

UDK 681.513.675

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MATHEMATICAL MODELS OF UNEQUIVALENT TECHNOLOGICAL PROCESSES AS VARIATION INEQUALITIES AND THEIR CALCULABLE REALIZATION ON THE BASIS OF METHODS OF OPTIMIZATION

Abstract. The approach to the solution of the class of spatially-distributed non-steady disparities which one is offered make mathematical models of physical processes of a directional effect. The approach is grounded on optimization looked up of a maximum of a Hamiltonian function from a function of space of a condition.

Keywords: mathematical model, variation, variation inequality, principle of maximum, functional.

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МАТЕМАТИЧЕСКИЕ МОДЕЛИ НЕРАВНОВЕСНЫХ ТЕХНОЛОГИЧЕСКИХ ПРОЦЕССОВ В ВИДЕ ВАРИАЦИОННЫХ НЕРАВЕНСТВ И ИХ ЧИСЛЕННАЯ РЕАЛИЗАЦИЯ НА БАЗЕ МЕТОДОВ ОПТИМИЗАЦИИ

Аннотация. Предложены математические модели класса неравновесных технологических процессов в виде вариационных неравенств, а также подход к их численной реализации. Подход основан на поиске максимума функции Гамильтона от функций пространства состояний.

Ключевые слова: математическая модель, вариационное неравенство, принцип максимума, функционал.

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МАТЕМАТИЧНІ МОДЕЛІ НЕРІВНОВАГОВИХ ТЕХНОЛОГІЧНИХ ПРОЦЕСІВ У ВИГЛЯДІ ВАРІАЦІЙНИХ НЕРІВНОСТЕЙ ТА ЇХ ЧИСЕЛЬНА РЕАЛІЗАЦІЯ НА БАЗІ МЕТОДІВ ОПТИМІЗАЦІЇ

Анотація. Запропоновано математичні моделі класу нерівновагових технологічних процесів у вигляді варіаційних нерівностей, а також підхід щодо їх чисельної реалізації. Підхід ґрунтується на пошуку максимуму функції Гамільтона від функцій простору стану.

Ключові слова: математична модель, варіаційна нерівність, принцип максимуму, функціонал.

Introduction. Analysis of physical phenomena characteristic for the class of physical processes with a pronounced directional operation (for example, the propagation of waves of different nature in heterogeneous environments, the deformation of elements of mechanical systems with variable structure, filtering highly paraffinic crude in the layers with partial conductivity of boundaries, etc.) makes it possible to consider the apparatus of variational inequalities [1–4] as an adequate mathematical description of these processes.

In this paper [5] we obtain and justify a generalized mathematical model (MM) to study a class of variational inequalities can be represented as follows.

Mathematical model of process and its transformation. Let the function $\psi(t, \bar{z})$, defined on a bounded open set Ω

of the space \mathfrak{R}^n , $n = 1, 2$, with smooth boundary Γ and the time interval $(0, t_k)$ for $t_k < \infty$, $Q = \Omega \times (0, t_k)$, $\Sigma = \Gamma \times (0, t_k)$ is the solution of the variational inequality

$$\psi \in K : \left(m(\bar{z}) \frac{\partial \psi}{\partial t}, v - \psi \right) + (B(\gamma)\psi, v - \psi) + j(v) - j(u) \geq (f, v - \psi) \quad \forall v \in H^1(\Omega), \quad (1)$$

$$\psi(0, \bar{z}) = \psi_0(\bar{z}), \quad (2)$$

where the operator $B(\gamma)$ specifies a linear transformation $B(\gamma): H^1(\Omega) \rightarrow H^1(\Omega)$ and is defined by the bilinear form:

$$(B(\gamma)\psi, v - \psi) = \int_{\Omega} \left(\sum_{i=1}^n \frac{\partial \psi}{\partial z_i} \cdot \frac{\partial (v - \psi)}{\partial z_i} \right) d\bar{z}, \quad (3)$$

where f – the driving function of the process, for which the operation $(f, v - \psi)$ coincides with the scalar product in $L^2(\Omega)$, i.e.

$$(f, v - \psi) = \int_{\Omega} [f(\bar{z}), v - \psi] d\Omega$$

or

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$$(f, v - \psi) = \int_{\Gamma} [f(\bar{z}), v - \psi] d\Gamma$$

where Γ — hereinafter, for simplicity, restrict ourselves to the tasks at the border; $j(\cdot)$ — convex functionals defining the kind of physical process in rheology and which are specified as follows

$$\begin{aligned} j(\cdot) &= \int_{\Gamma} \varphi(\psi, \bar{z}) \cdot \lambda(\psi) d\Gamma, \\ j(\cdot) &= \int_{\Omega} \varphi(\psi, \bar{z}) \cdot \lambda(\psi) d\Omega. \end{aligned} \quad (4)$$

In the relation (4) accept that $\varphi(\cdot)$ — is a continuous function, $\lambda(\cdot)$ — is continuous differentiable or not having the properties of differentiable functions.

Space of admissible functions $\varphi(\cdot)$ and $\lambda(\cdot)$ are defined as $\Delta \in L^\infty(\bar{Q})$, $\Lambda \in L^\infty(\bar{Q})$ where it is assumed that $\varphi(\cdot), \lambda(\cdot) \in L^\infty(\bar{Q})$, $\bar{Q} = \bar{\Omega} \times (0, t_k)$ and the spaces Δ and Λ are Banach with respect to the norm

$$\|\varphi(\psi, \bar{z})\|_{\Delta} = \|\varphi(\psi, \bar{z})\|_{L^\infty(\bar{Q})}.$$

The proposed method for solving variational inequalities of the form (1), (2) is based on the proof of the following statements.

To find the optimal solution $\psi(t, \bar{z})$ of the variational inequality (1), (2) there must exist a nonzero continuous function $p(t, \bar{z})$, so that at any time t in the interval $0 \leq t \leq T$ (T — time of physical processes) the Hamiltonian function \tilde{H} in the spatial domain Ω (or on its boundary Γ) would take the maximum value, where

$$\begin{aligned} \tilde{H} &= \langle ((B(\gamma)\tilde{\psi}, \tilde{v} - \tilde{\psi}) + \phi(\tilde{v}) - \phi(\tilde{\psi}) - \\ &- (\theta(\tilde{\psi}, \tilde{v}), \tilde{v} - \tilde{\psi}) - (f, (\tilde{v} - \tilde{\psi}))), \tilde{p} \rangle \end{aligned}$$

Carry out a preliminary series of reforms to simplify the original formulation of the problem. Introduce the notation

$$\varphi(t, \bar{z}) \cdot \lambda(\psi) = \Phi(\psi), \quad \varphi(t, \bar{z}) \cdot \lambda(v) = \Phi(v)$$

and

$$\phi(\psi) = \int_{\Gamma} \Phi(\psi) d\Gamma, \quad \phi(v) = \int_{\Gamma} \Phi(v) d\Gamma.$$

In addition, introduce an additional unknown function $\theta(\psi, v)$, the structure corresponding to the functionals $j(\cdot)$, such that

$$(\theta(\psi, v), v - \psi) \geq 0 \quad \forall v \in K.$$

Taking into account the executed

transformations introduce the relations (1), (2) in the form

$\psi \in K$:

$$\begin{aligned} &\left(m(\bar{z}) \frac{\partial \psi}{\partial t}, v - \psi \right) + (B(\gamma), v - \psi) + \phi(v) - \phi(\psi) - \\ &- (\theta(\psi, v), v - \psi) = (f, v - \psi) \quad \forall v \in K. \end{aligned} \quad (5)$$

$$\psi(0, \bar{z}) = \psi_0(\bar{z}), \quad (6)$$

To solve the problem of finding a state function $\psi(t, \bar{z})$, use an optimization procedure of the Pontryagin maximum principle [6], for which choose the following performance criterion

$$J = \min \int_0^T \int_{\Gamma} |v - \psi| dt d\Gamma. \quad (7)$$

The physical meaning of this criterion follows from the next. The trial function $v(t, \bar{z})$ is some approximation of the unknown function $\psi(t, \bar{z})$, reflecting only the essence of physics in the specific process. Therefore, the adequacy of physical processes caused by the action of functions $v(t, \bar{z})$, and $\psi(t, \bar{z})$, is provided up to the accuracy within the difference between these functions. In this case, the integral difference between the trial $v(t, \bar{z})$ and the unknown $\psi(t, \bar{z})$ functions can be regarded as a quantitative measure or a penalty for the deviation of the actual flow of the process from its true value.

Obtain the necessary optimality conditions of the problems (5) (6), (7).

According to [6], introduce a new coordinate

$$\frac{\partial^2 \sigma}{\partial t \partial z} = |v - \psi|^2 \Big|_{z \in \Gamma}. \quad (8)$$

Thus, the original problem will be considered in $(n+1)$ -dimensional space with the equation of dynamics

$\tilde{\psi} \in K$:

$$\begin{aligned} &\left(m(\bar{z}) \frac{\partial \tilde{\psi}}{\partial t}, \tilde{v} - \tilde{\psi} \right) + (B(\gamma), \tilde{v} - \tilde{\psi}) + \phi(\tilde{v}) - \phi(\tilde{\psi}) - \\ &- (\theta(\tilde{\psi}, \tilde{v}), \tilde{v} - \tilde{\psi}) = (f, \tilde{v} - \tilde{\psi}) \quad \forall \tilde{v} \in K, \end{aligned} \quad (9)$$

where

$$\tilde{\psi} = (\sigma, \psi_1, \dots, \psi_n), \quad \tilde{v} = (\sigma, v_1, \dots, v_n)$$

with the initial conditions

$$\tilde{\psi}(0, \bar{z}) = [\sigma, \psi_0(\bar{z})].$$

Assume that we have found $\psi(t, \bar{z})$. This condition corresponds to the relation

$$\min \int_{\Gamma} \int_0^T |\tilde{v} - \tilde{\psi}|^2 dt d\Gamma \rightarrow J_{\min} = J^*.$$

At $t = \tau$ ($0 \leq \tau \leq T$) perform a needle-shaped variation with the duration ε . As a result of the variation performed the value of the functional J (7) changes

$$\hat{J} = \int_{\Gamma} \int_0^T |\tilde{v} - \tilde{\psi}| dt d\Gamma > J_{\min}.$$

Write down the detailed result of the variation

$$\delta \tilde{v} = \tilde{v} - \tilde{\psi} = \varepsilon \left\{ [B(\gamma)\tilde{\psi}, \tilde{v} - \tilde{\psi}] + \phi(\tilde{v}) - \phi(\tilde{\psi}) - (\theta(\tilde{\psi}, \tilde{v}), \tilde{v} - \tilde{\psi}) - (f, (\tilde{v} - \tilde{\psi})) \right\} - (B(\gamma)\tilde{\psi}, \psi) + \phi(\tilde{\psi}) - (\theta(\tilde{\psi}, \tilde{\psi}), \tilde{\psi}) - (f, \tilde{\psi}) \Big|_{t=\tau}. \quad (10)$$

Express \tilde{v} through the variation and optimal function of the state

$$\tilde{v} = \tilde{\psi} + \delta \tilde{v}. \quad (11)$$

Substituting (11) into (9), obtain

$$\tilde{\psi} \in K : \left(m(\bar{z}) \frac{\partial \tilde{\psi}}{\partial t}, (\tilde{\psi} + \delta \tilde{v}) - \tilde{\psi} \right) = (B(\gamma)\tilde{\psi}, (\tilde{\psi} + \delta \tilde{v}) - \tilde{\psi}) + \phi(\tilde{\psi} + \delta \tilde{v}) - \phi(\tilde{\psi}) - (\theta(\tilde{\psi}, (\tilde{\psi} + \delta \tilde{v})), (\tilde{\psi} + \delta \tilde{v}) - \tilde{\psi}) - (f, (\tilde{\psi} + \delta \tilde{v}) - \tilde{\psi}) \quad \forall \tilde{v} \in K \quad (12)$$

For further transformations use the coordinate-wise analog (12)

$\tilde{\psi}_i \in K :$

$$\left(m(\bar{z}_i) \frac{\partial \tilde{\psi}_i}{\partial t}, (\tilde{\psi}_i + \delta \tilde{v}_i) - \tilde{\psi}_i \right) = (B(\gamma)\tilde{\psi}_i, (\tilde{\psi}_i + \delta \tilde{v}_i) - \tilde{\psi}_i) + \phi(\tilde{\psi}_i + \delta \tilde{v}_i) - \phi(\tilde{\psi}_i) - (\theta(\tilde{\psi}_i, (\tilde{\psi}_i + \delta \tilde{v}_i)), (\tilde{\psi}_i + \delta \tilde{v}_i) - \tilde{\psi}_i) - (f, (\tilde{\psi}_i + \delta \tilde{v}_i) - \tilde{\psi}_i) \quad \forall \tilde{v}_i \in K \quad i = 0, 1, \dots, n. \quad (13)$$

Expand (13) in Taylor series and restrict the consideration with the quantities of 1-th order of infinitesimality

$$m(z_i) \left(\frac{\partial \tilde{\psi}_i}{\partial t} + \frac{\partial \tilde{v}_i}{\partial t} \right) = (B(\gamma)\tilde{\psi}_i, \tilde{\psi}_i) + \phi(\tilde{\psi}_i) - (f, \tilde{\psi}_i) + \sum_{i=0}^n \frac{\partial [(B(\gamma)\tilde{\psi}_i, \tilde{\psi}_i) + \phi(\tilde{\psi}_i) - (f, \tilde{\psi}_i)]}{\partial \tilde{v}_i} \delta \tilde{v}_i, \quad i = 0, 1, \dots, n. \quad (14)$$

From (14) it follows that

$$m(z_i) \frac{\partial \tilde{v}_i}{\partial t} = \sum_{i=0}^n \frac{\partial [(B(\gamma)\tilde{\psi}_i, \tilde{\psi}_i) + \phi(\tilde{\psi}_i) - (f, \tilde{\psi}_i)]}{\partial \tilde{v}_i} \delta \tilde{v}_i, \quad i = 0, 1, \dots, n. \quad (15)$$

Now turn to $t = T$. Define a variation of the functional at $t = T$

$$\delta J_{t=T} = \hat{J} - J_{\min} > 0$$

or

$$-\delta J_{t=T} = -\delta \sigma_{Hb=f} \leq 0.$$

Introduce the variable $\tilde{p}(t, \bar{z})$ so that when $t = T$ this condition is satisfied

$$-\delta J_{t=T} = -\delta \sigma(T) = \langle \delta \tilde{v}, \tilde{p} \rangle_{t=T}. \quad (16)$$

Coordinate wise analog (16) is as follows

$$-\delta J_{t=T} = -\delta \sigma(T) = \langle \delta \tilde{v}_i, \tilde{p}_i \rangle_{t=T}, \quad i = 0, 1, \dots, n.$$

Since $\delta \sigma(T) > 0$, in order to satisfy this relation there should take place:

$$p^0(T, \bar{z}_i) = -1; \quad p_j(T, \bar{z}) = 0,$$

where $i = 0, 1, \dots, n; \quad j = 1, \dots, n$.

Thus, if the optimal solution is not found, then $-\delta J < 0$, and for the optimal solution $-\delta J = 0$ is valid, since the variation of functional must be zero for the optimal solution.

Associate a variable $\tilde{p}(t, \bar{z})$ to the dynamic equation of the process observed through trial function $v(t, \bar{z})$. Find a variable $\tilde{p}(t, \bar{z})$ which satisfies

$$\langle \delta \tilde{v}(t, \bar{z}), \tilde{p}(t, \bar{z}) \rangle = \langle \delta \tilde{v}(T, \bar{z}), \tilde{p}(T, \bar{z}) \rangle_{\tau+\varepsilon \leq t \leq T} = const.$$

Then we have

$$\frac{\partial}{\partial t} \langle \delta \tilde{v}(t, \bar{z}), \tilde{p}(t, \bar{z}) \rangle = \left\langle \frac{\partial \delta \tilde{v}(t, \bar{z})}{\partial t}, \tilde{p}(t, \bar{z}) \right\rangle + \left\langle \frac{\partial \tilde{p}(t, \bar{z})}{\partial t}, \delta \tilde{v}(t, \bar{z}) \right\rangle_{\tau+\varepsilon \leq t \leq T} = 0. \quad (17)$$

Coordinate wise analog (17) is

$$\sum_{i=0}^n \frac{\partial \delta \tilde{v}_i(t, \bar{z})}{\partial t} \tilde{p}_i(t, \bar{z}) + \sum_{i=0}^n \delta \tilde{v}_i(t, \bar{z}) \frac{\partial \tilde{p}_i(t, \bar{z})}{\partial t} = 0, \quad i = 0, 1, \dots, n. \quad (18)$$

Substitute in (18) the value of the derivative

$$\frac{\partial \delta \tilde{v}(t, \bar{z})}{\partial t} \text{ from (15)}$$

$$\begin{aligned}
 & m(z_i) \sum_{i=0}^n \tilde{p}_i \times \\
 & \times \sum_{i=0}^n \frac{\partial [(B(\gamma)\tilde{\psi}_p, \tilde{\psi}_i) + \phi(\tilde{\psi}_i) - (f, \tilde{\psi}_i)]}{\partial \tilde{v}_i} \delta \tilde{v}_i + \\
 & + \sum_{i=0}^n \delta \tilde{v}_i \frac{\partial \tilde{p}}{\partial \alpha} = 0, \\
 & i = 0, 1, \dots, n. \quad (19)
 \end{aligned}$$

Change the order of summation in (19)

$$\begin{aligned}
 & m(z_i) \sum_{i=0}^n \delta \tilde{v}_i + \\
 & + \left[\sum_{i=0}^n \tilde{p}_i \frac{\partial [(B(\gamma)\tilde{\psi}_p, \tilde{\psi}_i) + \phi(\tilde{\psi}_i) - (f, \tilde{\psi}_i)]}{\partial \tilde{v}_i} + \right. \\
 & \left. + \frac{\partial \tilde{p}}{\partial \alpha} \right] = 0, \quad i = 0, 1, \dots, n
 \end{aligned}$$

Finally get

$$\begin{aligned}
 & \frac{\partial \tilde{p}_i}{\partial \alpha} = \\
 & = - \sum_{i=0}^n \frac{\partial [(B(\gamma)\tilde{\psi}_p, \tilde{\psi}_i) + \phi(\tilde{\psi}_i) - (f, \tilde{\psi}_i)]}{\partial \tilde{v}_i} \tilde{p}_i, \\
 & i = 0, 1, \dots, n.
 \end{aligned}$$

Note that this equation is the dual of (5), and the variable $\tilde{p}(t, \bar{z})$ is expressed through the function of phase.

Again turn to the variation of functional (7) at $t = T$

$$-\delta J_{t=T} = \langle \delta \tilde{v}(t, \bar{z}), \tilde{p}(t, \bar{z}) \rangle_{t=T} = 0.$$

Replace the variation $\delta \tilde{v}$ with the value of (10), reduce by ε and, since τ can be arbitrary, obtain

$$\begin{aligned}
 & \langle ((B(\gamma)\tilde{\psi}, \tilde{v} - \tilde{\psi}) + \phi(\tilde{v}) - \phi(\tilde{\psi}) - \\
 & - (\theta(\tilde{\psi}, \tilde{v}), \tilde{v} - \tilde{\psi}) - (f, (\tilde{v} - \tilde{\psi}))), \tilde{p} \rangle_{t=\tau} - \\
 & - \langle ((B(\gamma)\tilde{\psi}, \tilde{\psi}) + \phi(\tilde{\psi}) - (f, \tilde{\psi})), \tilde{p} \rangle_{t=T} = 0. \quad (20)
 \end{aligned}$$

From (20) it follows that the second summand in it corresponds to the optimal solution of the variational inequality (5). In the case when the optimal solution $\psi(t, \bar{z})$ is found, variation of functional J will be zero, i.e. $\delta J = 0$. Given this, the first summand in (20), defined by the Hamiltonian function

$$\begin{aligned}
 \tilde{H} = & \langle ((B(\gamma)\tilde{\psi}, \tilde{v} - \tilde{\psi}) + \phi(\tilde{v}) - \phi(\tilde{\psi}) - \\
 & - (\theta(\tilde{\psi}, \tilde{v}), \tilde{v} - \tilde{\psi}) - (f, (\tilde{v} - \tilde{\psi}))), \tilde{p} \rangle, \quad (21)
 \end{aligned}$$

should take the maximum value. Thus, the above statement is proven. Let's show the possibility of determining the maximum value

of Hamiltonian function.

Coordinate wise analog (21) is defined by

$$\begin{aligned}
 \tilde{H} = & \langle ((B(\gamma)\tilde{\psi}_i, \tilde{v}_i - \tilde{\psi}_i) + \phi(\tilde{v}_i) - \phi(\tilde{\psi}_i) - \\
 & - (\theta(\tilde{\psi}_i, \tilde{v}_i), \tilde{v}_i - \tilde{\psi}_i) - (f, (\tilde{v}_i - \tilde{\psi}_i))), \tilde{p}_i \rangle, \\
 & i = 0, 1, \dots, n. \quad (22)
 \end{aligned}$$

To maximize the value of the function \tilde{H} , it's necessary to set all the partial derivatives of this function to zero by a testing variable $v(t, \bar{z})$, that taking into account (22) gives the system of equations

$$\frac{\partial \tilde{H}}{\partial v_i} = 0, \quad i = 0, 1, \dots, n. \quad (23)$$

Coordinate wise analog (22) contains $(n+1)$ of v_i functions, $(n+1)$ of θ_i functions and $(n+1)$ of p_i functions. Since the equations (23) are only $(n+1)$, and the unknown are $(3n+3)$, then the system (23) cannot be solved. To solve (23) define also the partial derivatives

$$\frac{\partial \tilde{H}}{\partial \theta_i} = \tilde{p}_i, \quad i = 0, 1, \dots, n. \quad (24)$$

$$\begin{aligned}
 \frac{\partial \tilde{H}}{\partial p_i} = & \left[m(\bar{z}_i) \frac{\partial \tilde{\psi}_i}{\partial \alpha}, \tilde{v}_i - \tilde{\psi}_i \right], \\
 & i = 0, 1, \dots, n. \quad (25)
 \end{aligned}$$

In this case, the solution of (23) can be obtained.

As a result of the reasoning done, the scheme of the algorithm for solving variational inequality (5) using the maximum principle can be represented as follows:

1. The dynamic equation (9), subject to the additional coordinate σ is written down.

2. An auxiliary function (Hamilton) \tilde{H} in accordance with the expression (22) is compiled.

3. A test function $v(t, \bar{z})$ that delivers maximum \tilde{H} functions in accordance with the expression (23) is determined. For the redefinition of the independent variables θ and p the system (23) is supplemented with equations (24) and (25).

4. The unknown variable $\psi(t, \bar{z})$ is determined by the test variable $v(t, \bar{z})$, which gives the maximum value of function \tilde{H} .

Conclusion. Thus, a method and an algorithm implementing it is proposed for

solving a class of variational inequalities, which are mathematical models of the above physical processes with a pronounced directional effect. The proposed method is based on the optimization procedure of the maximum principle. The choice of optimality criterion for solving the external problem is justified.



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Received 24.02.2012