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REPRESENTATION OF MATHEMATICAL MODELS OF NONLINEAR UNILATERAL TECHNOLOGICAL PROCESSES IN THE FORM OF VARIATIONAL INEQUALITIES AND OPTIMIZATION METHOD FOR NUMERICAL IMPLEMENTATION

Abstract. Mathematical models of a class of nonlinear unilateral technological processes in the form of varitional inequalities, which adequately reflects the essence of physical phenomena. The developed method numerical implementation of mathematical models. The method is based on finding the maximum of the function of Hamilton functions of the state space.

Keywords: Mathematical model, Variation, Variation inequality, Optimization, Principle of maximum, Functional

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ПРЕДСТАВЛЕНИЕ МАТЕМАТИЧЕСКИХ МОДЕЛЕЙ НЕЛИНЕЙНО-ОДНОСТОРОННИХ ТЕХНОЛОГИЧЕСКИХ ПРОЦЕССОВ В ВИДЕ ВАРИАЦИОННЫХ НЕРАВЕНСТВ И ОПТИМИЗАЦИОННЫЙ МЕТОД ИХ ЧИСЛЕННОЙ РЕАЛИЗАЦИИ

Аннотация. Предложены математические модели класса нелинейно-односторонних технологических процессов в виде вариационных неравенств, что адекватно отражает суть происходящих физических явлений. Разработан метод численной реализации предложенных математических моделей. Метод основан на поиске максимума функции Гамильтона от функций пространства состояний.

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

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ПРЕДСТАВЛЕННЯ МАТЕМАТИЧНИХ МОДЕЛЕЙ НЕЛІНІЙНО-ОДНОБІЧНИХ ТЕХНОЛОГІЧНИХ ПРОЦЕСІВ У ВИГЛЯДІ ВАРІАЦІЙНИХ НЕРІВНОСТЕЙ ТА ОПТИМІЗАЦІЙНИЙ МЕТОД ЇХ ЧИСЕЛЬНОЇ РЕАЛІЗАЦІЇ

Анотація. Запропоновано математичні моделі класу нелінійно-однобічних технологічних процесів у вигляді варіаційних нерівностей, що адекватно відбиває сутність перебігу фізичних явищ. Розроблено метод чисельної реалізації запропонованих математичних моделей. Метод трунтується на пошуку максимуму функції Гамільтона від функцій простору стану.

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

1. Introduction

Nonlinear one-way flow characteristic for a number of important technological processes, particularly, in the oil industry, construction and ecology. Examples of such processes include: filtration of gas-liquid mixtures (carbonated oil), impregnation foundation of hydraulic structures subsurface waters, the spread of harmful impurities in the air. These processes, in the special literature [1, 2], is called anomalous.

Analysis of physical phenomena characteristic for the class of physical processes with

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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 variation inequalities [1-4] as an adequate mathematic-cal description of these processes.

In this paper [5] we obtain and justify a generalized mathematical model (MM) to study a class of processes, which in terms of the theory of variation inequalities can be represented as follows.

2. Mathematical model of process and its transformation

Let the functional $\psi(t,\bar{z})$, defined on a bounded open set Ω of the space \Re^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 variation inequality

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

$$\psi(0, \overline{z}) = \psi_0(\overline{z}), \tag{2}$$

 $B(\gamma)$ – specifies a linear transformation $B(\gamma): H^1(\Omega) \to H^1(\Omega)$ and is defined by the bilinear form;

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

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.

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

(hereinafter, for simplicity, restrict ourselves to the tasks at the border Γ);

 $j(\cdot)$ – convex functional defining the kind of physical process in rheology and which are specified as follows

$$j(\cdot) = \int_{\Gamma} \varphi(\psi, \bar{z}) \cdot \lambda(\psi) \, d\Gamma,$$
$$j(\cdot) = \int_{\Omega} \varphi(\psi, \bar{z}) \cdot \lambda(\psi) \, d\Omega. \tag{4}$$

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 $\Delta \in L^{\infty}(\overline{Q})$, $\Lambda \in L^{\infty}(\overline{Q})$ where it is assumed that $\varphi(\cdot)$, $\lambda(\cdot) \in L^{\infty}(\overline{Q})$, $\overline{Q} = \overline{\Omega} \times (0, t_k)$ and the spaces Δ and Λ are

Banach with respect to the norm

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

The proposed method for solving variation 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 variation inequality (1), (2) there must exist a nonzero continuous function $p(t,\bar{z})$, so that at any time t in the interval $0 \le t \le T$ (T – time of physical processes) the Hamiltonian function \widetilde{H} in the spatial domain Ω (or on its boundary Γ) would take the maximum value, where

$$\begin{split} \widetilde{H} &= \left\langle \left(\left(B(\gamma) \widetilde{\psi}, \widetilde{v} - \widetilde{\psi} \right) + \phi(\widetilde{v}) - \phi(\widetilde{\psi}) - \left(\theta(\widetilde{\psi}, \widetilde{v}), \widetilde{v} - \widetilde{\psi} \right) - \left(f, \left(\widetilde{v} - \widetilde{\psi} \right) \right) \right), \widetilde{p} \right\rangle. \end{split}$$

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

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

and

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

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

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

Taking into account the executed transformations introduce the relations (1), (2) in the form

$$\psi \in K$$
:

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

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

3. Numerical method the implementation of mathematical models in the form of varitional inequalities

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

$$J = \min \int_{\Gamma} \int_{0}^{T} |v - \psi| dt d\Gamma.$$
 (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

$$\frac{\partial^2 \sigma}{\partial \partial z} = \left| v - \psi \right|^2 \bigg|_{z \in \Gamma}.$$
 (8)

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

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

$$\left(m(\overline{z})\frac{\partial\widetilde{\psi}}{\partial t},\widetilde{v}-\widetilde{\psi}\right)+\left(B(\gamma),\widetilde{v}-\widetilde{\psi}\right)+\phi(\widetilde{v})-\phi(\widetilde{\psi})-\left(\theta(\widetilde{\psi},\widetilde{v}),\widetilde{v}-\widetilde{\psi}\right)=\left(f,\widetilde{v}-\widetilde{\psi}\right)\quad\forall\widetilde{v}\in K,\quad(9)$$
where

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

with the initial conditions

$$\widetilde{\psi}(0,\overline{z}) = [0,\psi_0(\overline{z})].$$

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

$$\min \int_{\Gamma} \int_{0}^{T} |\widetilde{v} - \widetilde{\psi}|^{2} dt d\Gamma \to J_{\min} = J^{*}.$$

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

$$\hat{J} = \iint_{\Gamma} |\widetilde{v} - \widetilde{\psi}| dt d\Gamma > J_{\min}.$$

Write down the detailed result of the variation

$$\delta \widetilde{v} = \widetilde{v} - \widetilde{\psi} = \varepsilon \{ [(B(\gamma)\widetilde{\psi}, \widetilde{v} - \widetilde{\psi}) + \phi(\widetilde{v}) - \phi(\widetilde{\psi}) - (\theta(\widetilde{\psi}, \widetilde{v}), \widetilde{v} - \widetilde{\psi}) - (f, (\widetilde{v} - \widetilde{\psi}))] - (B(\gamma)\widetilde{\psi}, \psi) + \phi(\widetilde{\psi}) - (\theta(\widetilde{\psi}), \widetilde{\psi}) - (f, \widetilde{\psi}) \}_{t=\tau}.$$

$$(10)$$

Express \tilde{v} through the variation and

optimal function of the state

$$\widetilde{v} = \widetilde{\psi} + \delta \widetilde{v} . \tag{11}$$

Substituting (11) into (9), obtain

$$\widetilde{\psi} \in K : \left(m(\overline{z}) \frac{\partial \widetilde{\psi}}{\partial t}, (\widetilde{\psi} + \delta \widetilde{v}) - \widetilde{\psi} \right) =$$

$$= \left(B(\gamma) \widetilde{\psi}, (\widetilde{\psi} + \delta \widetilde{v}) - \widetilde{\psi} \right) + \phi(\widetilde{\psi} + \delta \widetilde{v}) - \phi(\widetilde{\psi}) -$$

$$- \left(\theta(\widetilde{\psi}, (\widetilde{\psi} + \delta \widetilde{v})), (\widetilde{\psi} + \delta \widetilde{v}) - \widetilde{\psi} \right) -$$

$$- \left(f, (\widetilde{\psi} + \delta \widetilde{v}) - \widetilde{\psi} \right) \quad \forall \widetilde{v} \in K$$
(12)

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

$$\widetilde{\psi}_{i} \in K: \qquad \left(m(\overline{z}_{i}) \frac{\partial \widetilde{\psi}_{i}}{\partial t}, (\widetilde{\psi}_{i} + \delta \widetilde{v}_{i}) - \widetilde{\psi}_{i} \right) =$$

$$= \left(B(\gamma) \widetilde{\psi}_{i}, (\widetilde{\psi}_{i} + \delta \widetilde{v}_{i}) - \widetilde{\psi}_{i} \right) + \phi(\widetilde{\psi}_{i} + \delta \widetilde{v}_{i}) - \phi(\widetilde{\psi}_{i}) -$$

$$- \left(\theta(\widetilde{\psi}_{i}, (\widetilde{\psi}_{i} + \delta \widetilde{v}_{i})), (\widetilde{\psi}_{i} + \delta \widetilde{v}_{i}) - \widetilde{\psi}_{i} \right) -$$

$$- \left(f, (\widetilde{\psi}_{i} + \delta \widetilde{v}_{i}) - \widetilde{\psi}_{i} \right) \quad \forall \widetilde{v}_{i} \in K$$

$$i = 0, 1, ..., n. \qquad (13)$$

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

$$m(z_{i})\left(\frac{\partial \widetilde{\psi}_{i}}{\partial t} + \frac{\partial \widetilde{v}_{i}}{\partial t}\right) = \left(B(\gamma)\widetilde{\psi}_{p}\widetilde{\psi}_{i}\right) + \\ + \phi(\widetilde{\psi}_{i}) - \left(f,\widetilde{\psi}_{i}\right) + \\ + \sum_{i=0}^{n} \frac{\partial \left[\left(B(\gamma)\widetilde{\psi}_{i},\widetilde{\psi}_{i}\right)_{i} + \phi(\widetilde{\psi}_{i}) - \left(f,\widetilde{\psi}_{i}\right)\right]}{\partial \widetilde{v}_{i}} \delta \widetilde{v}_{i},$$

$$i = 0, 1, ..., n. \tag{14}$$

From (14) it follows that

$$m(z_{i})\frac{\partial \widetilde{v}_{i}}{\partial t} = \sum_{i=0}^{n} \frac{\partial \left[\left(B(\gamma)\widetilde{\psi}_{p}\widetilde{\psi}_{i}\right) + \phi(\widetilde{\psi}_{i}) - \left(f,\widetilde{\psi}_{i}\right)\right]}{\partial \widetilde{v}_{i}} \partial \widetilde{v}_{i},$$

$$i = 0, 1, ..., n. \tag{15}$$

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

$$\delta J_{t=T} = \hat{J} - J_{\min} > 0 \quad \text{or}$$
$$-\delta J_{t=T} = -\delta \sigma_{H=I} \leq 0.$$

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

$$-\delta J_{t=T} = -\delta \,\sigma(T) = \left\langle \delta \widetilde{v}, \, \widetilde{p} \right\rangle_{t=T}. \tag{16}$$

Coordinate wise analog (16) is as follows

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

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

$$p^{0}(T, \bar{z}_{i}) = -1; p_{j}(T, \bar{z}) = 0,$$

where i = 0, 1, ..., n; j = 1, ..., 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 $\widetilde{p}(t,\overline{z})$ to the dynamic equation of the process observed through trial function $v(t,\overline{z})$. Find a variable $\widetilde{p}(t,\overline{z})$ which satisfies

$$\begin{split} &\left\langle \delta \widetilde{v}(t,\bar{z}), \widetilde{p}(t,\bar{z}) \right\rangle = \\ &= \left\langle \delta \widetilde{v}(T,\bar{z}), \widetilde{p}(T,\bar{z}) \right\rangle_{\tau+\varepsilon \leq t \leq T} = const \; . \end{split}$$

Then we have

$$\frac{\partial}{\partial z} \langle \delta \widetilde{v}(t, \overline{z}), \widetilde{p}(t, \overline{z}) \rangle = \left\langle \frac{\partial \delta \widetilde{v}(t, \overline{z})}{\partial z}, \widetilde{p}(t, \overline{z}) \right\rangle + \left\langle \frac{\partial v \widetilde{p}(t, \overline{z})}{\partial z}, \delta \widetilde{v}(t, \overline{z}) \right\rangle_{z + c \leq t \leq T} = 0.$$
(17)

Coordinatewise analog (17) is

$$\sum_{i=0}^{n} \frac{\partial \delta \widetilde{v}_{i}(t,\bar{z})}{\partial t}, \widetilde{p}_{i}(t,\bar{z}) +$$

$$+ \sum_{i=0}^{n} \delta \widetilde{v}_{i}(t,\bar{z}) \frac{\partial \widetilde{p}_{i}\widetilde{v}_{i}(t,\bar{z})}{\partial t} = 0,$$

$$i = 0, 1, ..., n.$$
(18)

Substitute in (18) the value of the derivative $\frac{\partial \delta \widetilde{v}(t,\bar{z})}{\partial t}$ from (15)

$$m(z_{i}) \sum_{i=0}^{n} \widetilde{p}_{i} \times \times \sum_{i=0}^{n} \frac{\partial \left[\left(B(\gamma) \widetilde{\psi}_{p} \widetilde{\psi}_{i} \right) + \phi(\widetilde{\psi}_{i}) - \left(f, \widetilde{\psi}_{i} \right) \right]}{\partial \widetilde{v}_{i}} \delta \widetilde{v}_{i} + \sum_{i=0}^{n} \delta \widetilde{v}_{i} \frac{\partial \widetilde{p}}{\partial t} = 0,$$

$$i = 0, 1, ..., n. \tag{19}$$

Change the order of summation in (19)

$$\begin{split} & m(z_{i}) \sum_{i=0}^{n} \delta \widetilde{v}_{i} + \\ & + \left[\sum_{i=0}^{n} \widetilde{p}_{i} \frac{\partial \left[\left(B(\gamma) \widetilde{\psi}_{p} \widetilde{\psi}_{i} \right) + \phi(\widetilde{\psi}_{i}) - \left(f, \widetilde{\psi}_{i} \right) \right]}{\partial \widetilde{v}_{i}} + \\ & + \frac{\partial \widetilde{p}_{i}}{\partial t} \right] = 0, \\ & i = 0, 1, ..., n \end{split}$$

Finally get

$$\frac{\partial \widetilde{p}_i}{\partial t} =$$

$$=-\sum_{i=0}^{n}\frac{\partial\left[\left(B(\gamma)\widetilde{\psi}_{i},\widetilde{\psi}_{i}\right)+\phi(\widetilde{\psi}_{i})-\left(f,\widetilde{\psi}_{i}\right)\right]}{\partial\widetilde{v}_{i}}\widetilde{p}_{i},$$

i = 0, 1, ..., n.

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

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

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

$$\langle ((B(\gamma)\widetilde{\psi},\widetilde{v}-\widetilde{\psi})+\phi(\widetilde{v})-\phi(\widetilde{\psi})-(\theta(\widetilde{\psi},\widetilde{v}),\widetilde{v}-\widetilde{\psi})-(f,(\widetilde{v}-\widetilde{\psi})),\widetilde{p}\rangle_{t=\tau}-(((B(\gamma)\widetilde{\psi},\widetilde{\psi})+\phi(\widetilde{\psi})-(f,\widetilde{\psi})),\widetilde{p}\rangle_{t=T}=0. (20)$$

From (20) it follows that the second summand in it corresponds to the optimal solution of the variation 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

$$\widetilde{H} = \langle ((B(\gamma)\widetilde{\psi}, \widetilde{v} - \widetilde{\psi}) + \phi(\widetilde{v}) - \phi(\widetilde{\psi}) - (\theta(\widetilde{\psi}, \widetilde{v}), \widetilde{v} - \widetilde{\psi}) - (f, (\widetilde{v} - \widetilde{\psi}))), \widetilde{p} \rangle,$$
(21)

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 $\widetilde{H} = \langle ((B(\gamma)\widetilde{\psi}_i, \widetilde{v}_i - \widetilde{\psi}_i) + \phi(\widetilde{v}_i) - \phi(\widetilde{\psi}_i) - (\theta(\widetilde{\psi}_i, \widetilde{v}_i), \widetilde{v}_i - \widetilde{\psi}_i) - (f, (\widetilde{v}_i - \widetilde{\psi}_i))), \widetilde{p}_i \rangle,$ $i = 0, 1, ..., n. \tag{22}$

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

$$\frac{\partial \widetilde{H}}{\partial v_i} = 0 , \quad i = 0, 1, ..., n .$$
 (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

$$\frac{\partial \widetilde{H}}{\partial \theta_{i}} = \widetilde{p}_{i},$$

$$i = 0,1,...,n. \qquad (24)$$

$$\frac{\partial \widetilde{H}}{\partial p_{i}} = \left[m(\overline{z}_{i}) \frac{\partial \widetilde{\psi}_{i}}{\partial t}, \widetilde{v}_{i} - \widetilde{\psi}_{i} \right],$$

$$i = 0,1,...,n. \qquad (25)$$

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

As a result of the reasoning done, the scheme of the algorithm for solving variation 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) \widetilde{H} in accordance with the expression (22) is compiled.
- 3. A test function $v(t, \overline{z})$ that delivers maximum \widetilde{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 functions \widetilde{H} .

4. Conclusion

Thus, a method and an algorithm implementing it is proposed for solving a class of variation 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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