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Numerical Modeling of Hydrogen Embrittlement of a Hollow Cylinder

Assia A. Lakhdari[a,*], Ilya I.Ovchinnikov[b], Aissa Seddak[a], Igor G. Ovchinnikov[b]

[a] Department of Mechanical Engineering, Université des Sciences et de la Technologie d'Oran Mohamed Boudiaf , USTO-MB, BP 1505 El M'naouer, 31000 Oran, Algeria

[b] Department of Transportation Constructions, Saratov State Technical University Gagarin Y.A., Russia

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Abstract

In this work, the behavior of a thick-walled tube in a hydrogenated medium was simulated. The study focused on the deformation and the rupture of the hydrogenated material at ambient temperature, taking into account the appearance of heterogeneity of the mechanical properties. For this, the influence of stress states on mechanical properties and diffusion in materials has been taken into account. During the development of the methodology of calculation of the thick wall tube, the work of the structure was presented in the form of three successive stages. Numerical simulation shows that the most dangerous case is the simultaneous action of hydrogen and the charge on the inner surface of the wall of the hollow cylinder due to the fact that the combination of the action of constraints of traction and hydrogen leads to an intense degradation of the material. It should be noted that such a case of the influence of charge and hydrogen is most typical for real conditions.

Keywords: *hydrogen; embrittlement; degradation; diffusion; stress state; mechanical properties; durability*.

1. Introduction

The hydrogenated environment has a destructive impact on the materials and structures. Furthermore, hydrogen can act on the structures at high temperatures and pressures, as well as at normal temperatures which are generally called low [1-7].

During its interaction with the structure materials, the hydrogen at high temperatures and pressures, can cause what is known as corrosion by hydrogen, during which decarburization takes place of section part, leading thus to decreasing the tensile strength, modulus of elasticity, the deformation pattern of transverse deformation coefficient, creep curves, the plastic limit and the limit of deformation. Following these changes, the stress-strain state in the structures changes and reduces longevity. The different experimental data on the effect of hydrogen at high temperature are given by [8-11].

To date, a number of deformation and fracture models of structures in the conditions of corrosion with hydrogen at high temperature has been developed; the review and analysis can be found in publications [12-15].

Unlike hydrogen at high temperature, hydrogen at low temperatures has a selective effect on the material structures so that the mechanical properties are not changed in the compressed regions, but they change in the stretched areas. However, the magnitude of the variation depends on the hydrogen concentration and the stress state diagram in such point. For only one and the same figure of the stress state, a high hydrogen concentration causes a large variation in mechanical properties, and for only one and the same concentration of hydrogen, a more rigid stress state diagram causes a significant mechanical properties change.

The review and analysis of experimental data on the hydrogenation effect at low temperature on the mechanical properties of materials that cause stress corrosion cracking, are presented in the work [16, 17].

The analysis shows the following possible cases of the hydrogen interaction with metals:

- During electrochemical processes at low-temperature, when hydrogen atoms are adsorbed- the surface of the structures become absorbed by the metal (this mechanism occurs in particular cases, such as hydrogenation etching, degreasing and galvanizing)
- During corrosion, when there is a chemical release of hydrogen, then it happens to penetrate into the metal;
- By direct contact of metal with hydrogen or hydrogen media where hydrogen enters the metal under its own pressure (many accidents known in the petroleum industry, due to the extraction of oil with high content hydrogen, which led to material losses and sometimes can cause losses of human lives).

* Corresponding author e-mailamina.lakhdari@univ-usto.dz.

Such a negative effect of hydrogen on the mechanical properties of metals leads for the need to take this effect into account in the design and calculation of structures; this will ensure better security for structures work. To date, there have been a number of developed models for the structure calculation subjected to hydrogenation. In the research done by [16] a method of calculating a cylindrical vessel has been proposed, taking into account the effect of hydrogen, the state of stress and temperature on the metal plasticity.

The authors [17] have developed a model of the hydrogen influence, taking into account the effect of hydrogen on the structure stretched zone as a function of the dependence of the mechanical properties of the hydrogen concentration. In the investigation [16] a model was proposed for the interaction of structures with a hydrogen environment, taking into account not only the influence of the sign, but also of the state of stress diagram on kinetics of change the properties of the structure during its interaction with the hydrogen. The authors of the work [17] proposed a theory of plasticity of materials exposed to hydrogen embrittlement, leading to the appearance of a different capacity for resistance of materials

In the above investigations, we tried to take into account the influence of the hydrogen concentration and the stress state diagram of material properties change, but without considering the influence of the stress state on the penetration of hydrogen in the volume of the structure.

2. Model of deformation and fracture of materials subjected to hydrogenation

When developing the models, it is important to take into consideration the following effects of the interaction of structures with hydrogen:

- The hydrogen penetrates into the structure of the activated diffusion mechanism, in which there is a diffusion of hydrogen in areas with a predominance of traction components, and optionally the extraction of hydrogen from the areas with predominantly compressive components, that is to say that the diagram of the state of stress influences the hydrogenation kinetics;
- The hydrogen penetrating into the metal leads to a deterioration in strength and plasticity according to the concentration of hydrogen, and in addition the change in mechanical properties depends on the hydrogen concentration and not of the nature of the hydrogenation process;
- The type and the state of the stress impact level on the interaction of the metal with hydrogen, in that during the predominance of compression components, the metal, and after an intensive hydrogenation retains its properties, but with a predominance of traction components, the strength and plasticity properties decrease, and in addition to the tightening of the stress state diagram, the change in properties is most important.

To develop deformation models and fracture of structures subjected to hydrogenation; an approach [17] is used, based on the systems of the examined: penetration model hydrogen, model of deformation of the material, progression model of limit state model of the constructive element.

2.1. Hydrogen permeation model in the material of the structure

The hydrogen permeation kinetics in the structure is described by the diffusion form as given in the following equation:

$$\frac{\partial C}{\partial t} = div(DgradC) \qquad (1)$$

With the initial conditions and the appropriate limits see work [17].

Where: D is a diffusion coefficient, which is a function of local parameters; C is concentration; T is temperature; t is time.

To reflect the influence of the stress-strain state of the hydrogen permeability, different approaches are used.

A process of diffusion of the hydrogen has been suggested by [17], in the field of elastic stresses, which is described by the equation:

$$\frac{\partial C}{\partial t} = D\nabla^2 C - \left(\frac{DV_H}{RT}\right)\nabla C\nabla\sigma_0 - \left(\frac{DV_H}{RT}\right)C\nabla^2\sigma_0 \qquad (2)$$

Where V_H – Hydrogen partial molar volume, $\sigma = (\sigma_x + \sigma_y + \sigma_z)/3$- mean stress, R - Gas constant.

The hydrogen equilibrium concentration C_δ in the field of elastic stresses σ_0 is determined by the expression:

$$C_\delta = C_0 \exp\left(\frac{\sigma_0 V_H}{RT}\right) \qquad (3)$$

Where C_0 – equilibrium concentration of hydrogen in the absence of stress field.

In equation (2), the last two members reflect the directed broadcast hydrogen in areas with predominance of the traction component ($\sigma_0 > 0$) and the extraction of hydrogen from areas with predominance of the compression component ($\sigma_0 < 0$). For the equation (3), the initial conditions and the appropriate limits must be taken into account.

Another approach for taking into account the influence of the stress state on the hydrogen permeation is to assume that the hydrogen diffusion coefficient D and the hydrogen absorption limit of C_* are functions a special dimensionless parameter:

$$S = \frac{3\sigma_0}{\sigma_U} \qquad (4)$$

Characterizing the pattern of the stress state, σ_u- stress intensity.

Parameter values S for certain patterns of the stress state are given in table 1.

Table 1: Parameter values S for certain patterns of the stress state

schema of the state of stress	biaxial compression	uniaxial compression	cisaillement	uniaxial traction	biaxial traction
S	-2	-1	0	+1	+2

The expressions for D and C_* are taken in the form:

$$D = D_0(1 + \alpha S^\beta) \qquad (5)$$

$$C_* = C_*^0(1 + \gamma S^\delta) \qquad (6)$$

D_0 and C_*^0- values of D and C_* in the idle state (non-constraint state), $\alpha, \beta, \gamma, \delta$ - coefficients.

In this case, equation (1) takes the form:

$$\frac{\partial[\frac{C}{C_*(S)}]}{\partial t} = div\left(D(S)grad\left[\frac{C}{C_*(S)}\right]\right) \quad (7)$$

2.2. Material model deformation under the influence of the hydrogenation

For model elaboration, we apply the deformation theory of A. A. Iliouchine, whose basic assumptions are adjusted to reflect the influence of hydrogen:

- First hypothesis: the spherical deformation tensor is proportional to spherical stress tensor, and the coefficient of proportionality is a function of the parameter S and the hydrogen concentration C:

$$\sigma_0 = K(S,C)3\varepsilon_0 \quad (8)$$

Where ε_0- average strain, $K(S, C)$ - three-dimensional elastic modulus.

$$K(S,C) = \begin{cases} K_0, S \le S_0 \\ K_1(S,C), S > S_0 \end{cases} \quad (9)$$

$S \le S0$ - value of the parameter S, corresponds to the diagram of the state of stress with predominance of compression components, which starts the degradation of properties of the metal under the influence of hydrogen.

- Second hypothesis: In any point of the body, the stress deviator is directly proportional to the deflection deformation. Below the scalar form is written as follows:

$$\sigma_x - \sigma_0 = \frac{2\sigma_u}{3\varepsilon_u}(\varepsilon_x - \varepsilon_0) \quad ; \quad \tau_{xy} = \frac{\sigma_u}{3\varepsilon_u}\gamma_{xy} \quad (10)$$

$$\sigma_x - \sigma_0 = \frac{2\sigma_u}{3\varepsilon_u}(\varepsilon_y - \varepsilon_0) \quad ; \quad \tau_{yz} = \frac{\sigma_u}{3\varepsilon_u}\gamma_{yz} \quad (11)$$

$$\sigma_z - \sigma_0 = \frac{2\sigma_u}{3\varepsilon_u}(\varepsilon_z - \varepsilon_0) \quad ; \quad \tau_{zx} = \frac{\sigma_u}{3\varepsilon_u}\gamma_{zx} \quad (12)$$

Where: σ_x, σ_y, σ_z, τ_{xy}, τ_{yz}, τ_{zx} - components of the stress tensor, ε_x, ε_y, ε_z, γ_{xy} γ_{yz}, γ_{zx} - components of the tensor deformations.

- Third hypothesis: Assume that the intensity of σu stresses is a function of the deformation intensity of εu of pattern setting for stress state S and the hydrogen concentration C:

$$\sigma_u = \varphi(\varepsilon_u, S, C) \quad (13)$$

This function has the following form:

$$\varphi(\varepsilon_u, S, C) = \begin{cases} \varphi_0(\varepsilon_u); \quad S \le S_0 \\ \varphi_1(\varepsilon_u, S, C), \ S > S_0 \end{cases} \quad (14)$$

It is obvious that in order to determine the functions $\varphi_0(\varepsilon_u)$ and the $\varphi_1(\varepsilon_u, S, C)$, we need the experimental curves of metal deformation for different *S* state of stress patterns and concentration of hydrogen *C* in the test samples.

In the particular case, we can take:

$$\varphi_1(\varepsilon_u, S, C) = \varphi_0(\varepsilon_u).y(S,C) \quad (15)$$

where : φ0(εu) - approximating the function of the material deformation curve for S ≤ S0 and the function of the influence of the pattern of the stress state and the hydrogen concentration y(S, C) is defined as:

$$y(S,C)\begin{cases} 1, \quad then\ S \le S_0 \\ \exp[-KC^{\alpha}(S-S_0)^b, \quad then\ \ S > S_0 \end{cases} \quad (16)$$

Where k, a, b – constants.

The type of the function y (S, C) in the equation (16) has been suggested by [17], on the basis of the experimental data analysis on the influence of the pattern of the stress state and hydrogen concentration on the mechanical properties of materials.

2.3. Progression model limit state

Much attention has been paid by the authors of the work [17], to the problem of developing models limit state of structures under the hydrogenation conditions. To develop the limit state model, we will consider the fact observed experimentally that the material located in a plastic state before hydrogenation, under the influence of hydrogen, is weakened. To reflect this, we introduce the fragility parameter:

$$\xi(S,C) = \sigma_B(S,C) / \sigma_B^0 \quad (17)$$

Representing the resistance ratio of the rupture strength of the material after hydrogenation $\sigma_B(S, C)$ to the initial rupture resistance σ_B^0 of the material before hydrogenation.

In the absence of hydrogenation effects $\sigma_B(S, C) = \sigma_B^0$, and the embrittlement parameter ξ =1. Under the action of hydrogen on the material under stress, there is a reduction $\sigma_B(S, C)$ and a decrease in the parameter ξ.

By analogy with equation (13) can be taken:

$$\sigma_B(S,C) = \sigma_B^0\psi(S,C) \quad (18)$$

Where: $\psi(S, C)$ - influence function of the form equation (16).

Resistance condition of the material subjected to hydrogenation, we take the form:

$$\sigma_U\,\xi + (1-\xi)\,\sigma_1 \le \sigma_B^0(S,C) \quad (19)$$

One can see that for ξ =1, the condition (19) becomes a plastic material condition resistance $\sigma_U \le \sigma_B^0$, and during hydrogen embrittlement as a measure that ξ decreases, a second term is included in the condition (19), reflecting the process of hydrogen embrittlement. Taking into account equation (15), the equation (17) can be transformed into the form:

$$\sigma_U + (\frac{1}{\xi} - 1)\sigma_1 \le \sigma_B^0 \quad (20)$$

If, at the end, and taking into account the equation (14), equation (15), equation (16), then resistance condition can be written permanently as follows:

$$\sigma_U \le \sigma_B^0 \quad then\ S \le S_0 \quad (21)$$

$$\sigma_U + \{exp[kC^{\alpha}(S-S_0)^b] - 1\}\,\sigma_1 \le \sigma_B^0 \quad then\ S > S_0$$

2.4. Delayed fracture model of metals in a hydrogenated medium

Delayed rupture of structures under the influence of hydrogen accounts for the process of accumulation of scattered damage, whose kinetics is determined by the pattern of the stress state and the hydrogen concentration.

During the simulation of delayed fracture in hydrogen, we assume that the assumptions are correct:

1. The influence of hydrogen on the mechanical properties of metals is the same for the short-term loading as for long-term loading;

2. In the case of the predominance of compressive components ($S \leq S_0$), the metal retains, its long term properties regardless of the concentration of hydrogen.
3. In the case of the predominance of traction components ($S > S_0$), under the influence of hydrogen, long-term mechanical properties are reduced, and the degree of reduction increases with the rigidity of the pattern of the *S* constrained state and the hydrogen concentration *C*.

To describe the kinetics of delayed fracture, one can use either the L.M. Kachanov approach, based on the use of the continuity of ψ parameter or the Y.N. Rabotnov approach based on the use of damage parameter Π or the A.R. Rzhanitsyn approach, based on the use of the concept of instantaneous resistance *R* of the material see reference [16].

Since the interaction process metal structures with hydrogen causes a change in mechanical properties, resulting in a change in the stress-strain state of the structure, and to describe the delayed fracture, it becomes important to use the model of the accumulation of damage of Moskvitin see reference [16], which is suitable for both stationary stress states and non-stationary.

The V. V. Moskvitin model applied to the case of delayed fracture of the metal in the hydrogen has the form:

$$\Pi = \int_0^t (t-T)^m \, \eta[\sigma_э(\tau), S(\tau), C(\tau)] d\tau \qquad (22)$$

The function η [$\sigma_э$, *S*, *C*] in this equation can be taken as:

$$\eta[\sigma_э, S, C] = \frac{m(S,C)+1}{t_r^{m(S,C)+1}(\sigma_э)} \qquad (23)$$

and dependence breakup time t_r depending on the equivalent stress (long-term resistance curve) is approximated by the following function:

$$t_r(\sigma_э) = \frac{A(S,C)}{\sigma_э^{b(S,C)}} \qquad (24)$$

Substituting equation (23) in equation (22) taking into account equation (24), we can write:

$$\Pi = \int_0^t \frac{[m(S,C)+1]\sigma_э^{b(S,C)[m(S,C)+1]}}{[A(S,C)+1]^{[m(S,C)+1]}} (t-T)^{m(S,C)} d\tau \qquad (25)$$

As can be seen, the effect of the hydrogenation is taken into account through the dependence of the coefficients *A*, *b*, *m* of the parameter diagram of the *S* state of stress and hydrogen concentration *C*.

In the case of the predominance of compressive components ($S \leq S_0$), equation (25) is simplified and reduced in the form:

$$\Pi = \frac{m_0+1}{A_0^{m_0+1}} \int_0^t \sigma_э^{b_0(m_0+1)} (t-T)^{m_0} d\tau \qquad (26)$$

Where the coefficients A_0, b_0 and m_0 correspond to the metal in the non-hydrogenated state.

3. Application of the developed model to the hydrogenation problem of a thick-walled tube

3.1. Basic equations for deformation of a thick-walled tube during hydrogenation

We examine the application of the model developed to the hydrogenation problem of a thick-walled tube subjected to an axisymmetric load in a hydrogenated medium. In this case, stress and strain tensors will have non-zero components σ_r, σ_φ, σ_z, ε_r, ε_φ. All three components of deformation, shear and tangential stresses will be equal to zero, due to symmetry with the tube axis and the constancy of the conditions along its axis. The relationship between the stresses and the deformations has the following form:

$$\varepsilon_r = \frac{1}{\psi}\left(\sigma_r - \nu\left(\sigma_\varphi + \sigma_z\right)\right)$$

$$\varepsilon_\varphi = \frac{1}{\psi}\left(\sigma_\varphi - \nu\left(\sigma_r + \sigma_z\right)\right) \qquad (27)$$

$$\varepsilon_z = \frac{1}{\psi}\left(\sigma_z - \nu\left(\sigma_r + \sigma_\varphi\right)\right)$$

Where: r, z - radial, circumferential and longitudinal coordinates, and $\psi(\varepsilon_u, C, S)$ - function of strain intensity ε_u, C - hydrogen concentration (in the traction zones of the hollow cylinder) = $S = \sigma_0/\sigma_u$ - parameter characterizing the stiffness state of stress state, σ0 - average stress, σu - stress intensity.

The function $\psi(\varepsilon_u, C, S)$ is taken as:

$$\psi(\varepsilon_u, C, S) = \begin{cases} A_0 - B_0\varepsilon_u^{m-1} & then\ S < S_0 \\ A_0 - B_0\theta^{1-m}(C,S)\varepsilon_u^{m-1} & then\ S \geq S_0 \end{cases} \qquad (28)$$

The transverse strain coefficient ν and is also taken as a function of ε_u, *C* and *S:*

$$\nu(\varepsilon_u, C, S) = \begin{cases} \nu_0 & then\ S < S_0 \\ \dfrac{1}{2} - \dfrac{1-2\nu_0}{\psi_0}\psi(\varepsilon_u, C, S) & then\ S \geq S_0 \end{cases} \qquad (29)$$

The function (*C*, *S*) in equation (28) is written in the form:

$$\theta(C, S) = \begin{cases} 1 & then\ S < S_0 \\ \exp(-kC^a(S-S_0)^b) & then\ S \geq S_0 \end{cases} \qquad (30)$$

Where: *k*, *a*, *b* - coefficients.

By expressing σ_z through σ_r and σ_φ in the third equation (27) and substituting it in the first two equations (27), it is found:

$$\varepsilon_r = \frac{1-\nu^2}{\psi}\left(\sigma_r - \frac{\nu}{1-\nu}\sigma_\varphi\right) - \nu\varepsilon_z,$$
$$\varepsilon_\varphi = \frac{1-\nu^2}{\psi}\left(\sigma_\varphi - \frac{\nu}{1-\nu}\sigma_r\right) - \nu\varepsilon_z. \qquad (31)$$

By substituting the expressions of ε_r and ε_φ in the continuity equation of the deformation:

$$\frac{d\varepsilon_\varphi}{dr} = \frac{(\varepsilon_r - \varepsilon_\varphi)}{r} \qquad (32)$$

And taking into consideration, that according to the equation of equilibrium:

$$\frac{d\sigma_r}{dr} + \frac{\sigma_r - \sigma_\varphi}{r} = 0 \quad (33)$$

$$\sigma_\varphi = \sigma_r + r\frac{d\sigma_r}{dr}, \ \frac{d\sigma_\varphi}{dr} = 2\frac{d\sigma_r}{dr} + r\frac{d^2\sigma_r}{dr^2} \quad (34)$$

After some transformations, we obtain the following nonlinear equation of constraints.

$$\frac{d^2\sigma_r}{dr^2} + \lambda\frac{d\sigma_r}{dr} + \eta\sigma_r = F \quad (35)$$

The coefficients λ and η in this equation are nonlinear functions of ψ and ν and their derivatives:

$$\lambda = \frac{3}{r} - \frac{2\nu\nu'}{(1-\nu^2)} - \frac{\psi'}{\psi},$$
$$\eta = -\left((1-4\nu)\nu' + (1-\nu-2\nu^2)\psi'\big/\psi\right)\Big/ r(1-\nu^2) \quad (36)$$

Where: ν and ψ - derived from r.

The right part of F has the form:

$$F = \psi\varepsilon_z\nu'/r^2(1-\nu^2) \quad (37)$$

The longitudinal deformation ε_z is determined from the equilibrium conditions of the thick-walled tube in the longitudinal direction:

$$N = 2\pi\int_{r_1}^{r_2}\sigma_Z r dr \quad (38)$$

Hence, replacing by the expression of σ_z, we obtain:

$$\varepsilon_Z = \left(\frac{N}{2\pi} - \int_{r_1}^{r_2}\nu(\sigma_r + \sigma_\varphi)\right)\Bigg/\left(\int_{r_1}^{r_2}\psi r dr\right) \quad (39)$$

Where: r_1 and r_2 - internal and external radius of the thick-walled tube, respectively.

If the tube is loaded by external and internal pressures (fig.1.a) then the boundary conditions for the differential equation (35) are written as follows:

$$\sigma_r(r = r_1) = -P_1 \ , \quad \sigma_r(r = r_2) = -P_2 \quad (40)$$

The concentration distribution of hydrogen according to the tube thickness is determined from the diffusion equation (2), written in a cylindrical coordinate system and taking into account the influence of the stresses:

$$\frac{1}{D}\frac{\partial C}{\partial t} = \frac{\partial^2 C}{\partial r^2} + \frac{1}{r}\frac{\partial C}{\partial r} - \frac{V_H}{RT}\left(\frac{\partial C}{\partial r}\cdot\frac{\partial\sigma_0}{\partial r}\right)$$
$$-\frac{CV_H}{RT}\left(\frac{\partial^2\sigma_0}{\partial r^2} + \frac{1}{r}\frac{\partial\sigma_0}{\partial r}\right) \quad (41)$$

Where: σ_0 - mean stress determined from the expression: $\sigma_0 = (\sigma_r + \sigma_\varphi + \sigma_z)/3$

t - time, D - diffusion coefficient, R - gas constant.

The initial and boundary conditions must be added to equation (41), taking into account the action of the hydrogenous medium on the thick-walled tube.

If hydrogen acts on the inner and outer surfaces of the tube (fig.1.b), then the boundary and initial conditions will be:

$$C(r = r_1) = C(r = r_2) = C_\infty, \ C(t = 0) = C_{in} \quad (42)$$

If the hydrogen penetrates into the wall of the tube from the inside, and the reflux of the outer surface is not taken into account (fig. 1.c), then we have:

$$C(r = r_1) = C_\infty, \ \frac{\partial C}{\partial r}(r = r_2) = 0 \ , C(t = 0) = C_{in} \quad (43)$$

Under the action of hydrogen on the outer surface tube and the absence of the reflux of the inner surface (fig. 1.d)

$$\frac{\partial C}{\partial r}(r = r_1) = 0 \ , C(r = r_2) = C_\infty, \ C(t = 0) = C_{in} \quad (44)$$

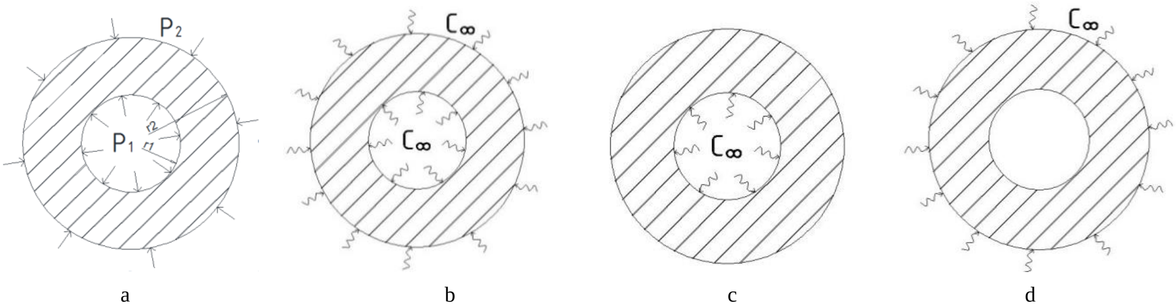

Figure1: Variants of the influence of the hydrogen medium and of the pressure on a thick-walled tube

3.2. Method of the thick-walled tube calculation, subjected to hydrogenation

When designing the method of calculating the thick-walled tube, subjected to a combined action of the filler and the hydrogen-containing medium, the work program of the structure is presented in the form of a succession of three stages [17]:

1. the stage of loading;
2. the stage of establishing the boundary conditions on the surfaces in contact with the hydrogenated medium;
3. stage of deformation of the thick-walled tube as a result of the change in the properties of the material under the influence of the hydrogenated medium in accordance with (28) and (29).

At the stage of application of the load, the calculation of the thick-walled tube is reduced to the solution of the homogeneous differential equation of the type:

$$\frac{\partial^2\sigma_r}{\partial r^2}+\lambda\frac{\partial\sigma_r}{\partial r}+\eta\sigma_r=0 \qquad (45)$$

With boundary conditions (40).

The coefficients λ and η are determined for the initial characteristics of the material.

The solution of the linear - elastic problem for the thick - walled tube is solved for the resolution of the non - linear part of the problems (45), (40), and as a zero approximation Of Blade), which has the form:

$$\sigma_r^o = I + J/r^2 \quad , \quad \sigma_\varphi^o = I - J/r^2 \qquad (46)$$

where :

$$I=(P_1r_1^2+P_2r_2^2)/(r_2^2-r_1^2) \quad ,$$
$$J=(P_2-P_1)r_1^2r_2^2/(r_2^2-r_1^2) \qquad (47)$$

For the resolution of the other part (problem at the limits) of the problems (45), (40), we use the method of scanning (algorithm of tridiagonal matrix), and in addition to find the derivatives one uses the formula of Lagrange, and the integrals in the expressions for λ and η by the Simpson formula of order 4.

At the next stage of the boundary conditions it is assumed that the concentration of hydrogen required on the surfaces of the tube is not established immediately, but during a certain t_d, given by the expression:

$$t_d = \Delta r/4D \qquad (48)$$

A suitable distribution of the mechanical parameters (and consequently the coefficients λ, η and the right part of the equation (35)) is found according to the concentration field of the hydrogenated medium at the corresponding time *tr*.

The third stage is devoted to the study of the deformation process of the thick-walled tube, caused by the action of the hydrogenated medium. The problem is solved by time increments. First, by the finite difference method, the diffusion equation (41) is solved with the initial conditions and with the corresponding limits, taking into account the distribution law of the mean stress σ0 according to the thickness of the wall of the tube. Depending on the found distribution of the hydrogen concentration C, taking into account the rigidity of the stress state diagram S according to formulas (36), (37), in the nodes of the network are found the values of the coefficients Λ and η and the right-hand part of F of equation (35), which is then solved by the scanning method. Then, the following time increment Δt is given and the calculation process is repeated.

The problem is solved by time increments until the In order to evaluate the reliability of the solution obtained, an example of calculation of a thick-walled tube of non-linear material was tested with the strain diagram $\sigma = A\varepsilon\text{-}B\varepsilon^m$, where A = 3 · 104 MPa, B = 2 · 105 MPa, m = 1.5. In the calculations we have taken $P_1 = 0$,

P_2 = 20 MPa, r_1 = 30 cm, r_2 = 60 cm, ν = 0.3.

In Figure 2, we present the results of our calculation in dotted lines, and in solid lines those of the work [17]. We observe a certain difference in the distribution of constraints, which is explained by the use by the authors of the work [17] of assumptions about the incompressibility of the material (ν = 0.5), and in our calculations ν = 0.2. The calculation for ν = 0.5 leads to a total similarity of the results.

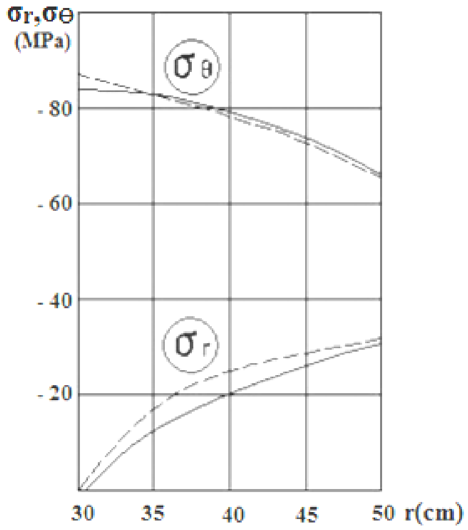

Figure 2: Calculation results for thick-walled tube

In order to evaluate the influence of the size of the finite difference network (depending on the wall thickness of the thick-walled tube) on the results of the calculation, a test calculation was made on a tube made of material with the In the calculations, we took P_1 = 20 MPa, P_2 = 0, r_1 / r_2 = 0.5. The results of the calculation are shown in Table 2.

Table 2. The results of the calculation

Number of nodes in the mesh	Values	
	σ_n/P_1	ε_n, %
11	2,1458	0,2255
21	2,1437	0,2218
41	2,1570	0,2241
81	2,1466	0,2220
161	2,1380	0,2225

Subsequently, the calculations are carried out on a network with 81 nodes.

3.3. Analysis of the influence of the state of stress on the permeability to hydrogen of the thick-walled tube (long hollow cylinder).

In order to evaluate the influence of the stress state on the hydrogen diffusion kinetics in the wall of the thick-walled tube, the calculation was carried out initially without taking into account the influence of the stress state on the Kinetics of diffusion, and then taking it again into consideration. The studies were carried out for three cases of loading and effects of the hydrogenated medium:

1. the charge P_1 and the hydrogen medium act on the inner surface of the thick-walled tube;
2. the charge acts on the outer surface of the thick-walled tube, and the hydrogen on the inner surface;
3. the charge acts on the inner surface of the thick-walled tube, and the hydrogen on the outer surface.

The pressure in all calculations is $P_1 = P_2 = 20$ MPa, the dimensions of the tube: $r_1 = 5$ cm, $r_2 = 10$ cm.

In Fig. 3, the graphs of the hydrogen concentration according to the tube radius for case 1 are presented, in the absence of the influence of the constraints on the diffusion kinetics (dotted line) and taking account of this influence (full line).

The analysis shows that the stress state has an intensifying effect on the hydrogen saturability of the tube wall, and with the increase of the time of the effect of the stresses, it increases and the increase reaches 34%.

The influence of the stress on the hydrogen saturation kinetics for case 2 is shown in fig.4.

In this case, there is a stress-inhibiting effect on the hydrogen saturability of the tube walls, because the load causes compression stresses to occur. The largest difference in the hydrogen concentration graphs is 29% for $t_3 / t_r = 0.31$.

Fig. 5 illustrates the influence of the stress state on the hydrogen diffusion kinetics for case 3, when the charge acts from the inside, and the hydrogen from the outside

As can be seen, at certain points on the wall of the tube, the difference in the magnitude of the hydrogen concentration can reach 50% (at $t_2 = 0.15$), and destruction $t_2 = t_r$ it reaches 26%.

The analysis carried out makes it possible to conclude that taking into account the influence of stress state on the hydrogen permeability of the structures is necessary both under the action of compressive stresses (fig.4). With the predominance of tensile stresses (figures 3 and 5).

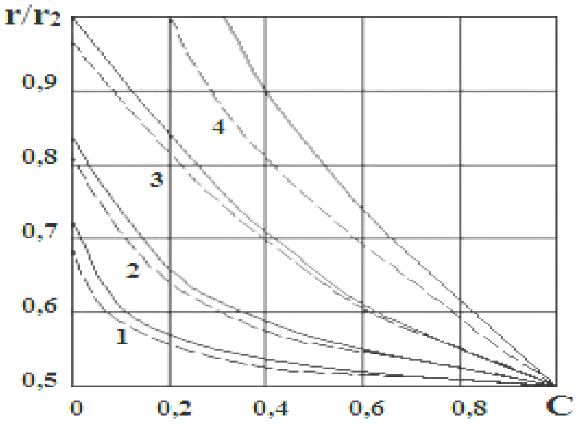

Figure 3: Concentration of hydrogen according to the thickness of the wall of the tube (case 1)
(dotted line - absence of the influence of constraints on the kinetics of diffusion, full line - with considering
(1 – t=0,076; 2 – t=0,15; 3 – t=0,31; 4 – t=tr=1)

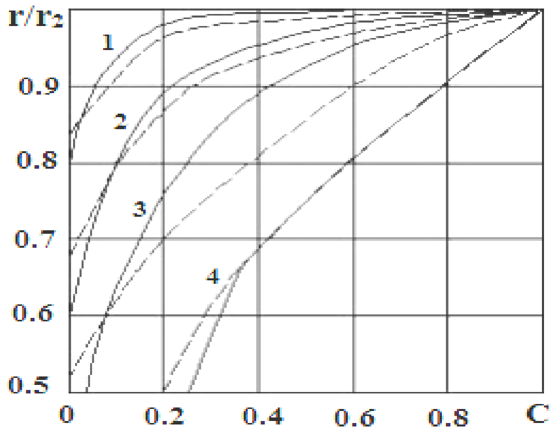

Figure 4: Concentration of hydrogen according to the wall thickness of the tube (case 2)
(dotted line - excluding the impact of stress, full line - with considering) , (1 – t=0,076; 2 – t=0,15; 3 – t=0,31; 4 – t=tr=1)

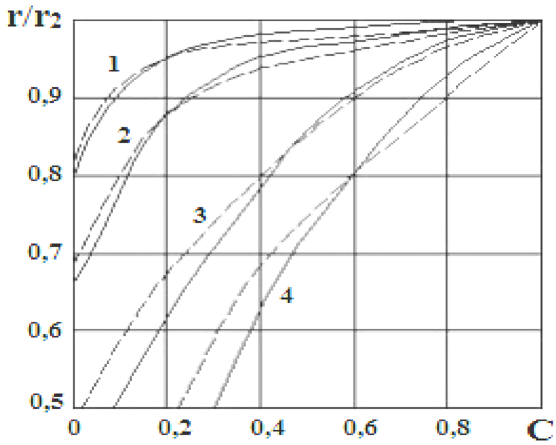

Fig.5: Concentration of hydrogen according to the wall thickness of the tube (case 3)
(dotted line - excluding the impact of stress, full line - with considering), (1 – t=0,076; 2 – t=0,15; 3 – t=0,31; 4 – t=tr=1)

3.4. Analysis of the influence of the loading scheme on the character of the stress state of a thick-walled tube under the action of the charge and the hydrogenation

In order to evaluate the effect of the stiffness of the stress state diagram that is characterized by the parameter *S*, the equations mentioned above, the mutual influence and the hydrogenated medium should be taken into consideration, which have been used on the mechanical characteristics of the material, and on the stress-strain condition, and the stress state on the hydrogen diffusion kinetics in the tube wall. That is to explain that the problem is part of non-linear deformation.

The same cases of loading and effects of the hydrogenated medium are examined as in paragraph 3.

For case 1 (the charge and the hydrogen acting from the inside), the results of the calculation in the form of diagrams of the concentration of hydrogen *C* and the circumferential stress σ are shown in Fig.6. It can be seen that in the zone close to the inner surface of the tube, on which the charge and the hydrogen are acting, the stress field is restructured, resulting in the most hydrogenated zones being discharged and the less hydrogenated - are charged.

In fig. 7, the hydrogen concentration diagrams *C*, the circumferential stresses σf and the longitudinal stresses σ_z for case 2 (external charge, hydrogen from the inside) are presented. As can be seen, in this case the change in the state of stress is less important, which is explained by the fact that the walls of the tube are in a compressed state and that is why the change in the mechanical characteristics is insignificant.

Finally, the illustrated fig.8 the character of the distribution of concentration hydrogen C, of the circumferential stresses σ_f according to the thickness of the wall of the tube for case 3 (charge from the inside, hydrogen from the outside). As can be seen, under the influence of the constraints of traction and hydrogenated medium a place a change of the mechanical properties of the material, resulting in a change in the character of distribution of the constraints. In addition, the greatest changes in the stress state occur in the internal zones of the tube wall and the values of these changes reach 18%.

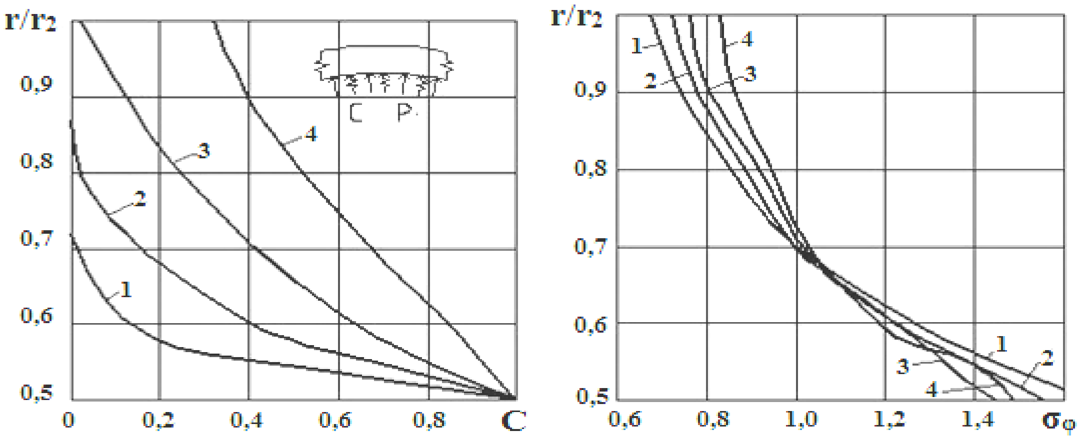

Figure 6: Hydrogen concentration and stresses σf at different times
(1 – *t*=0,076; 2 – *t*=0,15; 3 – *t*=0,31; 4 – *t*=t_r=1)

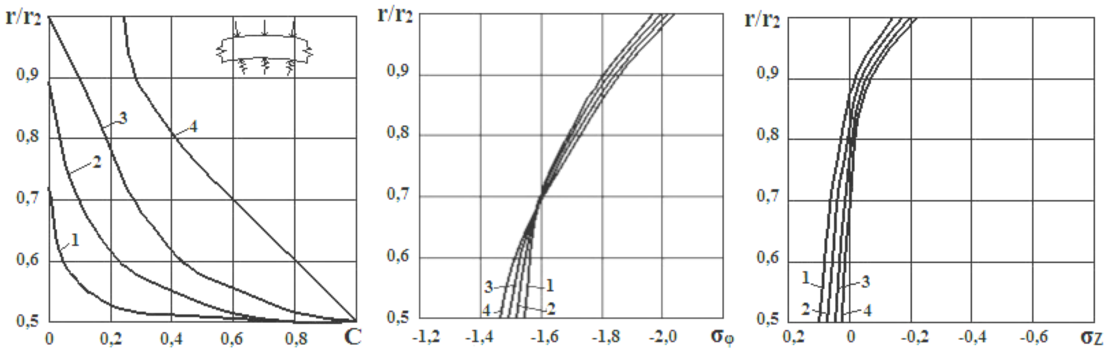

Figure 7: Concentration of hydrogen C, circumferential σf and longitudinal σz stresses in the tube
(case 2) at different times (1 – *t*=0,076; 2 – *t*=0,15; 3 – *t*=0,31; 4 – *t*=t_r=1)

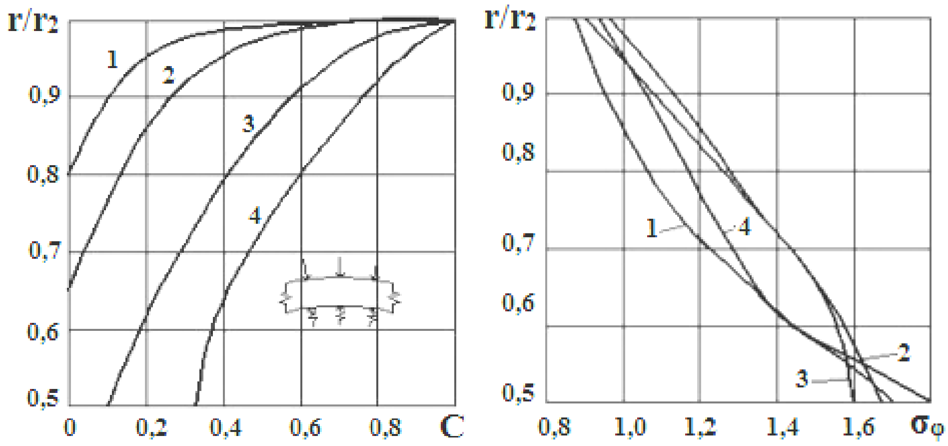

Figure 8: Hydrogen concentration and stresses σ_f at different times (case 3)
(1 – t=0,076; 2 – t=0,15; 3 – t=0,31; 4 – t=tr=1)

4. Conclusions

1. The elaborated model of material deformation in a hydrogenated medium takes into account the selective effect of hydrogen at low temperature on the mechanical characteristics of materials, leading to the appearance of an induced anisotropy and changing with saturation of the hydrogen material. The selectivity is expressed as a function of the value of the anisotropy induced not only by the concentration of hydrogen, but also by the state rigidity of the stress state.
2. In the proposed model, consideration is given to the influence of the type and level of stress state of the material on the penetration kinetics (permeation) of hydrogen in the material through the dependence of the coefficient of diffusion and the hydrogen absorption limit of the special parameter, characterizing the stress state diagram.
3. The analysis carried out shows that the established relations describe quite correctly the behavior of the thick-walled tube under the conditions of the combined action of the charge and of the hydrogenation taking into account the destructive action of hydrogen and allow to take into account the main effects, accompanying the interaction of the thick-walled tube with hydrogen.
4. The proposed method and the computational algorithm allow to perform a correct analysis of the kinetics of the hydrogenation changes and the stress state of a thick-walled tube taking into account the connectivity of the solved problem, I.e. the combined effect of hydrogen on the mechanical properties of the material and then on the state of stress of the tube and the influence of the state of stress on the diffusion kinetics of the material. Hydrogen in the walls of the thick-walled tube.
5. The numerical simulation carried out has shown that the most dangerous case is the case of the simultaneous action of the charge and of hydrogen on the surface Inside the wall of the thick-walled tube, because in this case the combination of the action of tensile stresses and hydrogen leads to the most intensive degradation of the tube material. It should be noted that such a case of the influence of the charge and of the hydrogenated medium is the most characteristic for the actual operating conditions of the thick-walled tubes.

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