infty, K_{10})\,, \end{cases}$$

where K_{10} is a small positive real constant.

In our numerical experiment $\xi = v(\cdot, l)$ was used, where v is the solution of the problem (I.1), (I.2), (I.3) and (I.4) with $\psi(v) = av$, a is a fixed positive real number and $\varphi(t) = 1$ on $\langle 0, t_0 \rangle$, $\varphi(t) = 0$ on $\langle t_0, T \rangle$. Using the Laplace transform, we obtain:

$$v(t, x) = \frac{2}{\sqrt{\pi}} \,.\, e^{(a/2b)x} \,.\, x \,.\, \int_{\max(0, t - t_0)}^{t} \frac{1}{4\sqrt{(b\tau^3)}} \,.\, e^{-(1/4b)\,[a^2\tau + (x^2/\tau)]}\, \mathrm{d}\tau\,. \tag{3.6}$$

In this case we can check the correctness of the numerical result by an immediate comparison.

Finally, let us look at the result of a particular example. Put: $\tau = 0{\cdot}01$, $h = 0{\cdot}1$, $b = 0{\cdot}5$, $l_1 = 15$, $T = 6$, $l = 4$, $L = 12$, $t_0 = 0{\cdot}7$, $K_1 = 0{\cdot}9$, $K_2 = 0{\cdot}01$, $K_3 = 0{\cdot}9$, $K_4 = 0{\cdot}1$, $K_5 = 0{\cdot}4$, $K_6 = 0{\cdot}6$, $K_7 = 0{\cdot}9$, $K_8 = 2$, $K_9 = 1$ and $K_{10} = 0{\cdot}1$. In this example the values of the function ξ are the approximative values of the function $v(\cdot, 4)$ with $a = 1$, calculated from (3.6) by means of simple Simpson's quadrature

Table 1. Iterations of the modified conjugate gradient method for the particular example described in the text

Item	a_1	a_2	a_3	$\tau^{-1}\check{I}(a_1, a_2, a_3)$
1	0·6000	0·1200	0·7500	0·001879
2	0·5694	0·1000	0·7435	0·001642
3	0·4484	0·1000	0·7144	0·001038
4	0·3275	0·1000	0·6854	0·000549
5	0·1288	0·1000	0·6377	0·000175
6	0·1047	0·1583	0·7054	0·000150
7	0·0919	0·1894	0·7416	0·000146
8	0·1036	0·2539	0·8153	0·000118
9	0·1153	0·3185	0·8891	0·000098
10	0·1170	0·3280	0·9000	0·000095
11	0·1163	0·4000	0·9000	0·000090
12	0·1157	0·4000	0·9000	0·000090

formula with the step 0·005. As we can see from Table 1, the computation is finished after the twelfth iteration. The vector $(a_1, a_2, a_3) = (0{\cdot}1157, 0{\cdot}4000, 0{\cdot}9000)$ gives a good approximation of the exact value $\psi' = 1$ ($k_1(x, a) = 1{\cdot}0157$ on $\langle -\infty, 0{\cdot}4\rangle$, $k_1(x, a) = 0{\cdot}9$ on $\langle 0{\cdot}9, \infty)$, $k_1(x, a) \in \langle 0{\cdot}9, 1{\cdot}0157\rangle$), the "best uniform" approximation gives the vector $(0{\cdot}1, 0{\cdot}4, 0{\cdot}9)$. Let us remark that the calculation of grad $\check{I}(a)$ was executed with help of the direct method.

Remark: For the convergence of the minimisation iterative methods the choice of the initial iteration is important. When it is convenient to have an initial iteration in our method in the form of a linear function ($\psi(u) = \hat{a}u$, $\hat{a} > 0$) we can use the fact that for all $x > 0$ and $a > 0$ there exists a unique point $T_{\max} \in (t_0, \infty)$ at which the function $v(\cdot, x)$ given by formula (3.6) has its maximum. The function $a \to T_{\max}$ with the fixed $x > 0$ is an injective mapping of the interval $(0, \infty)$ into the interval (t_0, ∞). The inverse mapping is defined by the formula

$$(3.7) \quad a = \{x^2/t_0 \cdot [-1/T_{\max} + 1/(T_{\max} - t_0)] + 6b \log [(T_{\max} - t_0)/T_{\max}]\}^{1/2} .$$

Let there exist precisely one point at which the function ξ has its maximum. Let us write $\hat{T}$ for this point. Then we can put

$$(3.8) \qquad \hat{a} = \{l^2/t_0[-1/\hat{T} + 1/(\hat{T} - t_0)] + 6b \log [(\hat{T} - t_0)/\hat{T}]\}^{1/2}$$

if the expression on the right hand side is defined.

APPENDIX

The appendix contains some theoretical results concerning our problem. *Lemma* 1 proves the existence of a solution of a certain integral equation which is, as *Lemma* 2 shows, the classical solution of the problem (I.1)–(I.4). The principle of monotonicity for parabolic operators contained in *Lemma* 3 is used to prove the uniqueness of the solution of (I.1)–(I.4) in *Lemma* 4. In *Theorem* 1 the results of *Lemmas* 2 and 4 are summarized and the correctness of the definition of the generalised solution is shown. *Theorem* 2 establishes conditions of existence of the solution of our optimal control problem.

Denote

(A.1)
$$T_1\,\varphi(t,x)=\frac{2}{\sqrt{\pi}}\int_0^t \frac{x}{4\sqrt{(b\tau^3)}}\,e^{-x^2/(4b\tau)}\,\varphi(t-\tau)\,\mathrm{d}\tau\,,\quad (t,x)\in\langle 0,T\rangle\times\langle 0,\infty)\,,$$

(A.2)
$$T_2\,v(t,x)=\frac{1}{\sqrt{\pi}}\int_0^t\int_{-\infty}^{+\infty} v(t-\tau,x-z)\,\frac{z}{4\sqrt{(b^3\tau^3)}}\cdot e^{-z^2/(4b\tau)}\,\mathrm{d}z\,\mathrm{d}\tau\,,\quad (t,x)\in\langle 0,T\rangle\times\langle 0,\infty)\,,$$

where φ and v are arbitrary functions such that the integrals on the right hand side of these relations exist. Let

(A.3)
$$h:\langle 0,T\rangle\times(-\infty,\infty)\to\langle 0,T\rangle\times\langle 0,\infty)\,,$$
$$h=(h_1,h_2)\,,\quad h_1(t,x)=t\,,\quad h_2(t,x)=|x|\,.$$

Lemma 1. *Let $\psi\in C^1(\mathbb{R}^1)$ and let ψ' be a bounded function on $\mathbb{R}^1$. Let $\varphi\in C(\langle 0,T\rangle)$ and $\varphi(0)=0$. Then there exists a unique continuous and bounded solution $u=u(t,x)$ of the integral equation*

(A.4) $$u(t,x)=T_1\,\varphi(t,x)+T_2(\psi\circ u\circ h)(t,x)\,,\ (t,x)\in\langle 0,T\rangle\times\langle 0,\infty\rangle\,.$$

Let u_0 be an arbitrary function, continuous and bounded on $\langle 0,T\rangle\times\langle 0,\infty\rangle$. Then the sequence of functions $\{u_n\}_{n=0}^{\infty}$ defined by the recursive formula

(A.5) $$u_n(t,x)=T_1\,\varphi(t,x)+T_2(\psi\circ u_{n-1}\circ h)(t,x)\,,\ (t,x)\in\langle 0,T\rangle\times\langle 0,\infty\rangle$$

converges uniformly to the function u.

Proof. Let $p\in\mathbb{R}^1$. Let us write $C^{(p)}_{T,\infty}$ for the Banach space of all functions that are continuous and bounded on the set $\langle 0,T\rangle\times\langle 0,\infty)$, with the norm $\|v\|=\sup\{|v(t,x)|\,e^{-pt};(t,x)\in\langle 0,T\rangle\times\langle 0,\infty)\}$. Let us define the operator $T:C^{(p)}_{T,\infty}\to C^{(p)}_{T,\infty}$, $Tu=T_1\varphi+T_2(\psi\circ u\circ h)$, $p=4b^{-1}\sup\{\psi'(\xi)^2;\xi\in\mathbb{R}^1\}$. Then for all $u,v\in C^{(p)}_{T,\infty}$ the inequality $\|Tu-Tv\|\leqq\frac{1}{2}\|u-v\|$ is valid. Using the Banach fixed point theorem, we obtain the assertion of the lemma.

Lemma 2. *Let $\psi\in C^2(\mathbb{R}^1)$, ψ' and ψ'' be bounded functions and* let *ψ'' be Lipschitz continuous.* Let *$\varphi\in C^1(\langle 0,T\rangle)$ and $\varphi(0)=0$. Then the continuous and bounded* *solution u of the equation* (A.4) *is the classical solution of the boundary value problem* (I.1), (I.2), (I.3) *and* (I.4); $\partial u/\partial x$ *is a bounded function on* $(0, T\rangle \times (0, \infty)$.

Proof. Let $u_0 = 0$ and $u_{n+1} = T_1\varphi + T_2(\psi \circ u_n \circ h)$. By elementary considerations and calculations we obtain the following results: the functions $\partial / \partial t[T_1\varphi]$, $\partial / \partial x[T_1\varphi]$, $\partial^2/\partial x^2[T_1\varphi]$ are defined, continuous and bounded in $(0, T\rangle \times (0, \infty)$; moreover $\partial / \partial t[T_1\varphi] = b\, \partial^2 / \partial x^2[T_1\varphi] = T_1\varphi'$; $\partial u_n / \partial x$ exists for all $n \in \mathbb{N}$ and $(t, x) \in (0, T\rangle \times (0, \infty)$; the function $\partial u_n/\partial x$ is continuous and bounded on its domain and satisfies

$$\frac{\partial u_{n+1}}{\partial x} = \frac{\partial}{\partial x}[T_1\varphi] + T_2\left[\frac{\partial(\varphi \circ u_n \circ h)}{\partial x}\right] \quad n = 0, 1, 2, \ldots .$$

Denote $L = \sup\left\{\left|\frac{\partial}{\partial x}[T_1\varphi]\right| . e^{-pt};\ (t, x) \in (0, T\rangle \times (0, \infty)\right\}$,

$$X_n = \sup\left\{\left|\frac{\partial u_n}{\partial x}\right| . e^{-pt}; (t, x) \in (0, T\rangle \times (0, \infty)\right\} \quad n = 0, 1, \ldots ,$$

$$Y_n = \sup\left\{\left|\frac{\partial u_{n+1}}{\partial x} - \frac{\partial u_n}{\partial x}\right| . e^{-pt}; (t, x) \in (0, T\rangle \times (0, \infty)\right\} \quad n = 0, 1, \ldots ,$$

$$Z_n = \sup\{|u_{n+1} - u_n|\, e^{-pt}; (t, x) \in (0, T\rangle \times (0, \infty)\} \quad n = 0, 1, \ldots,$$

$$p = 4b^{-1} \sup\{\psi'(\xi)^2; \xi \in \mathbb{R}^1\} .$$

Then it is evident that

(A.6)
$$Z_{n+1} \leqq \tfrac{1}{2}Z_n , \quad Z_n \leqq (\tfrac{1}{2})^n Z_0 , \quad X_{n+1} \leqq \tfrac{1}{2}X_n + L,$$

$$X_n \leqq (\tfrac{1}{2})^n X_0 + \sum_{i=0}^{n-1} (\tfrac{1}{2})^i L \quad n = 0, 1, 2, \ldots,$$

$$\frac{\partial u_{n+2}}{\partial x} - \frac{\partial u_{n+1}}{\partial x} = T_2\left[(\psi'(u_{n+1})\left(\frac{\partial u_{n+1}}{\partial x} - \frac{\partial u_n}{\partial x}\right) + (\psi'(u_{n+1}) - \right.$$

$$\left. - \psi'(u_n))\frac{\partial u_n}{\partial x}\right) \circ hh_2'\Big] \; n = 0,1, \ldots .$$

Since ψ'' is a bounded function and the sequence $\{X_n\}$ is bounded (see (A.6)), there exists a positive constant R so that $Y_{n+1} \leqq \frac{1}{2}Y_n + RZ_n$. Hence we have $Y_{n+1} \leqq \frac{1}{2}Y_n + RZ_0(\frac{1}{2})^n$, $Y_n \leqq (\frac{1}{2})^n Y_0 + n(\frac{1}{2})^{n-1} RZ_0$, $n = 0, 1, \ldots$. This fact evidently implies the uniform convergence of the sequence $\{\partial u_n / \partial x\}_{n=0}^{\infty}$ on $(0, T\rangle \times (0, \infty)$. Further, it is clear that $\partial u/\partial x$ exists on $(0, T\rangle \times (0, \infty)$, $\partial u/\partial x$ is continuous and bounded on its domain, $\partial u_n/\partial x \rightrightarrows \partial u/\partial x$,

$$\frac{\partial u}{\partial x} = T_2\frac{\partial(\psi \circ u \circ h)}{\partial x} + \frac{\partial}{\partial x}[T_1\varphi] .$$

Analogously we can prove the existence of continuous and bounded functions $\partial^2 u_n/\partial x^2$, $\partial u_n/\partial t$ (for all $n \in \mathbb{N}$), $\partial^2 u/\partial x^2$ and $\partial u/\partial t$ defined on $(0, T\rangle \times (0, \infty)$ and the uniform convergence of the sequences $\{\partial^2 u_n/\partial x^2\}$ and $\{\partial u_n/\partial t\}$ to $\partial^2 u/\partial x^2$ and $\partial u/\partial t$, respectively. In addition, we have

$$\frac{\partial^2 u}{\partial x^2}(t, x) = T_2\left[\frac{\partial^2(\psi \circ u \circ h)}{\partial x^2}\right] + \frac{\partial^2}{\partial x^2}[T_1\varphi] + \frac{2}{\sqrt{(b\pi)}}\int_0^t \frac{\partial\psi(u(t-\tau, 0))}{\partial x} \cdot$$

$$\cdot \frac{x}{4b\sqrt{\tau^3}} e^{-x^2/(4b\tau)} d\tau, \quad \frac{\partial u}{\partial t}(t, x) = T_2\left[\frac{\partial(\psi \circ u \circ h)}{\partial t}\right] + \frac{\partial}{\partial t}[T_1\varphi],$$

where

$$\frac{\partial u(t, 0)}{\partial x} \overset{\text{def.}}{=} \lim_{x \to 0+} \frac{\partial u(t, x)}{\partial x}.$$

By repeated use of integration by parts and other simple adjustments we obtain from the above formulae that u solves the equation (I.1). It is easy to see that u satisfies the conditions (I.2), (I.3) and (I.4).

Lemma 3. *Let functions a and c be defined on $(0, T\rangle \times (0, l)$. Let functions u and v be continuous on $\langle 0, T\rangle \times \langle 0, l\rangle$ and let $\partial u/\partial t$, $\partial v/\partial t$, $\partial^2 u/\partial x^2$ and $\partial^2 v/\partial x^2$ be continuous on $(0, T\rangle \times (0, l)$. Let b be a positive constant. Let*

$$\text{(A.7)} \qquad \frac{\partial u}{\partial t} - b\frac{\partial^2 u}{\partial x^2} - a(t, x)\,u - c(t, x)\frac{\partial u}{\partial x} < \frac{\partial v}{\partial t} - b\frac{\partial^2 v}{\partial x^2} - a(t, x)\,v - c(t, x)\frac{\partial v}{\partial x} \quad \text{on} \quad (0, T\rangle \times (0, l),$$

$$\text{(A.8)} \qquad u(t, 0) < v(t, 0) \qquad t \in \langle 0, T\rangle,$$

$$\text{(A.9)} \qquad u(t, l) < v(t, l) \qquad t \in \langle 0, T\rangle,$$

$$\text{(A.10)} \qquad u(0, x) < v(0, x) \qquad x \in \langle 0, l\rangle.$$

Then $u(t, x) < v(t, x)$ for all $(t, x) \in \langle 0, T\rangle \times \langle 0, l\rangle$.

Proof. Let us put $w = v - u$, $M = \{t \in (0, T\rangle; \exists\, x \in (0, l), w(t,x) \leqq 0\}$. We assume that M is a nonempty set. Let us denote $t_0 = \inf\{t, t \in M\}$. Then there exist sequences $\{t_n\} \subset M$, $t_n \to t_0$ and $\{x_n\} \subset (0, l)$ so that $w(t_n, x_n) \leqq 0$. We may suppose that $\{x_n\}$ converges. Let us denote $x_0 = \lim x_n$. Evidently, $(t_0, x_0) \in (0, T\rangle \times (0, l)$, $w(t_0, x_0) = 0$, $\partial w/\partial t(t_0, x_0) \leqq 0$, $\partial w/\partial x(t_0, x_0) = 0$, $\partial^2 w/\partial x^2(t_0, x_0) \geqq 0$. Hence we obtain a contradiction with our assumptions.

Lemma 4. *Let $\psi \in C^2(\mathbb{R}^1)$, $\varphi \in C(\langle 0, T\rangle)$ and $\varphi(0) = 0$. Let $u = u(t, x)$, $v = v(t, x)$ be classical solutions of the problem* (I.1), (I.2), (I.3) *and* (I.4). *Let $\partial u/\partial x$ be a bounded function.* Then $u = v$.

Proof. Let us put $w = u - v$. Then

$$\text{(A.11)} \begin{cases} \mathscr{L}w = \dfrac{\partial w}{\partial t} - b\dfrac{\partial^2 w}{\partial x^2} - a(t, x)\, w(t, x) - c(t, x)\dfrac{\partial w}{\partial x}(t, x) = 0, (t, x) \in (0, T\rangle \times \\ \quad \times (0, \infty)\,, \\ w(0, x) = 0\,, \quad w(t, 0) = 0\,, \quad x \in \langle 0, \infty)\,, \quad t \in \langle 0, T\rangle\,, \\ \limsup\limits_{x \to \infty} \{|w(t, x)|;\ t \in \langle 0, T\rangle\} = 0\,, \end{cases}$$

where

$$a(t, x) = -\psi''(\xi(t, x))\,.\,\partial u/\partial x(t, x)\,,$$
$$c(t, x) = -\psi'(v(t, x))\,,$$
$$\min(u, v) \leqq \xi \leqq \max(u, v)\,.$$

Let us assume that $a(t, x) \leqq 0$ on $(0, T\rangle \times (0, \infty)$. Let w_1 and w_2 be some solutions of the linear problem (A.11). Let us put $w_1^{(n)} = w_1 + t/n + 1/n$ for all $n \in \mathbb{N}$. Then we have $\mathscr{L}w_1^{(n)} \geqq (1/n) > 0 = \mathscr{L}w_2$, $w_1^{(n)}(0, x) = (1/n) > 0 = w_2(0, x)$, $w_1^{(n)}(t, 0) = (1/n)\,t + (1/n) > 0 = w_2(t, 0)$. There exists a sequence $\{\xi_n\}$, $\xi_n \to \infty$ such that $w_1^{(n)}(t, x) > w_2(t, x)$, $(t, x) \in \langle 0, T\rangle \times \langle \xi_n, \infty)$. Using *Lemma* 3 we obtain $w_1^{(n)} > w_2$ on $\langle 0, T\rangle \times \langle 0, \infty)$. Hence it is evident that $w_1 = w_2$.

If $a(t, x)$ is not a nonpositive function, then there exists a positive constant $\hat{c}$ such that $a(t, x) \leqq \hat{c}$ for all $(t, x) \in (0, T\rangle \times (0, \infty)$. Using the substitution $w(t, x) = \hat{w}(t, x)\,.\,e^{\hat{c}t}$, we return to the first case again.

Theorem 1. *Let $\psi \in C^2(\mathbb{R}^1)$, ψ' and ψ'' be bounded functions and let ψ'' be Lipschitz continuous.*

1. *Let $\varphi \in C^1(\langle 0, T\rangle)$, $\varphi(0) = 0$. Then there exists a unique classical solution of the boundary value problem* (I.1), (I.2), (I.3) *and* (I.4).

2. *Let $\varphi \in L_1(0, T)$. Then there exists a sequence $\{\varphi_n\}_{n=0}^{\infty} \subset C^1(\langle 0, T\rangle)$, $\varphi_n(0) = 0$ such that $\varphi_n \to \varphi$ in the space $L_1(0, T)$. Let us write u_n for the classical solution of the problem* (I.1), (I.2), (I.3) *and* (I.4) *for $\varphi = \varphi_n$. Let $L_{T,\infty}$ be the Banach space of all functions f such that $f(\cdot, x) \in L_1(0, T)$ for all $x \in \langle 0, \infty)$ and $\sup\{\int_0^T |f(t, x)|\,dt;\ x \in \langle 0, \infty)\} < \infty$, with the norm $\|f\| = \sup\{\int_0^T |f(t, x)|\,dt;\ x \in \langle 0, \infty)\}$. Then the sequence $\{u_n\}_{n=0}^{\infty}$ converges in the space $L_{T,\infty}$. Let us denote $u = \lim u_n$. The function u is independent of the particular choice of the sequence $\{\varphi_n\}$ with the above introduced properties.*

Proof. 1. This result is an immediate consequence of *Lemmas* 2 and 4.

2. Let us remark only that the integral representation of our problem makes it possible to derive the estimate.

$$\|u_n - u_m\|_{p,2} \leqq \tfrac{1}{2}\|u_n - u_m\|_{p,2} + \|\varphi_n - \varphi_m\|_{p,1}\,,$$

where $\|\tilde{u}\|_{p,2} \overset{\text{def.}}{=} \sup\left\{\int_0^T |\tilde{u}(t, x)|\,.\,e^{-pt}\,dt, x \in \langle 0, \infty)\right\}$,

$$\|\tilde{\varphi}\|_{p,1} \overset{\text{def.}}{=} \int_0^T |\tilde{\varphi}(t)| \cdot e^{-pt}\, dt\,,$$

$$p = 4b^{-1} \sup \{\psi'(\xi)^2, \xi \in \mathbb{R}^1\}\,.$$

Definition. *The function $u \in L_{T,\infty}$ defined in part 2 of Theorem 1 will be called the generalised solution of the problem* (I.1), (I.2), (I.3) *and* (I.4).

Lemma 5. *Let ψ fulfil the condition of Theorem* 1.

1. *Let $\varphi \in C(\langle 0, T\rangle)$, $\varphi(0) = 0$. Let u be the classical solution of the problem* (I.1)–(I.4). *Then for all $(t, x) \in \langle 0, T\rangle \times \langle 0, \infty)$, $\inf \{\varphi(\tau); \tau \in \langle 0, T\rangle\} \leqq u(t, x) \leqq \sup \{\varphi(\tau); \tau \in \langle 0, T\rangle\}$.*

2. *Let $\varphi \in L_\infty(0, T)$. Let u be the generalised solution of the problem* (I.1)–(I.4). *Then for all $x \in \langle 0, \infty)$, $u(\cdot, x) \in L_\infty(0, T)$, $\min \{0, \text{vraiinf} \{\varphi(\tau); \tau \in \langle 0, T\rangle\}\} \leqq u(t, x) \leqq \max \{0, \text{vraisup} \{\varphi(\tau); \tau \in \langle 0, T\rangle\}\}$ and $|u(t, x)| \leqq \text{vraisup} \{|\varphi(\tau)|; \tau \in \langle 0, T\rangle\}$ almost everywhere in $\langle 0, T\rangle$.*

Proof. 1. Let $(t_0, x_0) \in (0, T\rangle \times (0, \infty)$ and $u(t_0, x_0) = \sup \{u(t, x), (t, x) \in \langle 0, T\rangle \times \langle 0, \infty)\}$.

Put $\varepsilon = u(t_0, x_0) - \sup \varphi$, $v(t, x) = u(t, x) + \varepsilon(T - t)/(2T)$. Then $v(t_0, x_0) = u(t_0, x_0) + \varepsilon(T - t_0)/(2T) > \sup \varphi + \varepsilon/2 \geqq \sup \{v(t, x);\ t = 0 \text{ or } x = 0\}$. Thus, if $v(t_1, x_1) = \sup \{v(t, x);\ (t, x) \in \langle 0, T\rangle \times \langle 0, \infty)\}$ then $(t_1, x_1) \in (0, T\rangle \times (0, \infty)$, $\partial u/\partial t(t_1, x_1) = \partial v/\partial t(t_1, x_1) + \varepsilon/(2T) \geqq \varepsilon|(2T) > 0$, $\partial u/\partial x(t_1 x_1) = \partial v/\partial x(t_1, x_1) = 0$ $\partial^2 u/\partial x^2(t_1, x_1) = \partial^2 v/\partial x^2(t_1, x_1) \leqq 0$ and $[\partial u/\partial t + \psi'(u)\, \partial u/\partial x - b\, \partial^2 u/\partial x^2]$ $(t_1, x_1) \geqq \varepsilon/(2T)$ which contradicts our assumption.

2. Let $\varphi_n \in C^1(\langle 0, T\rangle)$, $\varphi_n(0) = 0$, $\varphi_n \to \varphi$ in $L_1(0, T)$. Denote $M = \max \{0, \text{vraisup} \{\varphi(\tau); \tau \in \langle 0, T\rangle\}\}$, $\psi_n = \inf (M, \varphi_n) \in C(\langle 0, T\rangle)$, $\psi_n(0) = 0$.

Let $\xi_n \in C^1(\langle 0, T\rangle)$, $\xi_n(0) = 0$, $\sup |\psi_n - \xi_n| \to 0$ for $n \to \infty$. Then $\xi_n \to \varphi$ in $L_1(0, T)$. We can suppose that the sequence $\{\sup \xi_n\}$ is convergent and for all $\varepsilon > 0$ there exists $n_0 \in \mathbb{N}$ so that $n \geqq n_0 \Rightarrow u_n \leqq \sup \xi_n \leqq M + \varepsilon$ where u_n is the classical solution of (I.1)–(I.4) with $\varphi = \xi_n$. If $x \in \langle 0, \infty)$, $\mu(t, u(t, x) > M + 2\varepsilon) = \delta > 0$ then $\int_0^T |u(t, x) - u_n(t, x)|\, dt \geqq \varepsilon\delta$ for all $n \geqq n_0$.

Theorem 2. *Let $\psi\colon \mathbb{R}^1 \times K \to \mathbb{R}^1$ and let K be a compact subset of $\mathbb{R}^n$. For all $a \in K$ let $\psi_a = \psi(\cdot, a) \in C^2(\mathbb{R}^1)$, ψ'_a and ψ''_a be bounded functions and let ψ''_a be Lipschitz continuous.* Let $\varphi \in L_\infty(0, T)$. *Let us write u_a for the generalised solution of the boundary value problem* (I.1), (I.2), (I.3) *and* (I.4) *for $\psi = \psi_a$. For all $a_0 \in K$ and $\varepsilon > 0$ let there exist $\delta > 0$ such that for all $x \in \mathbb{R}^1$ and $a \in K$ the following implication holds: $\|a - a_0\| < \delta \Rightarrow |\psi(x, a) - \psi(x, a_0)| < \varepsilon$. Let $\xi \in L_\infty(0, T)$ and let l be a positive real number. Then there exists $\alpha \in K$ so that for all $a \in K$ the inequality $\int_0^T (u_\alpha(t, l) - \xi(t))^2\, dt \leqq \int_0^T (u_a(t, l) - \xi(t))^2\, dt$ is valid.*

Proof. From the integral expression of the problem (I.1)–(I.4) we obtain by simple estimations that the mapping $a \to u_a$ of the set K into $L_{T,\infty}$ is continuous. Therefore, the mapping $a \to u_a(\cdot, l)$ of the set K into $L_1(0, T)$ is continuous as well. Further, for all $x \in \langle 0, \infty)$ the inequality vraisup $\{|u_a(t, x)|;\ t \in \langle 0, T\rangle\} \leqq$ vraisup $\{|\varphi(t)|;\ t \in \langle 0, T\rangle\}$ holds. Thus $|\Phi(u_\alpha) - \Phi(u_\beta)| \leqq \|u_\alpha(\cdot, l) - u_\beta(\cdot, l)\|_{L_1(0,T)} \cdot$ $\cdot\ [2\ \text{vraisup}\ |\varphi| + 2\ \text{vraisup}\ |\xi|]$ for all $\alpha, \beta \in K$. The just introduced facts imply the continuity of the functional $I : K \to \mathbb{R}^1, I(a) = \int_0^T (u_a(t, l) - \xi(t))^2 \, dt$.

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Souhrn

NUMERICKÁ IDENTIFIKACE KOEFICIENTU V PARABOLICKÉ KVASILINEÁRNÍ ROVNICI

JAN NEUMANN

V článku je studován následující problém optimálního řízení: určit v kvasilineární parciální diferenciální rovnici parabolického typu jistý koeficient tak, aby řešení určité okrajové úlohy pro tuto rovnici minimalizovalo daný integrální funkcionál. Kromě návrhu a rozboru numerické metody obsahuje práce i řešení základních problémů spojených s formulací úlohy (existence a jednoznačnost řešení okrajové úlohy, existence řešení úlohy optimální regulace).

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