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MODELING HEAT AND MASS EXCHANGE PROCESSES IN METAL-HYDRIDE INSTALLATIONS

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Hydrogen as an environmentally friendly energy carrier is increasingly used in various sectors of the economy of industrialized countries, primarily to improve the environmental situation. Regardless of the field of application, metal hydride installations are energy conversion facilities, which is why the development of the scientific and technical principles of their creation is a new scientific direction of industrial heat and power engineering. The paper considers the peculiarities of the heat and mass exchange process in a hydrogen-metal system, which takes place in metal-hydride installations. A mathematical model of non-stationary heat and mass exchange processes in metal hydride complex-design devices is proposed. The results of the calculation and theoretical research performed by the authors about the prospects of using modern metal hydride technologies are presented. On the basis of the calculation and theoretical research, the influence of the accuracy of setting the heat transfer factor on the dynamics of hydrogen desorption is analyzed. The main factors that influence the choice of the geometric dimensions of a metal hydride element are identified. One of the peculiarities of the model is its versatility, which makes it possible to use it in modeling various types of energy-converting metal-hydride installations, as well as optimizing the design and operating modes of the designed metal-hydride systems. The introduction of the proposed technological solutions for creating metal hydride equipment opens up prospects of creating a wide range of specialized energy conversion installations, which will increase the level of utilizing secondary energy resources at different industrial enterprises, create real prerequisites for reducing thermal pollution of the environment and be an important step towards the implementation of Ukraine's economic integration into the Pan-European system.

Keywords: energy conversion installations, heat and mass exchange processes, hydrogen, metal hydride, mathematical modeling.

Introduction

Attention to the use of hydrogen as an alternative fuel has existed for more than a decade. This is due to both the recent technological progress in the area under consideration and economic circumstances resulted from the high price of fossil energy resources and political aspects of the energy market formation. Not least, the prospects clean energy development are determined by the environmental pollution caused by combustion products and projected climate changes as a result of the greenhouse effect. Hydrogen energy will provide a higher and stable rate of economic development, reduce the threat of irreversible climate changes. The use of advanced metal-hydride technologies will significantly intensify the development of hydrogen energy. Metal-hydride devices, regardless of their application, are energy-transforming objects, which is why the development of the scientific and technical principles of their creation is a new scientific direction of modern heat and power engineering [1, 2]. In these devices, the main working unit is a metal hydride (MH), which plays the role of a power transforming element in which energy is consumed in the form of heat and then transformed into the potential energy of the compressed gas or partially into an energy-non-equilibrium hydrogen form.

Problem Formulation

When designing metal hydride devices, special attention is paid to the methods of mathematical modeling which make it possible to reduce material and time costs in comparison with various experimental researches. Based on the results of numerical experiments, it is possible to better understand the essence of physical processes occurring in devices, optimize designs and choose the best regime parameters. Due to the complexity of physico-chemical processes in metal hydride systems, the mathematical models describing the thermo-physical and hydraulic properties of the accumulating medium, kinetics of hydrogen sorption-desorption reactions, heat exchange

between the gas and solid phases have not yet been sufficiently studied. That is why the study of heat and mass exchange processes in the considered environments and creation of reliable mathematical models for their description are of paramount importance during the development of effective metal hydride systems.

Presentation of the Main Part of the Study

In the IPMash NASU, a mathematical model of the thermo-sorption interaction of hydrogen with a metal hydride has been developed, which is described by the equations of heat and mass transfer in the case of a viscous regime of hydrogen filtration through a metal hydride dispersion layer [3–7]. Unlike previously described, this model takes into account:

– convective transfer contribution to the total heat flow;

– equilibrium relations, which describe the connection between the pressure, temperature, and concentration of hydrogen in a metal hydride throughout the entire range of concentrations;

– chemical kinetics of sorption (desorption).

Such an approach corresponds to the real operational conditions of power transforming metal hydride systems. At this time, the model is implemented by a numerical method in the form of a Java program package in the Windows environment for IBM-PC-compatible personal computers [8–10].

The mathematical model of the process of heat and mass exchange in MH acquires the following form:

$$\frac{\partial T}{\partial \tau} = a\left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2}\right) + \frac{\beta c_{H_2}}{c\rho} J \frac{\partial T}{\partial r}; \qquad (1)$$

$$q_s \rho \frac{\partial \chi}{\partial \tau} = \lambda\left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2}\right) + \beta c_{H_2} J \frac{\partial T}{\partial r}; \qquad (2)$$

$$\chi(\Theta) = 2\ln\left(\frac{\Theta}{1-\Theta}\right) + \frac{\overline{H_1}(\Theta)}{RT}; \qquad (3)$$

$$\frac{1}{\xi R_{H_2}}\frac{\partial}{\partial \tau}\left(\frac{\Pi p}{T}\right) = \frac{Jp}{r} + p\frac{\partial J}{\partial r} + J\frac{\partial p}{\partial r} - \rho\frac{\partial \chi}{\partial \tau}; \qquad (4)$$

$$J = h\frac{\Pi^3}{\mu}\frac{p}{\xi R_{H_2} T}\frac{d_{ave}^2}{(1-\Pi)^2}\frac{\partial p}{\partial r}; \qquad (5)$$

$$\frac{d\chi}{d\tau} = A \cdot \frac{p(T,\chi)}{p_d(T,\chi) \cdot f_{sp} \cdot \Delta\tau \cdot \Delta\mu'}; \qquad (6)$$

$$\left(p + \frac{a}{v^2}\right)(v - b) = R_{H_2} T, \qquad (7)$$

where a – hydride thermal conductivity coefficient; β – correction factor; c_{H_2} – hydrogen heat capacity coefficient; c – hydride heat capacity coefficient; ρ – hydride density; J – hydrogen flow density; q_S – thermal effect of reaction of the thermo-chemical interaction of hydride with hydrogen; λ – thermal conductivity coefficient;

Θ – degree of filling the intermetallic metal hydride matrix with hydrogen atoms; $\overline{H_1}(\Theta)$ – concentration dependence of the partial molar enthalpy of interaction between hydrogen atoms; Π – metal hydride porosity; ξ – gas compressibility coefficient; h – filtration coefficient; d_{ave} – average hydride particle equivalent diameter; μ – viscosity dynamic coefficient; p_d – desorption pressure; f_{sp} – specific surface area; μ' – chemical potential; $A = \Delta G_0 + RT \ln p$ – complex value; ΔG_0 – Gibbs energy change; v – volume; a, b – virial coefficients.

The system of equations (1) – (7) is closed by the initial and boundary conditions of the third kind.

Performing heat engineering calculations of metal hydride systems involves not only the thermo-sorption, but also thermo-physical characteristics of the materials used. Available data on the thermo-physical properties of metal hydrides are fragmentary and do not take into account a number of factors essen-

tial for the processes of heat transfer during the interaction between a metal hydride and hydrogen. The absence of these data does not allow establishing the dependence of thermo-physical characteristics on the stage of the process in the real range of changes in the regime parameters, which introduces a significant error in the results of calculating the structure of metal hydride elements.

One of the most effective ways of identifying thermo-physical characteristics is the use of tools for inverse heat conduction problems, in particular, for determining the coefficients of effective heat conductivity of metal hydrides and its dependence on the parameters of the process of interaction with hydrogen [11]. The mathematical model of heat and mass exchange in a metal hydride in the nonlinear formulation is due to the dependence of the thermo-physical properties and structural characteristics of MG on the parameters of the thermo-sorption process.

Iterative Algorithm for Solving a System of Hydrogen-Metal Differential Equations

The above problem (1)–(7) is a boundary-value problem with the Stefan conditions at the boundary of the distribution of two metal hydride-hydrogen phases. In order to solve such a class of problems, there have been developed different numerical methods, which can be divided into two classes. The first one can include the methods that, in their network implementation, try to tune the grid one way or another in such a way that, for each time point, the grid model nodes pass along the boundary of phase distribution. Such methods are well-suited to solving one-dimensional problems. For two- and three-dimensional problems, the algorithms based on the reconstruction of grids in accordance with the limit of the distribution of two phases, in terms of conducting a computing experiment, are rather labor-intensive. The second class of problems includes such methods, which by means of certain transformations; replace a boundary-value problem with the Stefan conditions at the boundary of the distribution of two phases by a boundary-value problem with the coefficients taking into account the heat flux jump at the boundary of phase distribution [12, 13]. Using such an approach, the boundary-value problem can be rewritten in this form with the limiting and initial conditions of the third kind:

$$\left(c_{\mathrm{h}}\rho_{\mathrm{h}} + q_S\rho_{\mathrm{r}}\chi_0\delta\!\left(T - T^*\right)\right)\frac{\partial T}{\partial \tau} =$$

$$= div\left(\lambda \cdot \mathrm{grad}\; T\right) + \beta h\frac{d_{\mathrm{ave}}^{\;2}}{\xi R_{\mathrm{H}_2}}c_{\mathrm{H}_2}\frac{\Pi^3}{(1-\Pi)^2}\frac{p}{\mu T}\left\langle \mathrm{grad}\; p, \mathrm{grad}\; T\right\rangle$$

$$\frac{1}{\xi \cdot R_{\mathrm{H}_2}}\frac{\partial}{\partial \tau}\!\left(\frac{\Pi p}{T}\right) + \rho_{\mathrm{h}}\chi_0\delta\!\left(p - p^*\right)\frac{\partial p}{\partial \tau} = h\frac{d_{\mathrm{ave}}^{\;2}}{\xi \cdot R_{\mathrm{H}_2}}div\!\left(\frac{\Pi^3}{(1-\Pi)^2}\frac{p}{\mu T}\mathrm{grad}\; p\right), \qquad (8)$$

where $\delta\!\left(T - T^*\right)$ and $\delta\!\left(p - p^*\right)$ is the Dirac delta function; T^* and p^* are desorption temperature and pressure.

It is to be immediately noted that under such an approach the condition of connecting two phases at the contact boundary is taken into account. Thus, in [13] it is stated that during a numerical implementation, it is impossible to use the Dirac function as it is defined. Therefore, in the case of the numerical implementation of this approach, the smoothing of Dirac's functions is performed by different methods [12, 13].

For the numerical realization of the solution to a system of two nonlinear parabolic partial differential equations we apply an implicit difference scheme for the time coordinate. Then the system of two nonlinear parabolic partial differential equations can be written as a sequence of the systems of two nonlinear stationary partial differential equations

$$\left(c_{\mathrm{h}}\rho_{\mathrm{h}} + q_S\rho_{\mathrm{h}}\chi_0\delta\!\left(T_i - T^*\right)\right)\frac{T_i - T_{i-1}}{\Delta \tau} =$$

$$= div\left(\lambda \cdot \mathrm{grad}\; T_i\right) + \beta h\frac{d_{\mathrm{ave}}^{\;2}}{\xi R_{\mathrm{H}_2}}c_{\mathrm{H}_2}\frac{\Pi^3}{(1-\Pi)^2}\frac{p_i}{\mu T_i}\left\langle \mathrm{grad}\; p_i, \mathrm{grad}\; T_i\right\rangle$$

$$\left(\frac{1}{\xi \cdot R_{\mathrm{H}_2}}\frac{\Pi}{T_i} + \rho_{\mathrm{h}}\chi_0\delta\!\left(p_i - p^*\right)\right)\frac{(p_i - p_{i-1})}{\Delta \tau} = h\frac{d_{\mathrm{ave}}^{\;2}}{\xi \cdot R_{\mathrm{H}_2}}div\!\left(\frac{\Pi^3}{(1-\Pi)^2}\frac{p_i}{\mu T_i}\cdot \mathrm{grad}\; p_i\right), \qquad (9)$$

where T_{i-1} and p_{i-1} is the solution from the previous temporary layer; $\Delta\tau$ is the time step.

To solve a system of two stationary nonlinear equations at each time step, we linearize the system as follows:

$$\left(c_{\mathrm{h}}\rho_{\mathrm{h}} + q_S\rho_{\mathrm{h}}\chi_0\delta\left(T_{i,j-1} - T^*\right)\right)\frac{T_{i,j} - T_{i-1}}{\Delta\tau} =$$

$$= div\left(\lambda \cdot \mathrm{grad}\ T_{i,j}\right) + \beta h\frac{d_{\mathrm{ave}}^{\ 2}}{\xi R_{\mathrm{H}_2}}c_{\mathrm{H}_2}\frac{\Pi^3}{(1-\Pi)^2}\frac{p_i}{\mu T_{i,j-1}}\left\langle \mathrm{grad}\ p_{i,j-1}, \mathrm{grad}\ T_{i,j-1}\right\rangle$$

$$\left(\frac{1}{\xi \cdot R_{\mathrm{H}_2}}\frac{\Pi}{T_i} + \rho_{\mathrm{h}}\chi_0\delta\left(p_{i,j-1} - p^*\right)\right)\frac{\left(p_{i,j} - p_{i-1}\right)}{\Delta\tau} = h\frac{d_{\mathrm{ave}}^{\ 2}}{\xi \cdot R_{\mathrm{H}_2}}div\left(\frac{\Pi^3}{(1-\Pi)^2}\frac{p_{i,j-1}}{\mu T_{i,j-1}} \cdot \mathrm{grad}\ p_{i,j}\right), \qquad (10)$$

where $T_{i,j-1}$ and $p_{i,j-1}$ is the solution obtained in the previous iteration; $T_{i,j}$ and $p_{i,j}$ is the solution at the current iteration for each time step.

To start the iteration process in the first stage, for a certain time coordinate, and as an initial approximation, the solution from the previous time step is selected. To obtain the spatial dependence of the desired functions for each linear equation the finite element method can be applied [14]. The iterative process continues until the relative errors for the functions $T_{i,j}$ and $p_{i,j}$ become not less than ε_T and ε_p, respectively.

Numerical Experiment

Using a mathematical model of the thermo-sorbent interaction of a metal hydride with hydrogen, the calculation results have been compared with the experimental data on the process of hydrogen desorption for the $LaNi_5H_x$ MG. The numerical experiment was conducted under the following conditions: the construction of the small-sized generator-sorber (SSGS) having length L=0.15 m and an internal diameter d_{in}=0.04 m is equipped with a heat transfer matrix, which is constructed from copper finning plates with a thickness of δ=1.0·10⁻⁴ m. One finning plate package consists of 74 finning plates spaced by a distance of l=5.0·10⁻³ m between them. To thermally influence the SSGS metal-hydride by the heat-carrier flow, which washes its external surface, there is used a steel thin-walled tube, which forms a channel with the SSGS external surface. The thickness of the ring channel for the heat-carrier is 5.0·10⁻⁴ m. The flow of the heat-carrier which washes the outer SSGS surface has a temperature of 338 K, the initial temperature of the MG layer T_0=284 K, the initial hydrogen pressure p_1=0.1 MPa, the hydrogen desorption pressure p_2=0.36 MPa, the hot water flow rate G_{hw}=0.017 kg/s. The bulk density of the MG $LaNi_5H_x$ layer is ρ 3810 kg/m³ [15].

When solving heat and mass transfer problems in a metal hydride, an important fact is the correct setting of boundary conditions. Under the boundary conditions of the third kind which determine the law of free heat exchange with the environment at the boundaries of the reactor at any time, an important value is the heat transfer factor. Since the experiment conditions contained no heat transfer factor, according to [16], for the selected SSGS design, the value α was 3337 W/m²·K, which corresponds to the value of the Nusselt number for the laminar flow for a flat slit that is heated on one side.

Fig. 1 shows the estimated and experimental dependences of the mass flow M on the time τ [15].

The most intense reaction occurs in the range of 0–80 s. This is due to the property of hydrides to absorb and produce the initial portions of hydrogen at increased speeds. With the decrease in the temperature gradient near the reaction zone as it moves away from the heating surface, the hydrogen dynamics decreases. The desorbed hydrogen mass flow rate deviation obtained as a result of the calculation and experiment did not exceed 4%.

The correspondence of the developed mathematical model to the real nature of the investigated phenomenon allowed us to consider it as a very effective tool for analyzing the influence of various factors
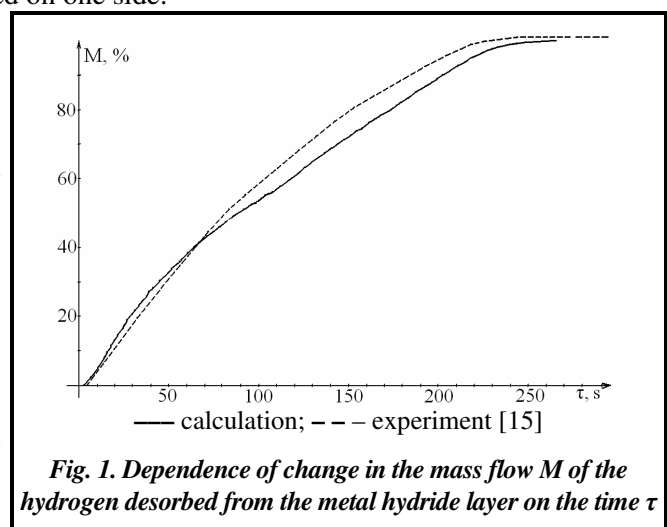

—— calculation; – – – experiment [15]

Fig. 1. Dependence of change in the mass flow M of the hydrogen desorbed from the metal hydride layer on the time τ

on the dynamics of hydrogen desorbed from the metal hydride layer.

With the help of a mathematical model, a research was carried out and it was determined how correct the heat transfer factor should be set when solving heat and mass transfer problems.

Fig. 2 shows the estimated dependences of the mass flow M of the hydrogen desorbed from the MG layer on the heat transfer factor. The values of the heat transfer factor were 3,337; 700; 500; 400 W/(m^2·K).

As can be seen from the figure, the heat transfer factor decreases as the time of hydrogen emission from the MG layer significantly increases. Calculations have shown that in the case of a decrease of α by 15%, the duration of the process increases by 35%. Consequently, it can be concluded that with the intense constant supply of heat to the heating surface there is a pronounced effect of the heat transfer factor on the rate of hydrogen emission from the MG layer.

The influence of the coolant temperature on hydrogen generation was investigated in Fig. 3.

When constructing metal hydride systems with a given metal hydride type, whose choice is due to thermo-sorption characteristics, it is necessary to strive to reduce the duration of hydrogen sorption-desorption cycles. This can be done by increasing the thermal loads realized in metal hydride elements, which is achieved by increasing the specific area of the heat transfer surface, per unit mass of a metal hydride.

For the above-described experimental conditions Fig. 4 shows contours of the thermal front advancement in the process of hydrogen desorption in the LaNi$_5$H$_x$ metal hydride layer. The contours are given for the time of 60, 90, 120, 150, 180, and 210 s.

1 − α=3,337 W/(m^2·K); 2 − α=700 W/(m^2·K); 3 − α=500 W/(m^2·K); 4 − α=400 W/(m^2·K)

Fig. 2. Dependence of change in the mass flow M of the hydrogen desorbed from the metal hydride layer on the heat transfer factor

1 − 353 K; 2 − 338 K; 3 − 323 K

Fig. 3. Dependence of change in the mass flow M of the hydrogen desorbed from the metal hydride layer at α=3,337 W/(m^2·K) from the coolant temperature

Fig. 4 illustrates the zonal nature of the phase transition in a metal hydride layer. Heat transfer by conduction in a metal hydride is carried out through the solid phase by the collision zones of the metal hydride particles and thermal conductivity in the gas pores filled with hydrogen. The distribution of heat due to hydrogen filtration by gas cavities obeys the laws of convective heat transfer taking into account the characteristics of gas dynamics due to the fine-dispersed structure and zone-by-zone mass exchange between the solid and gaseous phases. The zone width increases as it moves away from both the heating surface and finning plate.

The height of the finning plate, as well as the plate frequency, mainly affects the thermal front advancement in a MG. The heat enters the finning plates both from the heating surface and side surfaces of the depleted zones of the MG layer. But if one goes by increasing the length of the process proceeding from the thermal inertia of the MG layer, then, in addition to reducing productivity, it will lead to a reduction in efficiency due to the heat losses resultant from the overheating of the MG layers located near the heating surface.

The most significant influence on the dynamics of hydrogen production is exerted by the internal thermal and hydraulic metal hydride supports, which imposes restrictions on the geometric dimensions of a metal hydride element at the consumption characteristics of the system. Therefore, the height of the metal hydride layer should
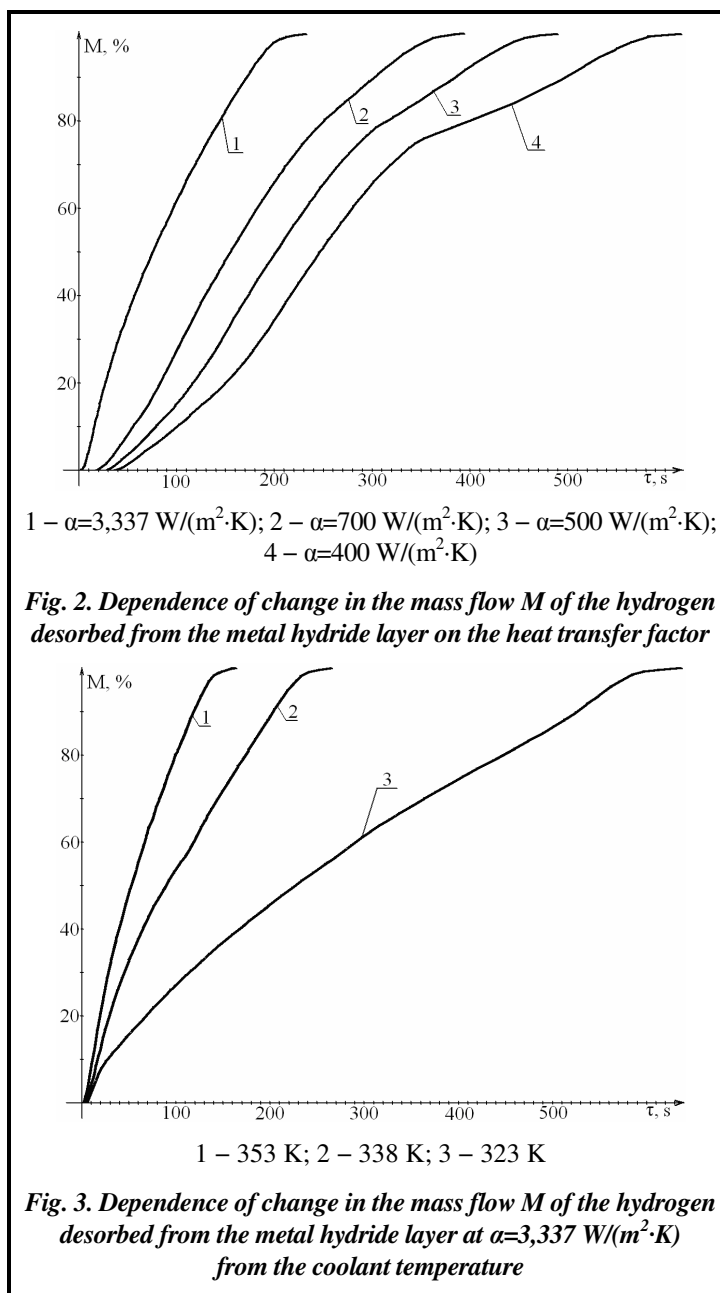
be selected based on the conditions for minimizing the energy losses caused by the overheating of the MG layer zones near the heating surface, as well as by optimizing the mass ratio of the metal structure to the hydride mass.

Conclusions

A mathematical model of non-stationary heat and mass exchange processes in relation to complex-design metal hydride devices has been developed. The influence of the heat transfer factor determination accuracy on the dynamics of hydrogen desorption is analyzed on the basis of a calculation-theoretical study. The main factors influencing the choice of the geometric sizes of a metal hydride element are highlighted. The presented mathematical model of the porous medium and software for its implementation can be further used to optimize the design and operating modes of the projected metal hydride devices in hydrogen transportation, storage and energy technology processing systems.

Fig. 4. Contours of the thermal front advancement in the process of hydrogen desorption in the $LaNi_5H_x$ metal hydrid layer

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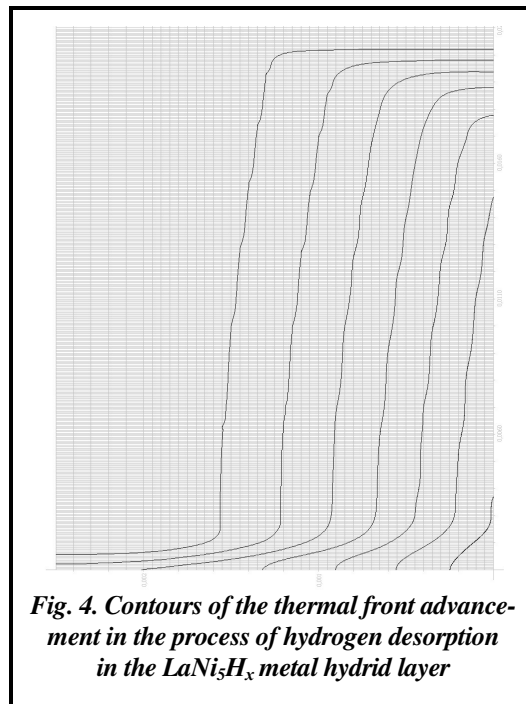
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Моделювання тепломасообмінних процесів у металогідридних установках

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Водень як екологічно чистий енергоносій знаходить все більш широке використання в різних сферах економіки індустріально розвинених краïн, в першу чергу, для поліпшення екологічної ситуації. Металогідридні установки незалежно від області застосування є енергоперетворювальними об'єктами, тому розробка науково-технічних принципів їх утворювання – новий науковий напрям промислової теплоенергетики. У роботі розглянуто особливості процесу тепломасообміну в системі «водень-метал», що протікає в металогідридних установках. Запропоновано математичну модель нестаціонарних процесів тепломасообміну стосовно металогідридних пристроїв складної конструкції. Наведено результати розрахунково-теоретичних досліджень, виконаних авторами щодо перспектив застосування сучасних металогідридних технологій. На підставі розрахунково-теоретичного дослідження проаналізований вплив точності задання коефіцієнта тепловіддачі на динаміку десорбції водню. Виділені основні чинники, що впливають на вибір геометричних розмірів металогідридного елемента. Особливістю моделі є її універсальність, що дає можливість застосування ïï під час моделювання різних типів енергоперетворювальних металогідридних установок, оптимізації конструкції та режимів роботи проектованих металогідридних пристроïв. Впровадження запропонованих технологічних рішень зі створення металогідридного устаткування відкриє перспективи широкого кола спеціалізованих енергоперетворювальних установок. Це дозволить підвищити рівень використання вторинних енергетичних ресурсів на підприємствах різних галузей, створить реальні передумови для зменшення теплового забруднення навколишнього середовища й буде важливим кроком на шляху реалізації програми інтеграції економіки України в єдину загальноєвропейську систему.

Ключові слова: енергоперетворювальні установки, тепломасообмінні процеси, водень, металогідрид, математичне моделювання.

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UDC 621.438-029.51

PECULIARITIES OF IDENTIFYING A POWER-GENERATING SINGLE-SHAFT GTE MATHEMATICAL MODEL

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The processes of designing and developing gas turbine engines (GTE) are based on using mathematical models (MM), reflecting the physical picture of engine operation processes. One of the ways of improving the MM validity is its identification on engine bench test results. Iden-tifying MMs of modern energy GTEs is a very demanding task due to the necessity to identify the main controllable engine parameters determined in the course of experimental studies, depending on a large number of the parameters that are not controlled during the experiment. In this regard, the actual direction of reducing the complexity of the process of identifying MMs is using identification software systems. Developed by the A. N. Podgorny Institute of Mechanical Engineering Problems of NASU, the methodology and means of identifying the parameters and characteristics of power plants, using experimental data (Otpimum software package), allows one to conduct a directed search for an optimal solution based on modern mathematical methods. This, in turn, leads to a reduction in identification execution time, in-creases the MM adequacy and allows one to more reliably determine the characteristics of engine components. The article proposes an approach to identifying a non-linear unit MM, with a detailed calculation of a turbine flow path to the level of blade rows on the D045 engine bench test results. It describes the choice of variable and controllable parameters as well as the ranges of their changes. The results of solving the identification problem showed the possi-bility of using the Optimum software for optimizing and identifying parameters and character-istics of power plants when identifying D045 GTE MMs. The use of the developed methodol-ogy for identifying GTE MMs that is based on bench test results, allows one to take into ac-count the maximum number of variable variables and significantly reduce the complexity and time of this process. The analysis of the results shows that with significant deviations of GTE characteristics from design values, a large amount of a priori information is needed to solve the identification problem. On the basis of the information, ranges of changes of variable and controllable parameters are assigned, as well as their values in the first approximation.

Keywords: mathematical model, identification, gas turbine engine, variable parameters, con-trollable parameters, objective function.