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Stressed state of a steel construction working in hydrogen containing environment

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Abstract. An approach is proposed to solve the problem of estimating the stress state of a shell structure loaded with a thermomechanical load and in contact with a hydrogen-containing medium. The stress state of the steel housing of the diffusion apparatus for the production of highly pure hydrogen was determined. The object of study is presented in the form of a composite shell of rotation, loaded by internal pressure and operating at elevated temperatures. The purpose of the work is to determine the stress state of the shell at normal and elevated pressure, taking into account changes in the mechanical properties of the combined effect of temperature and hydrogen. In the general case, the task of calculating such a structure under given operating conditions is related. In the phenomenological approach, the relationship between thermal diffusion and mechanical problems is manifested in a change in the parameters of the sample deformation diagram with increasing temperature and hydrogen concentration. The integration of differential equations of a boundary value problem for a shell under pressure is performed by the discrete orthogonalization method S.K. Godunov.

1. Introduction

Shell steel structural elements are widely used as structural elements in various branches of engineering. Sometimes such structural elements during operation work not only under the action of external mechanical loads but are also under the influence of heat and corrosive media. The influence of an aggressive environment on the mechanical properties of metals during the operation of structures is one of the important factors determining the design and residual life of many potentially dangerous objects.

It is known that the danger of hydrogen exposure to metal lies in the fact that this process takes place inside the metal and does not manifest itself by any external signs. Since no means is it not possible to fix the change in mechanical properties. Therefore, to assess the life of various structures operating in hydrogen-containing environments, it is necessary to build mathematical models based on the available experimental data showing the effect of hydrogen on the metal.

The relationship between stress $\sigma$, deformation $\varepsilon$ and concentration $c$ from hydrogen in a mechanically loaded structural element during operation, determined by the time $t$ for problems of high-temperature and low-temperature hydrogenation can be represented as $\sigma = f(\varepsilon, c, T, t)$.

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2. Formulation of the problem
The paper proposes an approach for determining the stress state of a thin-walled structure during its operation in a water-containing environment. It is assumed that the structure is a steel shell of revolution, with thickness \( h \), with variable geometrical and mechanical parameters along the generator. The shell is assigned to a continuous median surface with curvilinear orthogonal coordinates \( s \) (meridional) and \( \theta \) (circumferential). The coordinate in the direction of the outward normal to the surface of the shell is denoted by \( \gamma \), therefore \(-h/2 \leq \gamma \leq h/2\).

For a long time, the inner surfaces of the shell come into contact with an aggressive hydrogen-containing medium with an overpressure \( p \), with an elevated temperature \( T \), from which hydrogen diffuses into the material. It is necessary to determine the stress state of the shell, taking into account the mechanical properties of the material of the structure that change under the influence of hydrogen and heat.

The stress state of a thin-walled structure will be determined using the classical theory of shells in a geometric linear and physically nonlinear formulation. The solution of this related non-stationary problem can be represented as: 1) the solution of the heat conduction problem with the determination of the temperature distribution in the shell over time \( T(t) \); 2) solving the problem of hydrogen diffusion with determining the distribution of hydrogen concentration taking into account the heating \( c(t,T) \); 3) obtaining experimental dependences between stress \( \sigma \), deformation \( \varepsilon \), concentration \( c \) and temperature \( T \) for samples \( \sigma = f(t,T,c,\varepsilon) \) under the uniaxial stress state; 4) determine the stress state of the structure with regard to the physicomechanical properties of the material \( \sigma = f(t,T,c,p) \).

The process of heat distribution in the shell is described by the relation [1, 2]

\[
\frac{1}{H_1H_2} \left[ \frac{\partial}{\partial s} \left( H_2 \frac{\partial T}{\partial s} \right) + \frac{\partial}{\partial \theta} \left( H_1 \frac{\partial T}{\partial \theta} \right) + \frac{\partial}{\partial \gamma} \left( H_1H_2 \frac{\partial T}{\partial \gamma} \right) \right] = \frac{1}{a} \frac{\partial T}{\partial t},
\]

where \( H_1, H_2 \) are the Lame parameters, and \( a \) is the thermal diffusivity.

The effect of temperature on the surface of the shell at each time point must be specified by boundary conditions. In problems of heat conduction, three kinds of boundary conditions are usually used. In this paper, we will use the first kind, which consists in the fact that at each instant of time on the surface of the shell the temperature distribution

\[
T \left( \gamma = -\frac{h}{2}, t \right) = T_H,
\]

where \( T_H \) is the initial temperature on the surface of the shell.

As a result of contact of the shell with hydrogen, the process of hydrogenation of the metal occurs. Although the processes of heating and diffusion develop due to various physical carriers, however, when solving applied problems, the hypothesis is usually accepted that the mathematical description of the diffusion process can use the heat equation with constant coefficients [3 - 7]. Therefore, the diffusion process in the shell will be described by the equation

\[
\frac{1}{H_1H_2} \left[ \frac{\partial}{\partial s} \left( H_2 \frac{\partial c}{\partial s} \right) + \frac{\partial}{\partial \theta} \left( H_1 \frac{\partial c}{\partial \theta} \right) + \frac{\partial}{\partial \gamma} \left( H_1H_2 \frac{\partial c}{\partial \gamma} \right) \right] = \frac{1}{D} \frac{\partial c}{\partial t},
\]

where \( D \) is the diffusion coefficient, \( c \) is the concentration of hydrogen in the wall of the shell.

For the problem of diffusion on the surface of the shell, similarly to the problem of heat conduction, it is necessary to set the boundary conditions. The boundary conditions for the problem in equation (3) will serve as the hydrogen concentration \( c \), which should be known on the shell surface from certain
physical considerations [6]. If we accept the assumption of the rapid mixing of the hydrogen-containing medium, then we can set the boundary conditions of the first kind

\[ \bar{c} \left( \gamma = \frac{b}{2}, \bar{T} \right) = c_{\text{H}}, \]

where \( c_{\text{H}} \) is the initial concentration of hydrogen on the surface of the shell.

The stress-strain state of thin-walled structures when adopting various models of shells will be described by a system of differential equations of the form \([8,9]\)

\[ \frac{\partial \bar{Y}}{\partial s} = A_0(s, \theta) \bar{Y} + \sum_{m=1}^{m} A_m(s, \theta) \frac{\partial^m \bar{Y}}{\partial \theta^m} + \bar{f}(s, \theta), \quad (s_0 \leq s \leq s_L) \]

with boundary conditions

\[ B_1 \bar{Y}(s_0) = \bar{b}_1, \quad B_2 \bar{Y}(s_L) = \bar{b}_2. \]

Here \( \bar{Y} = \{Y_r, Y_0, \ldots, Y_n\} \) is the vector function of the desired solution, \( A_1 \) - matrices, which are determined by the geometric and mechanical characteristics of the shell; \( \bar{f} \) is a vector whose components depend on the surface loads applied to the shell and the integral characteristics of the temperature field; the dimension of the vector \( \bar{Y} \) and the order of the equations \( m \) depend on the chosen shell model, \( B_1, B_2 \) - the given matrices; \( \bar{b}_1, \bar{b}_2 \) - given vectors.

Thus, this thermal diffusion problem of determining the stress state for a shell structure in the form of a body of revolution during operation will be described by a set of equations for the three systems of differential equations \(1), (3) and (5) with different initial \(2), (4) and boundary \(6) \) conditions.

3. Accepted assumptions and methods for solving the problem

It is rather difficult to solve this nonstationary connected problem in a three-dimensional formulation. However, taking into account the design features of a particular problem, the axisymmetry of the stress state and the specificity of physical processes, its solution can be represented as a series of semi-connected problems. Since the speed of heat propagation is several orders of magnitude higher than the speed of propagation of diffusible hydrogen, although these problems are related, they can be solved separately.

As noted above, to solve the problem of determining the stress state of the shell, experimental dependences between strain stress, concentration and temperature are necessary. Such data can be obtained by simple tensile testing of specimens \( \sigma = f(\varepsilon) \) at fixed values of \( c \) and \( T \).

In order to solve this problem, we will use experimental data for steel given in [10]. It curves for tensile steel of the sample approximated bilinear curve with the points of yield strength \( \sigma_y, \varepsilon_y \) and ultimate strength \( \sigma_{\text{ult}}, \varepsilon_{\text{ult}} \) for three different concentrations of hydrogen: \( \sigma_y = 336 \text{ MPa}, \varepsilon_y = 0.00168, \sigma_{\text{ult}} = 514 \text{ MPa}, \varepsilon_{\text{ult}} = 0.2 \) at \( c = 1.68 \text{ ppm} \); \( \sigma_y = 372 \text{ MPa}, \varepsilon_y = 0.00186, \sigma_{\text{ult}} = 506 \text{ MPa}, \varepsilon_{\text{ult}} = 0.2 \) at \( c = 9.47 \text{ ppm} \); \( \sigma_y = 409 \text{ MPa}, \varepsilon_y = 0.002045, \sigma_{\text{ult}} = 414 \text{ MPa}, \varepsilon_{\text{ult}} = 0.2 \) at \( c = 15.93 \text{ ppm} \).

To solve the fourth problem, we consider the thin-walled construction in the framework of the classical shell model based on Kirchhoff - Love hypotheses. With axisymmetric deformation of the shell, the system \(5) \) takes the form of a system of ordinary differential equations of the sixth order \(8) \)

\[ \frac{d\bar{Y}}{ds} = A(s)\bar{Y} + \bar{f}(s), \quad \bar{Y} = \{N_x, N_y, M_s, u_x, u_y, \theta_s\}, \]

where \( N_x, N_y \) - radial and axial forces; \( u_x, u_y \) - similar displacement, \( M_s \) - meridional bending moment; \( \theta_s \) - normal rotation angle.

To integrate the system of equations \(7) \) it is also necessary to apply various numerical methods \([1, 2, 8]\). It is known that in the numerical solution of linear boundary value problems of shell statics there are boundary and local effects that cause a rapid growth of resolving functions. Currently, the method
of discrete orthogonalization of S. K. Godunov is often used to solve many boundary value problems \[11\], which "smoothes" the boundary effects and is used to solve various problems for shells \[12, 13\], etc. This method is also used for system integration (7).

In solving this problem, taking into account the possible plastic deformation, the nonlinear problem will also be described by a system of equations (7), and the relationship between stress and strain will be linearized by the method of additional strains. This relationship is presented in the form of Hooke's law, but with additional terms that take into account the dependence of the mechanical properties of the material on deformation and temperature \[1, 2\].

4. The results of the decision

As an example, the stress state of the steel body of the diffusion apparatus was determined. This device is intended for production of especially pure hydrogen. The body of the device is loaded with internal pressure. Operating temperature 200 °C.

At the first stage of the task calculation, the temperature field of the steel housing of the diffusion apparatus was determined during operation.

At the second stage, the diffusion problem was solved. Since the shell warms up to the 200th second of the device’s work in terms of thickness, it is almost the same, the diffusion coefficient over the wall thickness was assumed to be constant. Figure 1 shows the distribution of hydrogen concentration with the wall thickness for the cylindrical part of the shell after 3.3 hours of operation of the diffusion apparatus. Curves 1 - 2 correspond to the boundary conditions of the first and third kind.

A calculation was made to determine the stress-strain state of the diffusion apparatus casing. The calculation was made under the assumption that at some point in time of operation of the structure of the apparatus, the hydrogen concentration over the wall thickness becomes uniform and reaches a value of \(c = 1.68 \text{ ppm}, c = 10.0 \text{ ppm} \) and \(c = 16.0 \text{ ppm}\).

Figure 2 shows the change of the meridional \(\sigma_s\) and circumferential \(\sigma_\theta\) stresses along the coordinate \(s\) on the inner surface of the shell. With asterisks, stresses on the outer surface of the shell are shown. The calculation was performed at a hydrogen concentration \(c = 1.68 \text{ ppm}\) uniformly distributed over the wall thickness. At this overpressure, the problem becomes physically nonlinear. It takes 10 approximations of the solution of the nonlinear problem to achieve the required accuracy of the solution equal to 1%. In this case, plastic deformation zones appear in the shell.

![Figure 1](image1.png)

**Figure 1.** The distribution of hydrogen concentration over the wall thickness after 3.3 hours of operation of the diffusion apparatus.

![Figure 2](image2.png)

**Figure 2.** Distribution of meridional \(\sigma_s\) and circumferential \(\sigma_\theta\) stresses on the inner and outer surface of the shell \((c = 1.68 \text{ ppm, } P = 5 \text{ MPa})\).
5. Conclusion
The proposed approach for solving a non-stationary coupled physicomechanical problem of hydrogenation of a loaded thin-walled structure made it possible to determine the stress state of a steel structural element of a diffusion apparatus during operation.

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