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DEVELOPMENT OF A METHODOLOGY FOR CALCULATING THE STRESS STATE AND RESOURCE OF A HYDROGEN GENERATOR USING THE FINITE ELEMENT METHOD

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An experimental stand was created to study the thermobaric and chemical influence of hydrogen on the identification of hydrocarbon production. The said stand allows to reproduce chemical-technological processes as close as possible to real formation ones. This stand makes it possible to study the kinetics of not only hydrogen, thermobaric and chemical effects, but also other thermal gas chemical processes, including hydrogen generation. The main element of the experimental stand is a hydrogen generator, the components of which work at high pressures and temperatures under conditions of hydrogen embrittlement of mechanical properties and an aggressive environment that causes corrosion of its inner surface. Based on this, the development of a methodology for calculating the thermal stress state of the generator, its strength under hydrogen embrittlement conditions, and its resource becomes relevant. Based on the finite element method, a methodology for calculating non-stationary temperature fields and the thermal stress state that occur in the hydrogen generator during thermobaric and chemical processes of varying intensity is proposed. The methodology allows to take into account the features of the geometry of the structure, the time-varying temperature and pressure distributions of the reaction products, the temperature dependence of the thermophysical and mechanical properties of the hydrogen generator material. Thanks to the application of the developed software, a study of the hydrogen generator thermal stress state during two real thermobaric and chemical processes of different intensity was carried out. Graphs of temperature and pressure changes of the reaction products of hydroreactive substances in the generator over time, which were registered during the experiment conduction, were used. The distribution of non-stationary temperature fields and stresses in the hydrogen generator elements was obtained. Areas of maximum load of generator elements are defined. It was established that during the flow of the studied thermobaric and chemical processes, pressure makes a greater contribution to the thermal stress state. The obtained results and the developed theory and software can be used in the study of generators of other designs with other thermobaric and chemical processes occurring in them.

***Keywords**: hydrogen generator, thermobaric and chemical process, temperature fields, thermal stress state, resource.*

Introduction

The most effective technologies for increasing hydrocarbon production are those that combine thermal, chemical and mechanical effects on the producing horizon. One of the most promising technologies is based on the effect of hydrogen activation of processes in the porous medium of the producing horizon during the exothermic reaction in the well [1, 2].

In A. Pidhornyi Institute of Mechanical Engineering Problems of the National Academy of Sciences of Ukraine, an experimental stand for the study of hydrogen thermobaric and chemical effects, which allows to reproduce chemical and technological processes as close as possible to real formation ones, was created [3]. This stand makes it possible to study the kinetics of not only hydrogen, thermobaric and chemical effects on the identification of hydrocarbon production, but also other thermal gas chemical processes, including hydrogen generation. The experiments conduction methodology is based on the sequential mixing of two technological fluids in the reactor, measurement and fixation of the thermobaric and chemical process main parameters and reproduces the said process as close as possible to the real one, that is, the one that takes place in the well [4].

The most important and responsible element of the experimental stand is the hydrogen generator. Its components are constantly exposed to high pressures and temperatures in conditions of hydrogen embrittlement of mechanical properties and an aggressive environment that causes corrosion of its inner surface. Based on this, the development of a methodology for calculation the generator thermal stress state, which takes into account real load conditions, its strength and resource, is an urgent and important problem.

During the operation of metal structures, due to their interaction with the environment, surface destruction occurs: an aggressive environment penetrates into the metal volume, which leads to a deterioration of its mechanical characteristics, a change in the stress-strain state, load-bearing capacity, and a decrease in the structures resource. The corrosion process is significantly activated under the action of tensile stresses [5, 6].

It should be noted that the danger of this type of corrosion is that it is very difficult to detect in structural elements, and the equipment in a number of cases fails in a short time. This is explained by the fact that corrosion cracks are directed perpendicular to the tensile stresses, and the time to failure depends on the level of tensile stresses [5]. In addition, corrosion cracking is often accompanied by hydrogen embrittlement, which leads to brittle destruction of structural elements [7].

It should be added that the hydrogen environment is quite aggressive, and the harmful effect of hydrogen on the metal is manifested in the reduction of its strength and plastic properties [6]. This can cause catastrophic brittle destruction of structures that have a sufficient safety margin under real load.

It was established that the development of existing defects and the nucleation of new defects are dramatically accelerated under the conditions of a three-dimensional stress state. Therefore, the evaluation of the hydrogen generator thermal stress state is important, since it constantly works under the influence of high pressure and temperatures.

Problem statement for calculation studies of the thermochemical hydrogen generator strength and resource

The cylindrical reactor of the hydrogen generator is a hollow cylinder approximately 1.5 m long, with an outer diameter of 73 mm and an inner diameter of 62 mm, made of 40Kh steel. The scheme of the hydrogen reactor is shown in Fig. 1. The internal volume of the reactor is divided into lower and upper chambers by ball valve 2. The reactor is equipped with a preheating system. Thermometry is carried out by thermocouples.

In the upper chamber, a process liquid with a higher density is placed for mixing in the lower chamber with a liquid with a lower density. The reactor is equipped with a block of the given initial pressure, which allows to simulate thermobaric and chemical processes.

The temperature in the chemical reaction zone, as well as the temperature of the reaction products, including gaseous ones, is measured by thermocouples. The reactor is pressurized to a pressure of 100 MPa. It is designed for pressures up to 50 MPa and temperatures up to 400 ^{o}C (for short-term action – up to 600 ^{o}C).

During research, temperature and pressure indicators, which are stored in the form of graphs for further review and analysis of the obtained results, are constantly monitored.

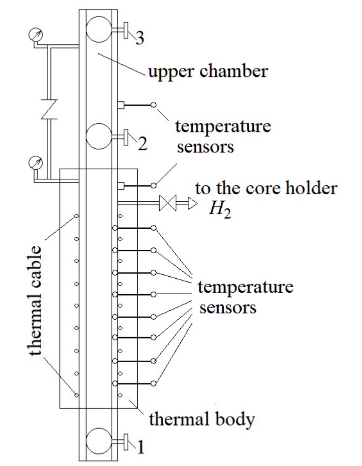

Fig. 1. Scheme of a hydrogen generator reactor:
1–3 – ball valves

Visualization of thermal thermobaric and chemical processes occurring in the reactor is shown in Fig. 2 and Fig. 3. Thus, the reaction takes place over a period of time from 9 to 45 minutes. The reactor design is equipped with a safety relief valve of a mechanical type, adjusted to a pressure of 50 MPa.

TWF-1 technological liquid with a density of 1.35 to 1.55 g/cm^3 is placed at the bottom of the reactor, TWF-2 liquid with a density of 1.6 to 1.9 g/cm^3 is placed in the upper chamber. Then high pressure is pumped into the reactor. After equalizing the pressure in the upper and lower chambers, valve 2 is opened (Fig. 1), TWF-2 liquid flows under the influence of gravity to the lower chamber and a multistage chemical process begins.

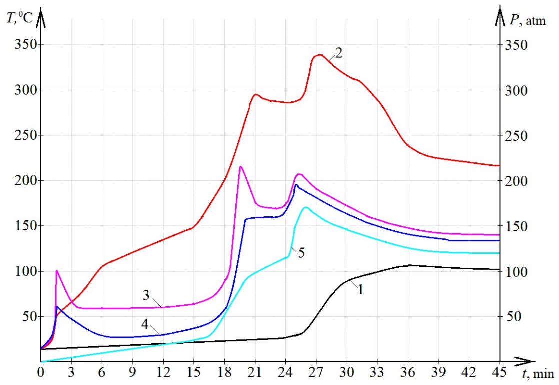

Fig. 2. Visualization of the thermobaric and chemical process with the basic composition of components of hydroreactive substances:
1 – T, °C in the reaction zone; 2 – T, °C temperature of gaseous reaction products; 3, 4 – T, °C temperature of the vapor-gas-liquid phase; 5 – pressure

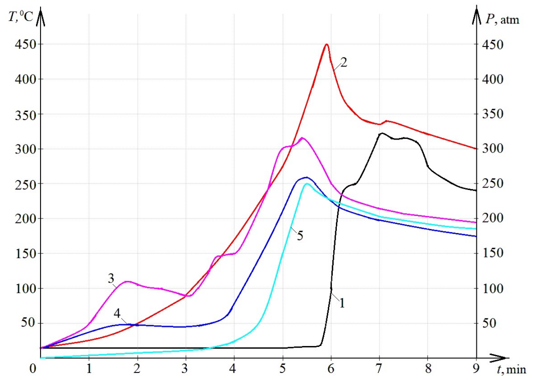

Fig. 3. Thermobaric and chemical process with activation of a hydroreactive substance and polymeric nitriles:
1 – T, °C in the reaction zone; 2 – T, °C temperature of gaseous reaction products; 3, 4 – T, °C temperature of the vapor-gas-liquid phase; 5 – pressure

Thus, a non-stationary internal pressure loading process takes place in the reactor (Graph 5, Fig. 2 and Fig. 3) and a change in the temperature of the reaction products over time (Graphs 1, 2, 3, 4, Fig. 2 and Fig. 3).

To calculate the thermal stress state of the hydrogen reactor body, it is necessary to solve the non-stationary problem of thermal conductivity under time- and height-variable boundary conditions of heat transfer of the third type (the temperature $T\,(h,\,\tau)$, °C of the reaction products and the heat exchange coefficients on the inner surface $\alpha(h,\,\tau)$ are set), which is carried out by the implicit step-by-step Crank-Nicolson method using the finite element method to obtain the temperature field of the reactor [8]. At the same time, the properties of thermal conductivity K (T, °C) and volume heat capacity ρc (T, °C) of 40Kh steel are specified depending on the temperature [8, 9].

At each time step, after solving the thermal conductivity problem, the thermal elasticity problem is solved. This takes into account the pressure load on the inner surface, which changes at each time step, as well as the thermal expansion of the reactor body material [9].

When calculating the reactor body strength, it is also necessary to take into account embrittlement and reduction of the strength limit of 40Kh steel due to flooding [10, 11, 12].

Since the products of the thermobaric and chemical reaction are an aggressive environment, corrosion of the material develops from the inner surface of the reactor, which reduces the load-bearing wall thickness of the reactor body, which affects its resource. The process and type of corrosion depend on many factors.

Computational model for determining the non-stationary temperature field and thermal stress state of the hydrogen generator using the finite element method

The design of the hydrogen generator reactor is shown in Fig. 1. The meridional section of the generator design is shown in Fig. 4. Discretization into finite elements of the middle fragment of the structure meridional section, which includes the coupling and ball valve, is shown in Fig. 5. The discretization has 127 finite elements along the z axis in the cylindrical coordinate system $r\theta z$. The axisymmetric calculation scheme from the middle of the lower to the middle of the upper ball valve along the axis has coordinates $0<z<190$ cm. The lower end $z=0$ is fixed ($u_z=0$), and axial stresses are applied to the upper end $z=190$ cm

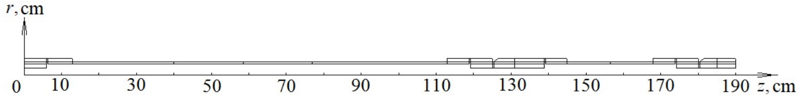

Fig. 4. Meridional section of the generator structure

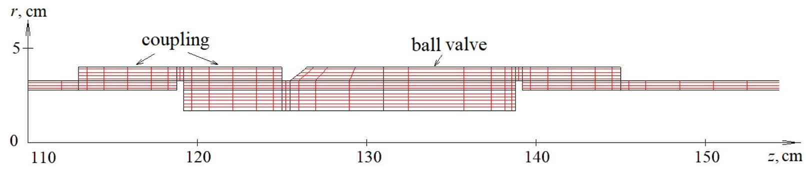

Fig. 5. Finite element discretization of the middle fragment of the structure meridional section, which includes coupling and ball valve

$$\sigma_z = \frac{P \cdot \pi \cdot r_u^2}{\pi\left(r_u^2 - r_l^2\right)} = \frac{P \cdot 1{,}9^2}{\left(4{,}45^2 - 1{,}9^2\right)} \text{MPa} = 0{,}2229 \cdot \text{P MPa},$$

where P is the pressure inside the reactor, which changes over time according to Graph 5 in Fig. 2 and 3 during the thermobaric and chemical process.

Thermophysical properties of steel, which depend on temperature, are given in Table 1.

The mechanical properties of 40KhN steel are given in Table 2, where – $\rho=8\cdot10^{-8}$ – material density; $A_{11} = \frac{E(1-\nu)}{(1+\nu)(1-2\nu)}$; $A_{12} = \frac{\nu E}{(1+\nu)(1-2\nu)}$; $G = \frac{E}{2(1+\nu)}$; E – Young's modulus; ν – Poisson's ratio; α – coefficient of linear temperature expansion of steel. With the use of the developed software [9, 10], the calculations of the hydrogen generator non-stationary temperature state were performed for two cases of thermobaric and chemical processes shown in Fig. 2 and 3.

Table 1. Thermophysical properties of steel that depend on temperature

T, ºC	20	100	200	300	400	450
$k_n=k_z$, W/(sm·degree)	0.48	0.46	0.427	0.423	0.385	0.37
ρC, J/sm^3	3.8	3.9	4.1	4.4	4.6	4.7

Table 2. Mechanical properties of 40KhN steel

T, ºC	20	200	300	400	450
$\alpha\cdot10^{-5}$, 1/degree	1.19	1.25	1.32	1.38	1.395
A_{11}, MPa	269230	282690	269230	263616	249038
A_{12}, MPa	115385	121134	115385	109615	106731
G, MPa	76969	80769	74623	73076	71154

Table 3. Piecewise linear law of heat transfer change on the inner surface of the reactor

z, sm	0	40	58.5	77	190
α, W/(cm^2·degree)	0.1	0.15	0.2	0.175	0.035
	0.2	0.25	0.3	0.150	0.050

The temperature of the reaction products is given along the z axis by the piecewise constant law. On the segment 0<z<40 cm, the temperature that occurs in the reaction zone is taken, on the segments 40<z<58,5 cm and 58,5<z<77 cm – the temperature of the gas-liquid phase of the reaction is taken, and on the segment 77<z<190 cm – the temperature of gaseous reaction products is set.

The temperature of the reaction products changes over time according to Graphs 1–4 in Fig. 2 and 3, for which the piecewise linear approximation is adopted. The coefficients of heat exchange on the inner surface of the reactor are given for two options of heat exchange, which change along the z axis according to the piecewise linear law given in the Table 3. Smaller values of heat exchange are set for the thermobaric and chemical process shown in Fig. 2, and larger ones – in Fig. 3.

The air temperature on the outer surface of the reactor is assumed to be equal to 20 ºC, and heat exchange coefficients – α=0,005 W/(cm^2·degree).

When performing calculations, the number of uniform steps over time was equal to 30 in both cases.

Thermal stress state of the hydrogen generator during the thermobaric and chemical process that lasted 45 minutes with the basic composition of hydroreactive substances

The change in the temperature of the reaction products and the pressure in the generator over time is shown in Fig. 2. In the reaction zone and in the zone of the vapor-gas-liquid phase of the reaction products, the heating of the thin-walled elements of the reactor occurs almost in a quasi-stationary mode due to significant heat exchange coefficients. At time points from 18 to 21 min, when the rate of change in the temperature of the reaction products is maximum (about 70 ºC per minute), the change in the temperature of the metal lags behind the temperature of the reaction products by 5–10 ºC, and the temperature difference along the wall thickness of 5.5 mm is 1–2 ºC.

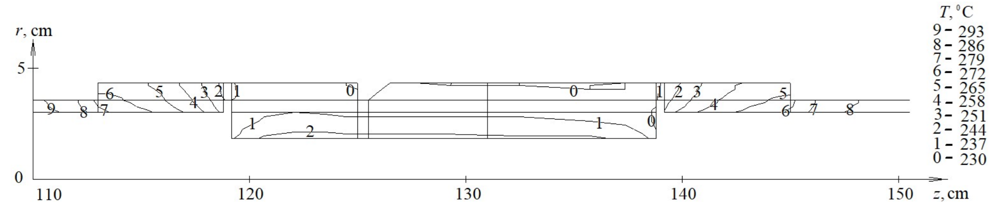

Fig. 6. Temperature distribution across the cross-section for the moment of time t=28 min in the area of the middle ball valve

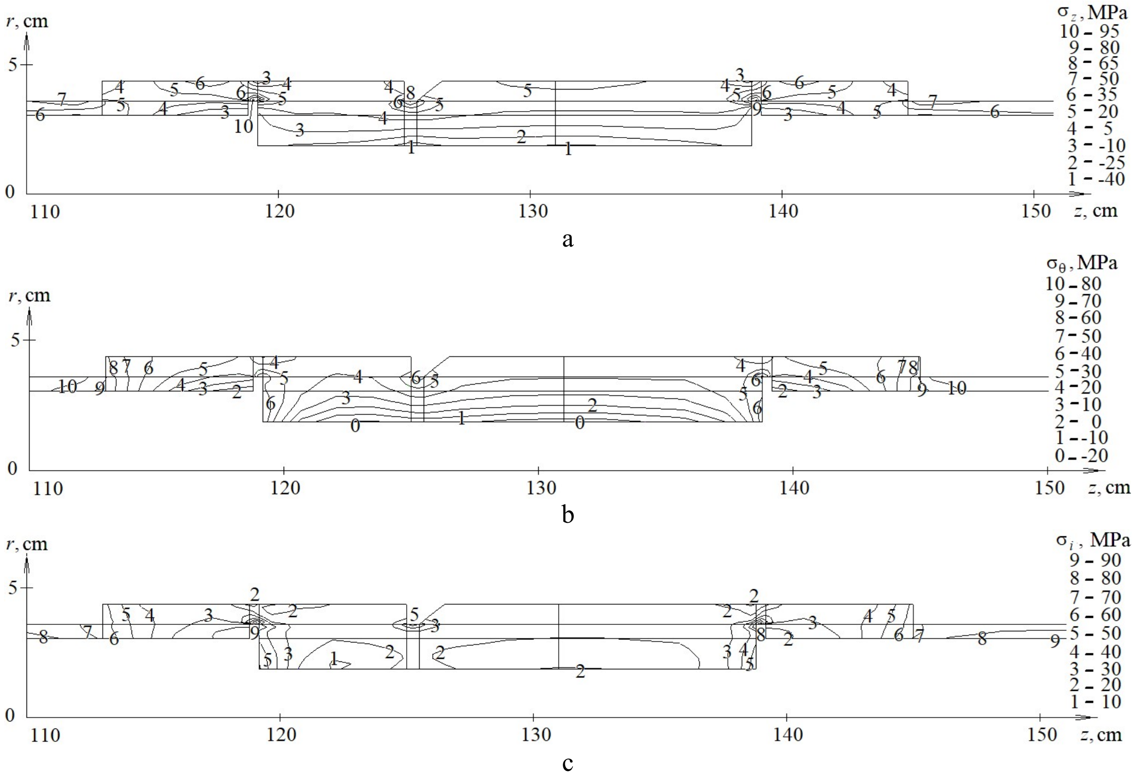

Fig. 7. Distribution of stresses in the area of the middle ball valve for the moment of time t=28 min:
a – axial stresses; b – circumferential stresses; c – equivalent stresses

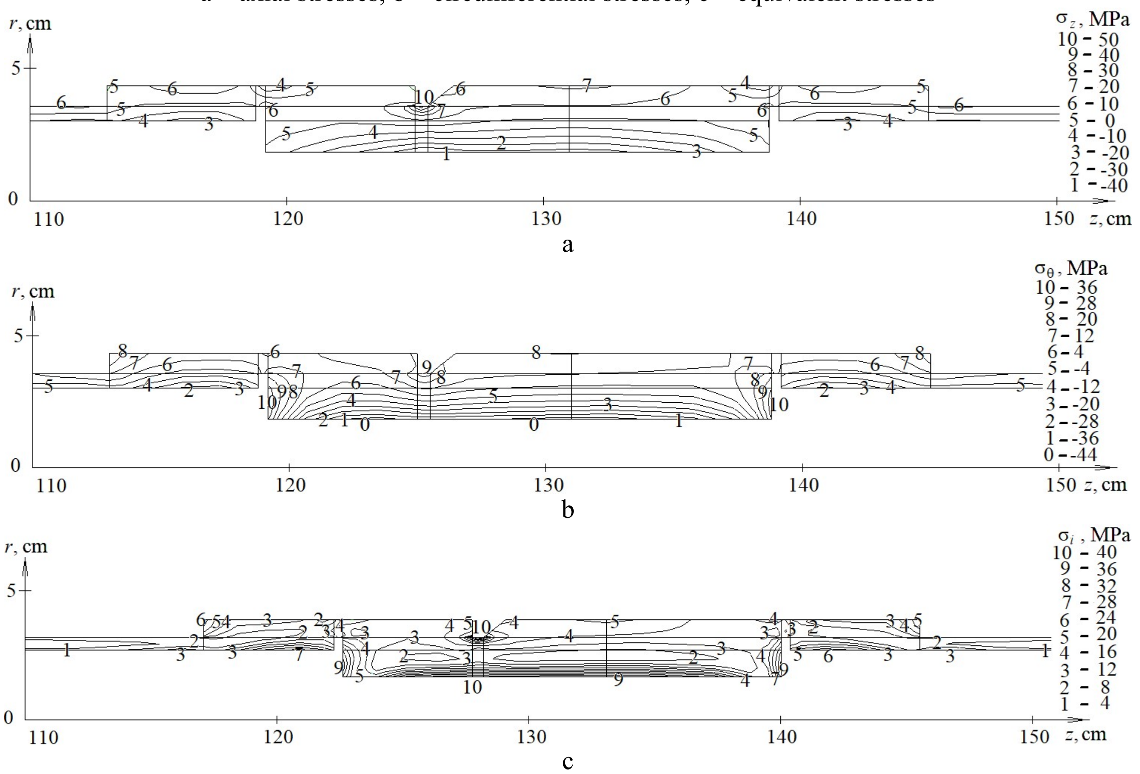

Fig. 8. Distribution of temperature stresses in the area of the middle ball valve:
a – axial stresses; b – circumferential stresses; c – equivalent stresses

In the zone of gaseous reaction products, where their temperature at the time t=28 min reaches 335 ºC and higher, the maximum temperature of the pipe metal is lower than the gas temperature by 30 ºC, and the temperature difference along the wall thickness is about two degrees. The maximum axial and circumferential stresses are equal to σ_z=60 MPa, σ_θ=100 MPa, respectively, the stress intensity is σ_i=110 MPa.

In the area of the coupling and the ball valve, where the cross-sectional area of the elements of the hydrogen reactor increases abruptly, the metal does not have time to warm up, and therefore its temperature is lower.

The cross-sectional temperature distribution for this moment in time in the area of the middle ball valve is shown in Fig. 6.

The distribution of axial, circumferential and equivalent stresses obtained using the Mises criterion [8], for the moment of time t=28 min is shown in Fig. 7.

The maximum contribution to the stressed state is given by the pressure of the reaction products inside the reactor. To estimate the contribution of temperature deformations, the calculation was performed at zero pressure of the reaction products.

The maximum temperature stresses in the pipe are σ_z=-25 MPa, σ_θ=-27 MPa, σ_i=28 MPa. The contribution of temperature stresses in the ball valve area is much higher. The distribution of temperature stresses in the region of the second ball valve is shown in Fig. 8.

The distribution of temperatures and stresses in the area of the upper ball valve is similar to the distribution in the area of the middle ball valve, but the maximum values are significantly lower due to the lower values of the heat exchange coefficients.

Thermal stress state of the hydrogen generator during the barochemical process with the activation of hydrogen-generating substances

In the case of a barochemical process with the activation of hydrogen-generating substances, the duration of the thermobaric and chemical process is 9 minutes. The change over time in the temperature and pressure of the reaction products in the hydrogen generator is shown in Fig. 3. The maximum value of the reaction products pressure occurs at the time t=5.7 min, and one of the metal temperatures – at t=6 min.

The temperature of the gaseous reaction products at the time t=5.7 min reaches 419 ºC and rises very quickly, so the maximum temperature in the reactor pipe, despite a higher heat exchange coefficient than in the previous case, reaches only 345 ºC (it lags behind the temperature of the reaction products by 74 ºC), and the temperature difference across the wall thickness is 7 ºC.

At the time of 6 minutes, the temperature of the reaction products is 430 ºC, it has reached a maximum and starts decreasing. At the same time, the maximum temperature of the metal reaches 386 ºC with a difference in wall thickness of 5 ºC (it lags behind the temperature of the reaction products by 44 ºC). The distribution of temperatures along the generator cross-section in the area of the middle ball valve at time points t=5.7 and 6 min is shown in Fig. 9.

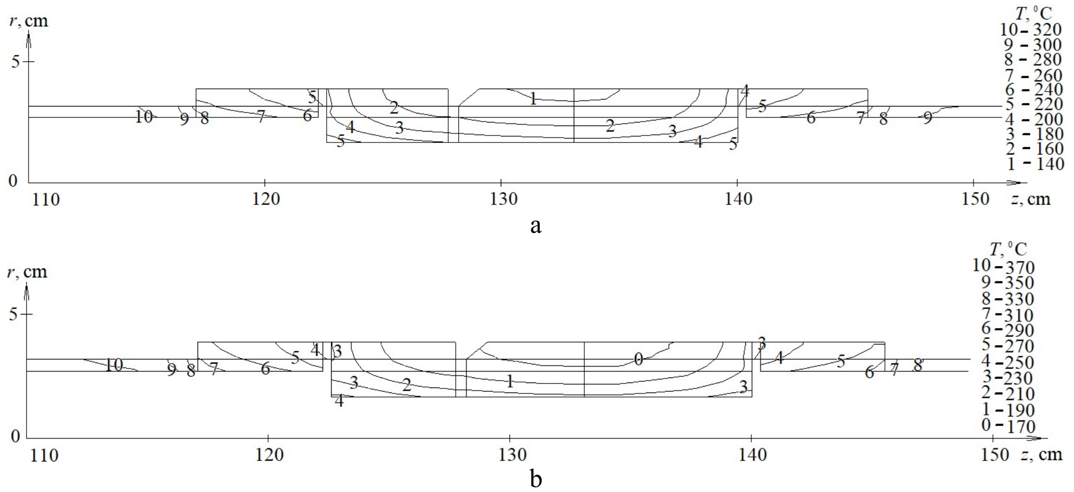

Fig. 9. Temperature distribution along the generator cross-section in the area of the middle ball valve:
a – time t=5.7 min; b – time t=6 min

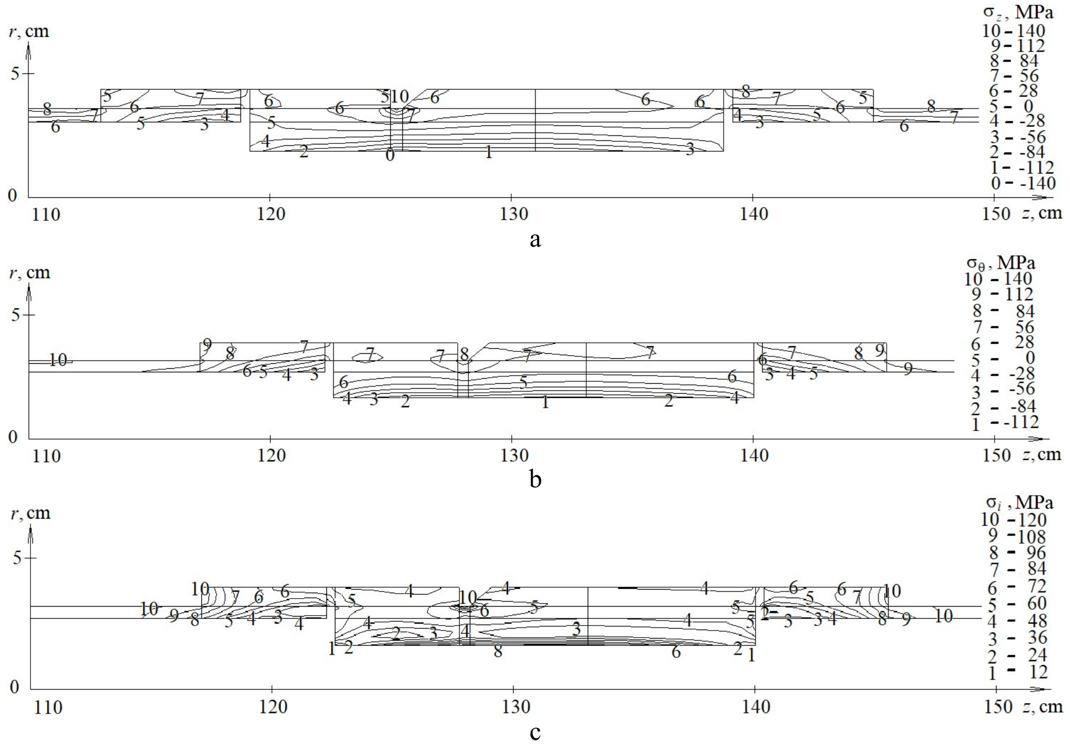

Fig. 10. Stress distribution at time t=5.7 min in the cross-section of the hydrogen generator in the area of the middle ball valve:
a – axial stresses; b – circumferential stresses; c – equivalent stresses

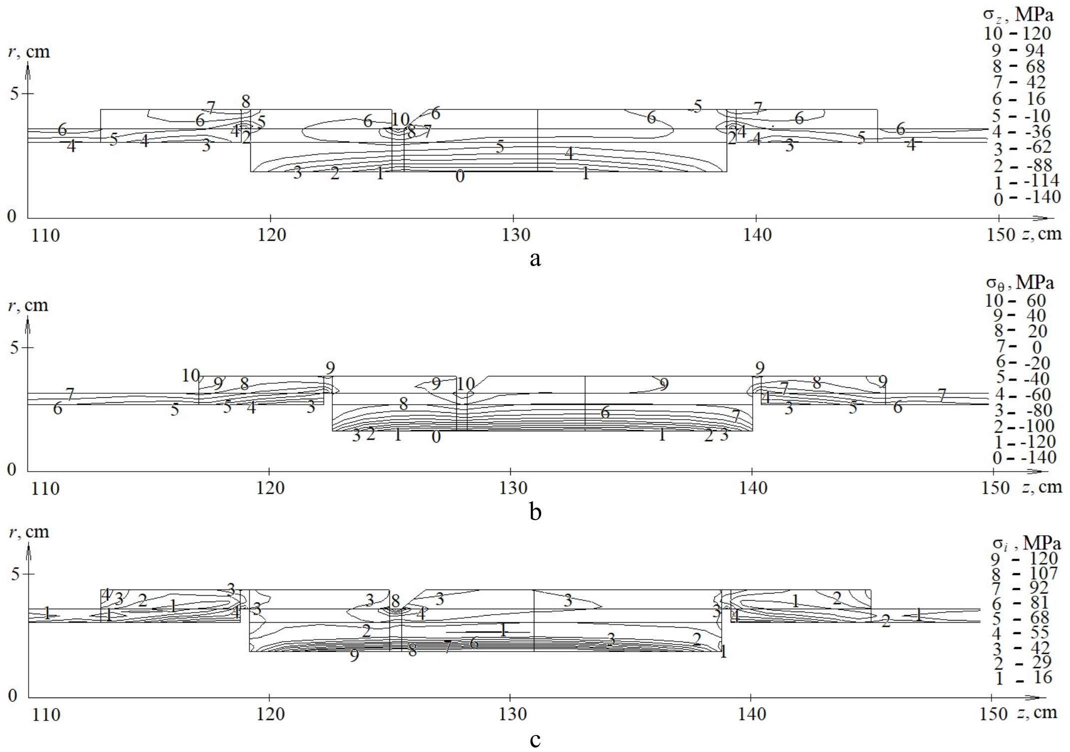

Fig. 11. Distribution of temperature stresses in the cross-section in the area of the generator middle ball valve at zero pressure:
a – axial stresses; b – circumferential stresses; c – equivalent stresses

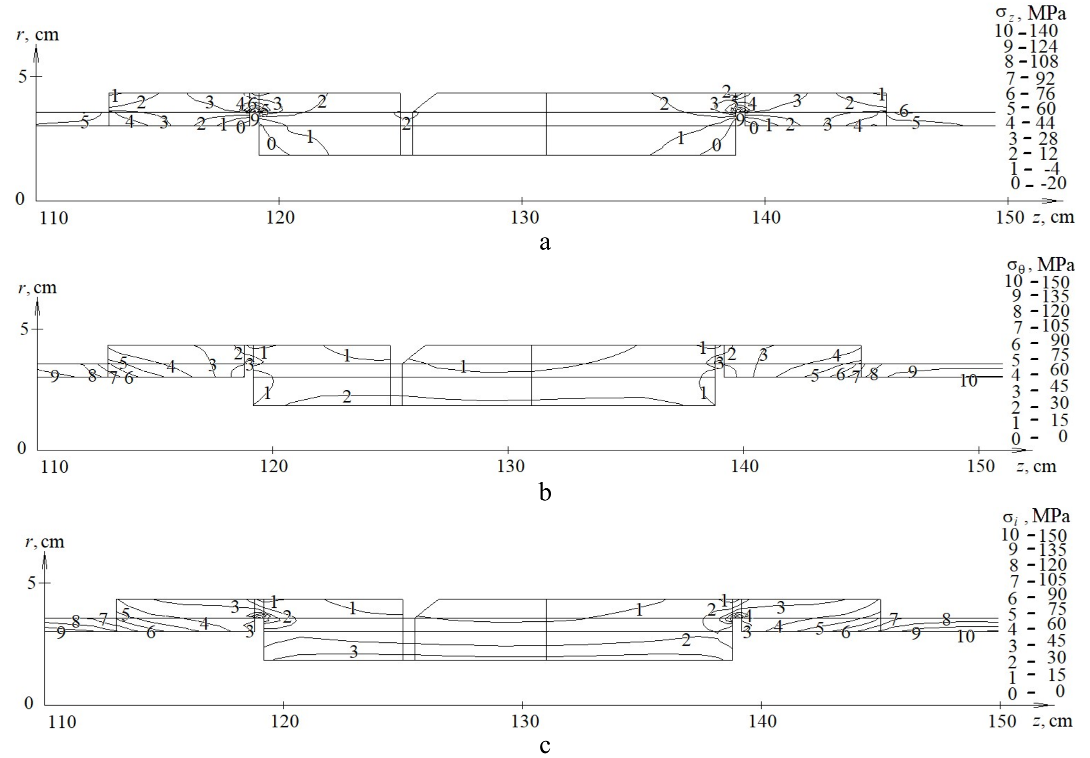

Fig. 12. Distribution of stresses in the area of the middle ball valve at a pressure of P=24.4 MPa and in the absence of a temperature field:
a – axial stresses; b – circumferential stresses; c – equivalent stresses

Maximum stresses on the inner surface of the pipe at time t=5.7 min at an internal pressure of 24.4 MPa σ_z=74.6 MPa, σ_θ=169 MPa, σ_i=163 MPa. In the case of the action of pressure P=24.4 MPa only, without taking into account the influence of temperature, the maximum stresses in the pipe are σ_z=63.1 MPa, σ_θ=150 MPa, σ_i=147.4 MPa.

The stress distribution at time t=5.7 min in the cross-section of the hydrogen generator in the area of the middle ball valve is shown in Fig. 10.

The distribution of temperature stresses at zero pressure at time t=5.7 min in the cross-section of the hydrogen generator in the area of the middle ball valve is shown in Fig. 11.

The distribution of stresses in the cross-section in the area of the middle ball valve of the generator at a pressure of P =24.4 MPa, without taking into account the temperature is given in Fig. 12.

The complex distribution of temperatures and stresses in the area of the generator middle ball valve should be noted. The pressure of gaseous reaction products has a greater contribution to the thermal stress state. At the same time, in areas of sharp change in the cross-sectional area, where significant temperature differences are observed, there is a significant contribution of temperature deformations.

A similar distribution of temperatures and stresses is also observed in the area of the upper ball valve of the hydrogen generator, but their level is somewhat lower due to lower heat exchange coefficients on the inner surface.

Conclusions

The main component of the experimental stand, intended for the study of chemical and technical processes that are as close as possible to real formation ones, which take place during the intensification of hydrocarbon production, is the hydrogen generator. Its elements work at high pressures and temperatures in conditions of hydrogen embrittlement and an aggressive environment. In view of this, the study of the thermal stress state, strength and resource becomes relevant.

The paper, based on the finite element method, presents a methodology for calculating non-stationary temperature fields and the thermal stress state observed in the hydrogen generator during thermobaric and chemical processes of varying intensity, which takes into account the features of the geometry of the structure, the time-varying temperature and pressure distributions of the reaction products, the temperature dependence of the thermophysical and mechanical properties of the hydrogen generator material.

A specific design was considered and a study of the thermal stress state during the flow of two real thermobaric and chemical processes of different intensity was performed. At the same time, graphs of temperature and pressure changes of the reaction products of hydroreactive substances in the generator over time, registered during the flow of the experiment, were used.

Non-stationary temperature fields and time-varying stress distribution in the elements of the hydrogen generator were obtained.

The moments and places of the maximum load of generator elements were determined. When the studied thermobaric and chemical processes take place, pressure makes a greater contribution to the thermal stress state.

The generator has a sufficient margin of strength under conditions of elastic deformations up to the yield point of steel. It should be noted that the generator can be used at temperatures and stresses greater than the considered values.

The developed theory and software can be used in the study of other options for the construction of generators and thermobaric and chemical processes occurring in them.

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Розробка методики розрахунку напруженого стану і ресурсу генератора водню методом скінченних елементів

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Для дослідження водневого термобарохімічного впливу на ідентифікацію видобутку вуглеводнів створено експериментальний комплекс, який дає змогу відтворити хіміко-технологічні процеси, максимально наближені до реальних пластових. Цей комплекс дозволяє досліджувати кінетику протікання не лише водневого і термобарохімічного впливу, а й інших термогазохімічних процесів, у тому числі з генеруванням водню. Головним елементом експериментального комплексу є генератор водню, складові якого працюють при високих тисках і температурах в умовах водневого окрихчування механічних властивостей і агресивного середовища, що породжує корозію його внутрішньої поверхні. Виходячи з цього набуває актуальності розробка методики розрахунку термонапруженого стану генератора, його міцності в умовах водневого окрихчування й ресурсу. На основі методу скінченних елементів запропоновано методику розрахунку нестаціонарних температурних полів і термонапруженого стану, що мають місце в генераторі водню при протіканні термобарохімічних процесів різної інтенсивності. Методика дозволяє враховувати особливості геометрії конструкції, змінні за часом розподіли температур і тиску продуктів реакції, залежність від температури теплофізичних і механічних властивостей матеріалу генератора водню. Завдяки застосуванню розробленого програмного забезпечення проведено дослідження термонапруженого стану генератора водню при протіканні двох реальних термобарохімічних процесів різної інтенсивності. Використано графіки зміни за часом температур і тиску продуктів реакції гідрореагуючих речовин у генераторі, які було зареєстровано при протіканні експерименту. Отримано розподіл нестаціонарних температурних полів і напружень в елементах генератора водню. Визначено області максимального навантаження елементів генератора. Установлено, що при протіканні досліджених термобарохімічних процесів більший внесок у термонапружений стан дає тиск. Одержані результати й розроблені методичне і програмне забезпечення можуть використовуватися при дослідженні генераторів інших конструкцій з іншими термобарохімічними процесами, що протікають у них.

***Ключові слова**: генератор водню, термобарохімічний процес, температурні поля, термонапружений стан, ресурс.*

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