

UDC 661.961; 861.968

DOI: 10.15587/1729-4061.2017.112200

*Одержано математичний опис процесів генерації водню у вигляді системи диференціальних рівнянь та вираз для передаточної функції генератора. За допомогою логарифмічних частотних характеристик генератора водню ідентифікована наближена математична модель генератора у вигляді амплітудно-частотної характеристики. Запропонований алгоритм контролю технічного стану генератора водню із використанням його наближеного математичного опису*

*Ключові слова: генератор водню, газогенератор, технічний стан, частотні характеристики, алгоритм контролю*

*Получено математическое описание процессов генерации водорода в виде системы дифференциальных уравнений и выражение для передаточной функции генератора. С помощью логарифмических частотных характеристик генератора водорода идентифицирована приближенная математическая модель генератора в виде амплитудно-частотной характеристики. Предложен алгоритм контроля технического состояния генератора водорода с использованием его приближенного математического описания*

*Ключевые слова: генератор водорода, газогенератор, техническое состояние, частотные характеристики, алгоритм контроля*

# DESIGN OF CONTROL ALGORITHM OVER TECHNICAL CONDITION OF HYDROGEN GENERATORS BASED ON HYDRO-REACTIVE COMPOSITIONS

**Yu. Abramov**

Doctor of Technical Sciences,  
Professor, Chief Researcher  
Research Center\*\*

**V. Borisenko**

PhD, Associate Professor\*

**V. Krivtsova**

Doctor of Technical Sciences, Professor\*

E-mail: basmanov@ukr.net

\*Department of Physical and  
Mathematical Disciplines\*\*

\*\*National University of Civil Protection of Ukraine  
Chernyshevska str., 94, Kharkiv, Ukraine, 61023

## 1. Introduction

One of the promising directions when creating high-efficiency power plants is to employ hydrogen as their working body [1]. Requirements to maximum autonomy and long-lasting operation of such systems at their minimal dimensions necessitated the use of systems for hydrogen storage in the chemically bound state. The main element in the systems for hydrogen storage and supply in the bound state is a hydrogen generator. Technical condition of the hydrogen generator in such systems largely determines the level of safety during operation of power plants in general. A set of experimental studies conducted, for example, at a rocket propulsion system bench [2], shows the relevance of ensuring their safe operating conditions.

With a view to the safe operation of power plants using hydrogen, such parameters and characteristics must be put in place that ensure serviceable technical condition of all their elements [3]. Guaranteed provision of technical specifications of one of the basic elements in the system of hydrogen storage and supply can be achieved through the implementation of appropriate control algorithm over its technical condition.

## 2. Literature review and problem statement

The processes of hydrogen generation in the storage and supply systems have been rather well examined. The main results of these studies are outlined in [4]. This paper, however, considers only conceptual issues on the benefits of utilizing hydrogen in energy systems. Quantitative indicators of such systems are given in the integral form only. Article [5] presents data on that it is very promising to apply methods of obtaining hydrogen from substances, in which it is in the chemically bound state, for the thermal elements of portable devices. By using a technology for obtaining H<sub>2</sub> from water employing Al modified with ceramic oxides as an example, it is shown that the side products of the reaction are chemically neutral while the yield of hydrogen may reach (3.7–4.8 %). The data presented are, however, the result of laboratory studies while control over hydrogen generation parameters is implemented with receiving indirect redundant information. This information is applied for the further study into hydrogen generation processes and is not used to solve the tasks on monitoring and diagnosis.

Paper [6] reports results of determining only certain thermodynamic characteristics of the hydrogen sorption

processes (constants of reaction rate, the activation energy, etc.). It lacks data that describe dynamic properties of such systems. Article [7] described the models of processes occurring in hybrid systems using isothermal charts. Such a description gives rise to quite serious obstacles for designing algorithms to control and diagnose these systems. These obstacles arise from the need to apply algorithms of informal logic, which leads to complexities in hardware and software support for control and diagnosis systems.

A special feature of hydrogen production using hydro-reactive formulations is the presence of hydrolysis reaction. This reaction is characterized by a pressure change in the cavity of a hydrogen generator in the range of (1–70) MPa [4]. Paper [8] pointed to the fact that the process of obtaining hydrogen by the hydrolysis can yield large amounts of heat (up to 15 MJ/kg). Such a mode of operation may predetermine potential emergencies [9]. In [10], attention is drawn to the fact that despite the use of hydrogen in transportation, the necessary infrastructure to ensure its efficient utilization is missing. Specifically, monitoring and diagnosis of equipment for hydrogen generation are trivial.

Authors of these papers, in order to ensure safe operation of systems and their elements, apply pressure monitoring sensors [4], temperature sensors [8], as well as hydrogen concentration sensors [9]. The industrial designs of hydrogen generators usually execute control over one or two parameters [11]. These sensors typically possess relay static characteristics with a preset implementation of control algorithms of the trivial type based on the principle “pass-no pass”. In doing so, such parameters are controlled that characterize local properties of hydrogen generators. Paper [12] showed that the automation and control over technical condition of complex technical systems make it possible to improve their technical readiness factor. However, there is no algorithm for solving this problem in the paper. In this regard, one of the challenges in ensuring the safe operation of power plants using hydrogen is such organization of technical inspection, which is based on the use of its integral properties. Characteristics that describe integral properties of power plants and their elements include frequency characteristics.

### 3. The aim and objectives of the study

The aim of present work is the design of control algorithm for technical inspection of the hydrogen generator taking into consideration its dynamic properties.

To achieve the set aim, the following tasks have to be solved:

- on the laws of preservation of mass and energy, to obtain a mathematical description of processes of hydrogen generation in the form of a system of differential equations;
- by using a transfer function of the hydrogen generator, to construct a model of hydrogen generator in frequency domain;
- to identify a simplified model of the generator in frequency domain and its parameters;
- by taking into consideration the approximated mathematical description of the hydrogen generator, to estimate its reaction to test-impacts in the form of impulse and harmonic changes in the area of its outlet, and to justify a criterion for determining its technical condition.

### 4. Design of control algorithm over a technical condition of the hydrogen generator

In order to describe an operation mode of the hydrogen generator, it is possible to employ a method of the so-called “zero-dimensional” ballistics, which is based on the hypothesis on using the generator characteristics averaged by volume [4].

In this case, for a quasi-constant composition of the gas generation reaction products, in accordance with the laws of preservation of mass and energy, it is possible to write in the first approximation

$$V \frac{dP}{dt} = kRT_* \chi S \rho U - k \sqrt{RT_*} \mu A_k P F; \quad (1)$$

$$\rho V \frac{dT}{dt} = (k \chi T_* - T) \rho S U - (k-1) \mu A_k P F \frac{T}{\sqrt{RT_*}},$$

where  $P$  and  $T$  are, respectively, pressure and temperature of the gaseous phase in the generator, averaged by volume;  $U$  is the rate of gas generation, averaged by volume;  $V$  is the free volume of cavity of the gas generator;  $k$  is the adiabatic index;  $R$  is the gas constant;  $T_*$  is the average temperature in the reaction zone at the inter-phase boundary;  $\chi$  is the heat loss coefficient, average by volume and time, in a cavity of the gas generator;  $S$  is the surface area of gas release;  $\mu$  is the coefficient of flow rate through the outlet;  $F$  is the outlet's cross-sectional area;  $\rho$  is the density of the gas generated;  $A_k$  is the function of isentropic index

$$A_k = \sqrt{k} \left( \frac{2}{k+1} \right)^{\frac{k+1}{2(k-1)}}.$$

To close the system of equations (1), it must be supplemented with a gas state equation in average magnitudes, that is,

$$P = \rho R T, \quad (2)$$

as well as with the equation that describes the law of gas release and which takes, for example, the following form:

$$U = c_0 + c_1 P + c_2 P^2, \quad (3)$$

where  $c_i, i = \overline{0,2}$  are the constants.

We shall linearize the system of equations (1) by expanding into a Taylor series of relatively small deviations:

$$\Delta P = \frac{\delta P}{P_0}; \quad \Delta U = \frac{\delta U}{U_0}; \quad \Delta F = \frac{\delta F}{F_0}; \quad \Delta T = \frac{\delta T}{T_0}, \quad (4)$$

where index “0” refers to a quasi-stationary state.

In the case of organizing a generation process with the possibility of a free release of the produced hydrogen from reaction volume, at each moment the yield of the gaseous reaction products will differ very little from its consumption. In this regard, we shall consider the quasi-stationary values to be such values of pressure, temperature, and density, at which the yield of the gaseous reaction products differs from the consumption by the magnitude that is small compared to the values of the yield and consumption.

In addition, we shall take into consideration that there is a correlation

$$\Delta U = \frac{P_0}{U_0} \left( \frac{\partial U}{\partial P} \right)_0 \Delta P. \tag{5}$$

Then the system of equations (1) can be reduced to the following system of 2 equations:

$$\begin{aligned} V_0 P_0 \frac{d\Delta P}{dt} + \left( k\mu A_k PF\sqrt{RT} \right)_0 - \left( k\rho\chi ST_* P \frac{\partial U}{\partial P} \right)_0 \Delta P = \\ = \left( k\mu A_k \rho F\sqrt{RT} \right)_0 \Delta F - \left( 0,5k\mu A_k PF\sqrt{RT} \right)_0 \Delta T; \\ V_0 P_0 \frac{d\Delta T}{dt} + \left( \rho SRTU \right)_0 + \left( 0,5(k-1)\mu A_k PF\sqrt{RT} \right)_0 \Delta T = \\ \left( \left( k\rho\chi RT_* SP \frac{\partial U}{\partial P} \right)_0 - \left( \rho SRT P \frac{\partial U}{\partial P} \right)_0 - \left( (k-1)\mu A_k PF\sqrt{RT} \right)_0 \right) \Delta P - \\ - \left( (k-1)\mu A_k PF\sqrt{RT} \right)_0 \Delta F. \end{aligned} \tag{6}$$

It should be noted here that the second equation of system (6) is recorded in this form taking into consideration expression (2).

If a notation is introduced:

$$K_p = \xi_T \left( \frac{\rho SP_0 \left( \frac{\partial U}{\partial P} \right)_0}{\dot{m}_0} - 1 \right) (k-1);$$

$$K_{F1} = \xi_p \left( 1 - \frac{\rho SP_0 \left( \frac{\partial U}{\partial P} \right)_0}{\dot{m}_0} \right)^{-1};$$

$$K_T = 0,5\xi_p; \quad \tau_T = \xi_T \tau_0; \quad K_{F2} = \xi_T (k-1); \quad \tau_p = \frac{\xi_p}{k} \tau_0;$$

$$\xi_T = \left( \frac{\rho SU_0}{\dot{m}_0} + \frac{k-1}{2} \right)^{-1};$$

$$\tau_0 = \frac{P_0 V_0}{\dot{m}_0 (\chi RT_*)}; \quad \dot{m}_0 = \frac{\mu A_k P_0 F_0}{\sqrt{RT_0}}$$

then the system of equations (6) is transformed to the form:

$$\begin{aligned} \tau_p \frac{d\Delta P}{dt} + \Delta P = -K_{F1} \Delta F - K_T \Delta T; \\ \tau_T \frac{d\Delta T}{dt} + \Delta T = K_p \Delta P - K_{F2} \Delta F. \end{aligned} \tag{7}$$

In this case, relation  $T_0 = \chi T_*$  is taken into consideration. System of differential equations (7) will be matched with a second-order differential equation that takes the form

$$\begin{aligned} \tau_T \tau_p \frac{d^2 \Delta P}{dt^2} + (\tau_T + \tau_p) \frac{d\Delta P}{dt} + (1 + K_T K_p) \Delta P = \\ = -\tau_T K_{F1} \frac{d\Delta F}{dt} + (K_T K_{F2} + K_{F1}) \Delta F. \end{aligned} \tag{8}$$

Then, in accordance with equation (8), we shall write a transfer function of the gas generator in the form

$$W(S) = \frac{\Delta P(S)}{\Delta F(S)} = \frac{(K_T K_{F2} + K_{F1}) - \tau_T K_{F1} S}{\tau_T \tau_p S^2 + (\tau_T + \tau_p) S + K_T K_p + 1}, \tag{9}$$

where

$$\Delta P(S) = L[\Delta P(t)]; \quad \Delta F(S) = L[\Delta F(t)]. \tag{10}$$

In expressions (10),  $L$  is the integral Laplace transform operator.

Proceeding to the standard form of representation of the transfer function, expression (9) will be transformed as follows:

$$W(S) = K \frac{1 - \tau_1 S}{(\tau_2 S + 1)(\tau_3 S + 1)}, \tag{11}$$

where the following notations are considered:

$$K = \frac{K_{F1} + K_T K_{F2}}{1 + K_T K_p}; \quad \tau_1 = \frac{\tau_T K_{F1}}{K_{F1} + K_T K_{F2}}; \tag{12}$$

$$a_1 = \frac{\tau_T + \tau_p}{1 + K_T K_p}; \quad a_2 = \frac{\tau_T \tau_p}{1 + K_T K_p};$$

$$\tau_3 = 0,5 \left[ a_1 + (a_1^2 - 4a_2)^{0,5} \right].$$

Transfer function (11) will be matched with a logarithmic amplitude-AFR(LAFR) of the hydrogen gas generator  $l(\omega)$

$$l(\omega) = 20 \lg A(\omega), \tag{13}$$

where  $A(\omega)$  is the amplitude-AFR(AFR) of the gas generator, the expression for which takes the form

$$A(\omega) = K \prod_{i=1}^3 A_i(\omega); \tag{14}$$

$$A_1(\omega) = (1 + \omega^2 \tau_1^2)^{0,5};$$

$$A_2(\omega) = (1 + \omega^2 \tau_2^2)^{-0,5};$$

$$A_3(\omega) = (1 + \omega^2 \tau_3^2)^{-0,5}. \tag{15}$$

Fig. 1 shows a graphic asymptotic dependence (13) for the case of vertically oriented reaction surfaces of hydro-reactive compositions (HRC) (hydrogen consumption is  $4 \cdot 10^{-4}$  kg·s<sup>-1</sup>, the ratio of the cross-sectional area of the hydrogen generator's outlet to the surface area of gas release is equal to 0.02). For such an operation mode of the gas generator, parameters of transfer function (11) are equal to [4]:  $K=1.33$  kg(m<sup>3</sup>·s<sup>2</sup>)<sup>-1</sup>;  $\tau_1=7.9$  ms;  $\tau_2=6.5$  ms;  $\tau_3=14.4$  ms.

It follows from an analysis of dependence  $l(\omega)$  that this dependence can be approximated by dependence  $l_0(\omega)$ , which corresponds to LAFR of aperiodic link with a coupling frequency  $\omega_0$ , determined from expression

$$\omega_0 = \omega_3 + 0,5(\omega_2 - \omega_1) = \tau_3^{-1} + 0,5(\tau_2^{-1} - \tau_1^{-1}) = \tau_0^{-1}, \tag{16}$$

where  $\tau_0$  is the time constant of the aperiodic link. For the examined case,  $\tau_0=12.0$  ms.

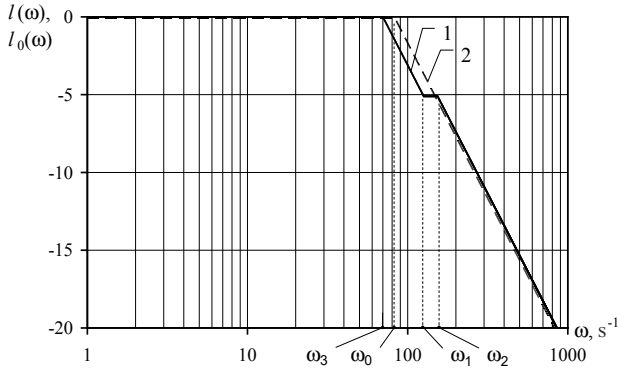


Fig. 1. LAFR of the gas generator based on HRC:  
1 -  $l(\omega)$ ; 2 -  $l_0(\omega)$

Fig. 2 shows dependences for between  $A(\omega)$  and between  $A_0(\omega)$  where

$$A_0(\omega) = K(1 + \omega^2 \tau_0^2)^{-0.5}. \quad (17)$$

Fig. 3 shows dependence for the error of misalignment between these frequency characteristics

$$\delta(\omega) = \text{mod} \left[ K^{-1} [A(\omega) - A_0(\omega)] \right]. \quad (18)$$

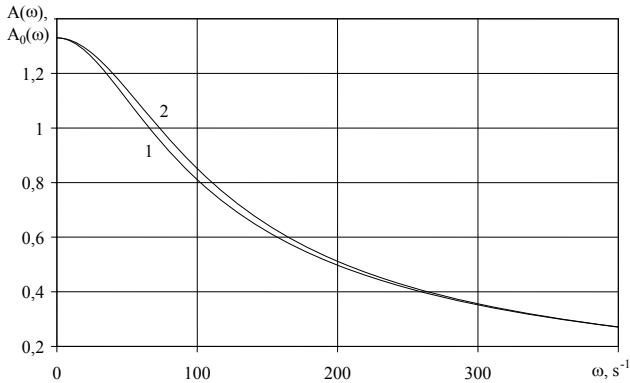


Fig. 2. LAFR of the gas generator based on HRC:  
1 -  $A(\omega)$ ; 2 -  $A_0(\omega)$

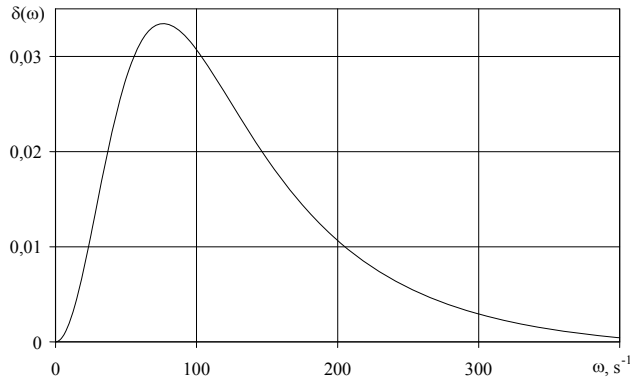


Fig. 3. Error of misalignment between  $A(\omega)$  and  $A_0(\omega)$

An analysis of these dependences indicate that the maximum value of the error of misalignment between  $A(\omega)$  and  $A_0(\omega)$  does not exceed 3.5 %.

Approximation of the characteristics of  $A(\omega)$  with function  $A_0(\omega)$  makes it possible to implement control algorithm over the technical condition of gas generator of the hydrogen

storage and supply system. Such a control algorithm can be implemented in the following way.

At the first stage, we change the area of outlet  $\Delta F(t)$  in accordance with expression

$$\Delta F(t) = A \sin \frac{\pi t}{t_0} [1(t) - 1(t - t_0)], \quad (19)$$

where  $A$ ,  $t_0$  are the amplitude and duration of a single pulse of a semi-sinusoidal form, respectively;  $1(\cdot)$  is the Heaviside function.

A change in area  $\Delta F(t)$ , in accordance with (19), will be matched with a change in pressure  $\Delta P(t)$  in the cavity of a gas generator, described by +expression

$$\Delta P(t) = L^{-1} [W_0(S) \Delta F(S)], \quad (20)$$

where  $L^{-1}$  is the operator of inverse integral Laplace transform;  $\Delta F(S)$  is the representation of function (19) by Laplace;  $W_0(S)$  is the transfer function of the gas generator whose AFR takes the form (17).

This expression after concretization is transformed as follows:

$$\begin{aligned} \Delta P(t) &= \frac{KA\pi}{t_0} L^{-1} \left[ \left[ S^2 + \left( \frac{\pi}{t_0} \right)^2 \right] (\tau_0 S + 1)^{-1} [1 - \exp(-S\tau_0)] \right] = \\ &= KA(t_0^2 + \pi^2 \tau_0^2)^{-1} \times \\ &\times \left[ \begin{aligned} &\left[ t_0^2 \sin \frac{\pi t}{t_0} + \pi \tau_0 t_0 \left( \exp \left( -\frac{t}{\tau_0} \right) - \cos \frac{\pi t}{t_0} \right) \right] 1(t) + \\ &\left[ t_0^2 \sin \frac{\pi(t-t_0)}{t_0} + \pi \tau_0 t_0 \left( \exp \left( -\frac{t-t_0}{\tau_0} \right) - \cos \frac{\pi(t-t_0)}{t_0} \right) \right] 1(t-t_0) \end{aligned} \right]. \quad (21) \end{aligned}$$

Upon completion of the transient processes and at time  $t = 0,5t_0$ , in line with (21), there is

$$\Delta P = KA t_0^2 (t_0^2 + \pi^2 \tau_0^2)^{-1}. \quad (22)$$

The magnitude  $\Delta P$  is measured. Then, at *a priori* assigned values of parameters  $A$  and  $t_0$ , as well as at known magnitude of transfer coefficient  $K$ , the magnitude of parameter  $\tau_0$  will be determined from expression

$$\tau_0 = \frac{t_0}{\pi} \left( \frac{KA}{\Delta P} - 1 \right)^{0.5}. \quad (23)$$

This ends the first stage of implementation of the control algorithm over technical condition of the gas generator.

At the second stage, we register area  $F_0 = \text{const}$  of the outlet of gas generator and measure pressure  $P_0 = \text{const}$  in its cavity. Next, we change area  $\Delta F(t)$  of the outlet of gas generator in line with the sinusoidal law at frequency  $\omega_0$  whose magnitude is determined from expression

$$\omega_0 = \tau_0^{-1} = \frac{\pi}{t_0} \left( \frac{KA}{\Delta P} - 1 \right)^{-0.5}, \quad (24)$$

that is, we change magnitude  $\Delta F(t)$  in line with expression [13]

$$\Delta F(t) = F_0 + F_m \sin \omega_0 t, \quad (25)$$

where  $F_m$  is the amplitude whose magnitude is *a priori* assigned.

A change in area  $\Delta F(t)$  under established operation mode of the gas generator will be matched with a change in pressure  $\Delta P(t)$  in its cavity, that is

$$\Delta P(t) = P_0 + P_m \sin(\omega_0 t + \phi), \quad (26)$$

where  $P_m$  is the amplitude of a variable component of pressure in the cavity of gas generator;  $\phi$  is the phase shift angle between  $\Delta P(t)$  and  $\Delta F(t)$ .

There is a relation between the parameters of expressions (25) and (26)

$$P_0 P_m^{-1} = F_0 A_0(0) [F_m A_0(\omega)]^{-1}, \quad (27)$$

which, considering (17) and (24), transforms this relation to the form

$$P_0 P_m^{-1} = \sqrt{2} F_0 F_m^{-1}. \quad (28)$$

The magnitude  $P_m$  is measured. Then, at *a priori* assigned small number  $\varepsilon$ , the result of control over technical condition of the gas generator in the hydrogen storage control system can be obtained by applying criteria

$$\left| P_0 P_m^{-1} - \sqrt{2} F_0 F_m^{-1} \right| \leq \varepsilon, \quad (29)$$

that is, if this condition is satisfied, then technical condition of the gas generator is accepted to meet regulatory requirements.

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### 5. Discussion of results of designing an algorithm for technical condition of hydrogen generators based on hydro-reactive formulations

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Development of the algorithm to control technical condition of the hydrogen generator was preceded by studies, earlier conducted by the authors, in the field of production, storage and supply of hydrogen. The results of these studies are given in the concentrated form in papers [4, 9]. Further development of the research was predetermined by the need to create hydrogen generators with improved performance characteristics. One of the directions of this work is to build effective control systems.

The designed control algorithm over technical condition has the following advantages:

- ease of implementation of test-impacts, which represent in one case a pulse of half sinusoidal form, and in the second – harmonic signal of constant frequency;
- in a standard variant of technical implementation of hydrogen generators, the frequency of a test-impact does not exceed 20 Hz, which is rather simply implemented in mechanical devices;
- technical condition of the hydrogen generator is assessed under dynamic mode of its operation;
- technical condition of the hydrogen generator can be estimated during its regular operation.

The developed algorithm for control over technical condition of the hydrogen generator [13] is a theoretical basis for constructing an automated control system for the devices of this type.

A signature of the devised control algorithm over technical condition of the hydrogen generator is the establish of belonging of a figurative point, which characterizes its dynamic state in some region. We propose using, as such a region, the region whose dimensions are limited by the magnitude of small parameter  $\varepsilon$  on the amplitude-frequency characteristic of the hydrogen generator. The center of this region is determined by two coordinates: the magnitude of pairing frequency and the value of amplitude-frequency characteristic of the hydrogen generator at this frequency.

If a figurative point of the hydrogen generator enters this region, its technical condition is considered to meet regulatory requirements.

It should be noted that the ideology underlying control algorithm over technical condition of the hydrogen generator has become feasible for implementation as a result of transition to a simpler mathematical description of the generator. Specifically, with such a simple mathematical description of properties of the generator, we employ only two parameters – a transfer coefficient and a time constant. The magnitude of time constant of the hydrogen generator is the magnitude inverse to its frequency of conjugation. When the (proposed) mathematical model of the hydrogen generator is applied, a time constant fully determines its dynamic properties. With a stricter hydrogen generator description, they use four parameters. When passing to a simplified mathematical model of the hydrogen generator, the error of misalignment for the typical values of its physical parameters does not exceed 3.5 %.

It should be noted that the possibility to employ a simpler mathematical description of the generator hydrogen appeared as a result of transition from a system of differential equations to the transfer function. This, in turn, allowed us to identify special features in the hydrogen generator when describing it in the frequency domain.

The proposed approach to building a control algorithm over technical condition of the hydrogen generator is valid assuming that its properties are described by a linear system of differential equations. This mathematical description, in turn, holds for small deviations in physical variables from their values under a quasi-stationary mode of hydrogen generation. In this regard, further development of studies into control over technical condition of hydrogen generators should be aimed at determining the borders of admissibility when using linear models. In addition, the very idea of the method of “zero-dimensional” ballistics is based on the characteristics of generator averaged by volume. That is why, when improving the proposed algorithm for technical inspection of the hydrogen generator, there may arise a task on assessing such averaging.

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### 6. Conclusions

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1. It is shown that according to the laws of preservation of mass and energy, the process of hydrogen generation from the substances in which it is in the chemically bound state can be described by a system of linear differential equations. Such a description of hydrogen generation processes opens up the prospects for using the methods of technical cybernetics in the study of linear systems.

2. By employing a transfer function of the hydrogen generator, we performed a transition from the time domain



of description of hydrogen generation processes to the frequency area. In the frequency domain, hydrogen generator properties are represented in the form of an asymptotic logarithmic frequency characteristic. Such a description of the hydrogen generator properties allows us to solve the task on identifying its simplified model, by reducing the number of model parameters from four to two.

3. We identified a simplified model of hydrogen generator in the frequency domain in the form of a model of equivalent dynamic link, and determined its parameter – the time constant, which fully reflects its dynamic properties, in particular, performance efficiency. A methodical inaccuracy, caused by the misalignment between models, does not exceed 3.5 %.

4. A mathematical description is obtained for the reaction of hydrogen generator to two kinds of test-impacts – in the form of a pulse of a semi-sinusoidal form, and in the form of a harmonic function of time. The first kind of test-impact makes it possible to identify the magnitude of time constant of the generator. The second type of test-impact whose frequency is determined by the magnitude of time constant of the hydrogen generator, makes it possible to obtain estimates for informational parameters – a constant and a variable of pressure components in its cavity. We proposed the criterion for determining a technical condition of the hydrogen generator, which implies entering of a figurative point that describes the current state of dynamic processes in the hydrogen generator, and is determined by using informational parameters.

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