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MATHEMATICAL MODELS OF TECHNOLOGICAL PROCESSES OF OIL REFINING AND THEIR QUALITATIVE ANALYSIS BASED ON THE GENERAL CONCEPT OF MODELS

Theorems of existence and uniqueness of the decision of system of the equations in the private derivatives, representing the generalized mathematical model of processes and devices of preprocessing of crude hydrocarbons are formulated and proved. Generalization gives the chance to apply the principle of unification and typification when developing a method of numerical realization of mathematical models of a class of processes (devices) of preprocessing of crude hydrocarbons, and the proof of the corresponding theorems (an essence — the qualitative analysis) provides a correctness of application of the generalized model in applied problems of mathematical modeling of studied processes (devices). Proofs of the formulated theorems are strict, logically true and are consistently executed within terms of the functional analysis. Practical applicability of theorems of existence and uniqueness of the decision as component of the qualitative analysis, is defined by possibility of research on their basis of adequacy of algorithmic means of mathematical modeling of a studied class of processes (devices).

Key words: *mathematical model, synthesis of the mathematical description, system of the equations in private derivatives, theorems of existence and uniqueness of the decision.*

1. Introduction. Solving the mathematical modeling problems are primarily and largely determined by the selected mathematical model (MM) of the object (or process). Adequately chosen MM provides the reliability of mathematical modeling. In addition, the results of mathematical modeling (in particular, its accuracy) is affected by numerical methods that implement the selected MM object (process). Therefore, the development of MM that meets the criteria, will improve the effectiveness of the workflow.

2. The research purpose and problem formulation. The purpose of this paper is to carry out a qualitative analysis (statement and proof of existence and uniqueness theorems) of generalized MM processes and apparatuses of primary processing of raw hydrocarbons presented in the form of a system of partial differential equations (PDEs).

To achieve this goal in this paper the problem of determining the conditions and scope of constraint region (CR) of PDE is solved with appropriate initial (IC) and the boundary conditions (BC), that is summarized formalizes the dynamics of a class of processes and machines of primary processing of crude hydrocarbons.

3. Main part. In modern industrial technologies during the initial processing of crude hydrocarbons (oil in particular) are applied processes such as desalination, dehydration and primary topping, with the first two processes are implemented under the scheme Built-in (thermal) desalting and dehydration [1]. By going on physico-chemical phenomena of technological devices that provide these processes can be categorized as follows:

- *surface* heat exchange machines in which heat exchange is performed at an interface specific reagents (phases). To this class of devices include, among others: recycling heat exchangers, heat exchangers of kerosene fraction, heat exchangers of diesel fraction, heat exchangers of weighted diesel fraction;
- *volumetric* heat exchange machines, in which heat exchange is performed within the total volume of the reactants involved. This class includes such devices: termodegidratory, electric dehydrators and mixers
- *dispersed* heat exchange machines, in which heat exchange is carried out on several individual surfaces. To this class of devices include, for example: column prior topping kerosene fraction, a column of the diesel fraction.

For each of the above classes of processes (devices) of primary processing of crude hydrocarbons (PPCH) MM developed in the form of a parabolic or hyperbolic PDE with the appropriate initial and boundary conditions [2, 3]. Analyzing MM considered an PPCH of devices has been identified the possibility of a generalized mathematical description that, in the future, involves unifying and typing approaches to computational and numerical implementation.

In this case, the generalized MM processes (machines) PPCH was formulated in the following way:

$$\frac{\partial \Phi(r,z,t)}{\partial t} = A\Phi(r,z,t) + f\ , \tag{1}$$

$$r, z \in \Omega \subset R^{M_k}\ ;\ t \in (0, t_k)\ ;\ \Phi(r,z,t) \le \Phi_{д}\ ;$$

$$\Phi(r,z,t)\Big|_{t=0} = \Phi_0(r,z),\ (r,z) \in \Omega\ ; \tag{2}$$

$$\Phi(r,z,t)\Big|_{\Sigma} = 0\ , \tag{3}$$

where $\Phi(r,z,t)$ — unknown function, for which the vector space coordinates $\bar{g} = \{r, z\}$ is defined on the open space Ω with the boundary Γ, which belongs to the space R^{M_k}. For fixed $t_k > 0$ shall consider the dynamics of the system (1)-(3) in a time interval $(0, t_k)$, which is a cylinder height $Q = \Omega \times (0, t_k)$ with the limit $\Sigma = \Gamma \times (0, t_k)$. The operator A — is hyperbolic (or parabolic-hyperbolic). If the statement A contains a parabolic component, we assume that the operator A can be unsymmetrical and time-invariant second order operator. The function f is the external excitation of the system.

As noted earlier, the study of technological devices PPCH processes are characterized by a complex mathematical formulation. Therefore, under these conditions, it is necessary to investigate the resulting generalized MM class of considered devices regarding to the inaccuracies of the methodological and computational nature. This kind of impropriety may arise in connection with a certain level of formalization, both on stage productions, as well as numerical solutions of the problem 4]. Considering the above, we carry out a qualitative analysis of the generalized MM processes (units) PPCH, the purpose of which is to investigate the existence and uniqueness of solutions of dynamical equations of the form (1) with initial and boundary conditions of the form (2), (3).

As noted above, the objectives of the study of technological devices MSRP processes are characterized by a complex mathematical formulation. Therefore, under these conditions, the resulting generalized MM class of devices considered is necessary to investigate regarding the inaccuracies of the methodological and computational nature. This kind of impropriety may arise in connection with a certain level of formalization, both on the stage of setting as well as the numerical solution of the problem [4]. Considering the above, we carry out a qualitative analysis of the generalized MM processes (units) MSRP, the purpose of which is to investigate the existence and uniqueness of solutions in dynamical equations of the form (1) with initial and boundary conditions of the form (2), (3).

In [5-7], we have investigated the existence, uniqueness and control systems similar to (1)-(3). However, these studies were performed without constraints on the phase coordinates and control variables, that is inherent in the physical processes that occur in devices MSRP [8]. In this regard, we formulate and prove the following theorem.

Theorem 1. For the system (1)-(3) are given functions Φ_0, Φ_d and f, where:

$$f \in L^2(Q)\,; \tag{4}$$

$$\Phi_0 \in H_0^1(\Omega) \cap L^p(\Omega), \quad p > 0\,; \tag{5}$$

$$\Phi_d \in L^2(Q)\,. \tag{6}$$

Then there is a function $\Phi = \Phi\left(\bar{g}, t\right)$, which satisfies the following conditions:

$$\Phi \in L^{\infty}\left(0, t_k; H_0^1(\Omega) \cap L^p(\Omega)\right), \tag{7}$$

$$\frac{\partial \Phi}{\partial t} \in L^{\infty}\left(0, t_k; H_0^1(\Omega) \cap L^p(\Omega)\right), \tag{8}$$

$$\Phi\left(\bar{g}, 0\right) = \Phi_0\left(\bar{g}\right), \tag{9}$$

$$\Phi\left(\bar{g}, t\right) \le \Phi_d . \tag{10}$$

In proving the theorem 1, we use the following sequence:

- Construct an «approximate» solutions;
- For the «approximate» solutions define a priori estimates;
- Go to the limit, based on the compactness property (this is necessary for the transition to the limit in nonlinear terms).

Proving of theorem 1.

1. *Construction of the «approximate» solutions.* To construct the «approximate» solutions use Faedo-Galerkin method [7, 8]. Consider a sequence $\varphi_1, \varphi_2, ..., \varphi_m$, which has the following properties:

$$\varphi_i \in H_0^1(\Omega) \cap L^p(\Omega), \quad \forall i, p > 0,$$

$\varphi_1, \varphi_2, ..., \varphi_m$ — linearly independent $\forall m$.

It is obvious that the linear combination $\varphi_i, \forall i > 0$ — are compact [9] in $H_0^1(\Omega) \cap L^p(\Omega)$. We look for «approximate» solutions $\Phi_m = \Phi_m(t)$, $\forall m = 1, 2, ...$ in the form of

$$\Phi_m(t) = \sum_{i=1}^{m} q_i(t) \varphi_i ,$$

where the functions $q_i(t)$ are selected so as to satisfy the relation

$$\left(\frac{d\Phi_m(t)}{\partial t}, \varphi_j \right) + a\left(\Phi_m(t), \varphi_j\right) = \left(f(t), \varphi_j\right), \quad 1 \le j \le m , \tag{11}$$

where $a\left(\Phi_m(t), \varphi_j\right) = \left\langle A\Phi_m(t), \varphi_j \right\rangle_{H_0^1(\Omega) \cap L^p(\Omega)}$.

The system (11) of non-linear ordinary differential equations is supplemented by initial and boundary conditions

$$\Phi_m(0) = \Phi_{0_m}; \ \Phi_{0_m} = \sum_{i=1}^{m} \alpha_{i_m} \varphi_i \to \Phi_0 \text{ в } H_0^1(\Omega) \cap L^p(\Omega), m \to \infty . \tag{12}$$

2. *Finding a priori estimates*. To do this, multiply each equation (11), which corresponds to an index j, on $q_i(t)$ and sum by j. Then we get

$$\left(\frac{d\Phi_m(t)}{dt},\ \Phi_m(t)\right)+a\left(\Phi_m(t),\Phi_m(t)\right)=\left(f(t),\Phi_m(t)\right),$$

i.e.

$$\frac{1}{2}\frac{d}{dt}\left|\Phi_m(t)\right|^2+a\left(\Phi_m(t),\Phi_m(t)\right)=\left(f(t),\Phi_m(t)\right). \qquad (13)$$

We set: $\|v\|=\sqrt{a(v,v)}$ (that is the norm in $H_0^1(\Omega)$ is equivalent to the norm $\|v\|_{H^1(\Omega)}$). According to (13) we write

$$\left(\left|\Phi_m(t)\right|^2+\left\|\Phi_m(t)\right\|^2\right)\le 2\alpha_m\left|\Phi_m(t)\right|^2+2\int_0^{t_k}\left|f(t),\Phi_m(t)\right|dt. \qquad (14)$$

From (12) it follows that the right-hand side of (14) does not exceed the $C+2\int_0^{t_k}\left|f(t),\Phi_m(t)\right|dt$ (the constant C doesn’t depend on m). Then we can write

$$\left(\left|\Phi_m(t)\right|^2+\left\|\Phi_m(t)\right\|^2\right)\le C+2\alpha_m\left|\Phi_{0_m}\right|^2+2\int_0^{t_k}\left|f(t),\Phi_m(t)\right|dt. \qquad (15)$$

Due to (14) we get $\int_0^{t_k}\left|f(t)\right|dt\le \text{const}$.

From (15) it follows that $\left|\Phi_m(t)\right|^2\le C+\left|\Phi_{o_m}\right|^2$.

The last expression implies that

$$\left|\Phi_m(t)\right|\le \text{const}, \qquad (16)$$

(where this constant doesn’t depend on m).

Returning to (15) we obtain

$$\left\|\Phi_m(t)\right\|\le \text{const}, \qquad (17)$$

(As in the previous case, to express (16) the given constant also depends on the index m).

It follows that $t_k=T$, and from inequalities(16) and (17) we get that for $m\to\infty$ the values Φ_m — are limited, that is, belong to a limited set in

$$L^\infty\left(0,t_k;H_0^1(\Omega)\cap L^p(\Omega)\right).$$

3. *Going to the limit.* In accordance with the Dunford-Pettis theorem [10], the space $L^\infty\left(0,t_k;H_0^1(\Omega)\cap L^p(\Omega)\right)$ (accordingly $L^\infty\left(0,t_k;L^2(\Omega)\right)$ is adjoin to $L^1\left(0,t_k;H_0^1(\Omega)\cap L^p(\Omega)\right)$ (and accordingly to

$L^1\left(0,t_k;L^2(\Omega)\right)$, and therefore, from sequence Φ_m possible to extract sequence Φ_μ, that

$$\Phi_\mu \to \Phi_d \text{ weakly in } L^\infty\left(0,t_k;H_0^1(\Omega)\cap L^p(\Omega)\right), \qquad (18)$$

that is

$$\int_0^{t_k}\left(\Phi_\mu(t),q(t)\right)dt \to \int_0^{t_k}\left(\Phi_m(t),q(t)\right)dt,\ \forall q\in L^1\left(0,t_k;H_0^1(\Omega)\cap L^p(\Omega)\right). \qquad (19)$$

Furthermore, from (16), in particular, follows, that values Φ_m are limited in, which implies that the sequence Φ_m belongs to a limited set in $H_0^1(\Omega)$.

However, known that enclosures $H_0^1(\Omega)$ in $L^2(\Omega)$ are compact (Rellich-Kondrashov theorem [7]). Thus, we can assume that the sequence Φ_μ, that is chosen from the sequence Φ_m, is satisfies condition $\Phi_\mu \to \Phi_d$ strong in $L^2(\Omega)$ and almost everywhere addition to (18) and (19).

We pass to limit (11) considering that $\mu = m$. Let j is fixed and $\mu > j$. Then, by (11) we have

$$\left(\frac{d\Phi_\mu(t)}{\partial t},\varphi_j\right)+a\left(\Phi_\mu(t),\varphi_j\right)=\left(f(t),\varphi_j\right),\quad 1\le j\le \mu, \qquad (20)$$

However, by (19)

$$a\left(\Phi_\mu,\varphi_j\right)\to a\left(\Phi_d,\varphi_j\right) \text{ weakly in } L^\infty(0,t_k)$$

and, thus

$$\left(\frac{d\Phi_\mu(t)}{dt},\varphi_j\right)\to\left(\frac{d\Phi_d}{dt},\varphi_j\right)\ \ D'(0,t_k).$$

From (20) we can obtain that

$$\left(\frac{d\Phi_d}{\partial t},\varphi_j\right)+a\left(\Phi_d,\varphi_j\right)=\left(f(t),\varphi_j\right),$$

And this is true for any fixed j. This, taking into account the density of the basis, this implies that

$$\left(\frac{d\Phi_d}{\partial t},\varphi\right)+a\left(\Phi_d,\varphi\right)=\left(f(t),\varphi\right),\ \forall\varphi\in H_0^1(\Omega)\cap L^p(\Omega).$$

As previously was assumed $\Phi(\bar{g},t)\le\Phi_d$, it can be concluded that the conditions of existence are obtained.

Thus, due to the proof of theorem 1 we obtain conditions for the existence of solutions of equation (1) with initial data (2) and boundary (3) conditions. It is not known whether these results provide a unique solution. Let us prove it. MM represent generalized as such (without losing nevertheless the loss of generality):

$$\frac{\partial\Phi(M,t)}{\partial t} = A\Phi(M,t) + f(M,t), \tag{21}$$

$$M \in \Omega \subset R^{M_k};\; t \in (0,t_k);\; \Phi(M,t) \le \Phi_{д};$$

$$\Phi(M,t)\Big|_{t=0} = \Phi_{0_M}, \quad M \in \Omega; \tag{22}$$

$$\Phi(M,t)\Big|_{\Sigma} = 0, \tag{23}$$

where M — randomly taken point, the coordinates of which satisfy the state vector of the system.

Then the following theorem is true.

Theorem 2. The problem's solution (21)-(23), which is continuous in the closed region Q with the boundary of Σ by variable $t \in (0,t_k)$, and, moreover, by the coordinates of the point M — is single.

Proof of theorem 2. Let us $\varphi_1(M,t)$ и $\varphi_2(M,t)$ — is the two solutions, which satisfy conditions of theorem 2, and $\varphi = \varphi_1 - \varphi_2$. Show that $\varphi(M,t) \equiv 0$ in region Q will satisfy the proof of an uniqueness of the solution (1)-(3).

For proof of theorem 2 we will use the first Green's formula [11] for function $\varphi = \varphi_1 - \varphi_2$. The result is (assuming that operator A — hyperbolic)

$$\begin{aligned} \int_Q \varphi A\varphi\, d\tau &= \int_Q (\varphi_1 - \varphi_2) A(\varphi_1 - \varphi_2)\, d\tau = \\ &= \int_Q \kappa\left[\nabla(\varphi_1 - \varphi_2)\right] d\tau - \int_Q \gamma(\varphi_1 - \varphi_2)\, d\tau + \int_\Sigma \kappa(\varphi_1 - \varphi_2)\frac{\partial(\varphi_1 - \varphi_2)}{\partial\eta} d\sigma, \end{aligned} \tag{24}$$

where functions $\kappa = \kappa(M) > 0$; $\gamma = \gamma(M) \ge 0$ are continuous in the region Q. For the problem of the form (21)-(23) Green's formula looks

$$\int_Q \varphi A\varphi\, d\tau = \int_Q \kappa\left[\nabla(\varphi_1 - \varphi_2)\right] d\tau - \int_Q \gamma(\varphi_1 - \varphi_2)\, d\tau. \tag{25}$$

Obviously that function $\varphi = \varphi_1 - \varphi_2$ is a solution of the homogeneous problem

$$\frac{\partial\Phi(M,t)}{\partial t} = A\Phi(M,t), \tag{26}$$

$$\Phi(M,t)\Big|_{t=0} = 0,\; \Phi(M,t)\Big|_{M=\Sigma} = 0. \tag{27}$$

Seeing $A\varphi = (\partial\varphi/\partial t)$, then from (25) we obtain

$$\int_Q \varphi \frac{\partial\varphi}{\partial t} d\tau = \int_Q \kappa(\nabla\varphi)\, d\tau - \int_Q \gamma(\nabla\varphi)\, d\tau . \qquad (28)$$

Integrating the identity (28) in the time variable t in the interval $(0, t_k)$ and using the identity $\varphi(M,0) = 0$, obtain

$$\int_Q \varphi(M,t_k)\, d\tau = \int_0^{t_k}\int_Q \kappa\left[\nabla\varphi(M,t_k)\right] d\tau\, dt - \int_0^{t_k}\int_Q \gamma\left[\nabla\varphi(M,t_k)\right] d\tau\, dt . \quad (29)$$

Since the right-hand side of (28) is nonpositive, and the left side — a non-negative, then

$$\int_Q \varphi(M,t_k)\, d\tau = 0 .$$

It follows the function $\varphi(M,t_k) \equiv 0$ for arbitrary $t_k > 0$. Thus, theorem 2 is proved.

4. Conclusion. For the class of processes and devices of primary processing of crude hydrocarbons, the generalized mathematical model in the form of partial differential equations, characterized by the presence of restrictions on the state functions and control variables. Given these characteristics of the generalized MM, the qualitative study is carried out, which resulted in the theorem proving the existence and uniqueness of solutions of equations defining the generalized MM.

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МАТЕМАТИЧНІ МОДЕЛІ ТЕХНОЛОГІЧНИХ ПРОЦЕСІВ НАФТОПЕРЕРОБКИ ТА ЇХ ЯКІСНИЙ АНАЛІЗ НА ОСНОВІ ЗАГАЛЬНОЇ КОНЦЕПЦІЇ МОДЕЛЕЙ

Сформульовано та доведено теореми існування та єдиності рішення системи рівнянь у приватних похідних, що представляють собою узагальнену математичну модель процесів та пристроїв попередньої обробки вуглеводневої сировини. Узагальнення дає можливість застосувати принцип уніфікації та типізації при розробці методу чисельної реалізації математичних моделей класу процесів (пристроїв) попередньої обробки вуглеводневої нафти та доведенні відповідних теорем (суть — якісний аналіз) забезпечує коректність застосування узагальненої моделі в прикладних задачах математичного моделювання досліджуваних процесів (пристроїв). Доведення сформульованих теорем є строгими, логічно вірними та послідовно виконуються в рамках функціонального аналізу. Практична застосовність теорем існування та єдиності рішення, як компонента якісного аналізу, визначається можливістю дослідження на їх основі адекватності алгоритмічних засобів математичного моделювання досліджуваного класу процесів (пристроїв).

Ключові слова: *математична модель, синтез математичного опису, система рівнянь у приватних похідних, теореми існування та єдиності рішення.*

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