Analytical and numerical solution to the problem of hydrogen diffusion in rotating cylindrical elastic bodies

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Abstract. The work is devoted to the solution of the problem of hydrogen diffusion in rotating cylindrical elastic bodies compressed by two distributed loads. The study includes the analytical determination of the stress state of the body on the basis of known stresses from the Hertz contact problem, the derivation of the hydrogen diffusion equation in a rotating body in the found field of elastic stresses, and the numerical solution of the obtained hydrogen diffusion equation. The numerical solution of the diffusion equation was carried out by the method of finite differences. According to the numerical solution of the diffusion equation, the effect of hydrogen concentration localization near the outer boundary was detected. This result is consistent with experimental studies of the distribution of hydrogen concentration in roller bearings. This problem is important for diagnostics of failures of rolling bearings due to hydrogen embrittlement.

Keywords: hydrogen diffusion, diffusion equation, rolling bearings, stress state

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1. Introduction

The content of hydrogen in metals and alloys leads to a decrease in the strength properties of the material. This problem is present in many machines and mechanisms, including rolling bearings. In particular, 75% of premature failures of wind turbine gearboxes are associated with the destruction of rolling bearings. Near-surface defects called white etching cracks have been found in damaged wind turbine bearings [1]. White etching cracks appear in the material under the combined influence of hydrogen and mechanical stresses. Studies show that increased hydrogen concentrations in bearing steels are a consequence of the diffusion of hydrogen into the metal due to the decomposition of the bearing grease as a result of a tribochemical reaction [2].

After the grease decomposes with the release of hydrogen atoms, the hydrogen begins to interact with the material, causing degradation of its mechanical properties. At the moment, there are several main approaches to describing the effect of hydrogen on the mechanical properties of materials: the HELP model of fracture due to local plasticity [3], the HEDE model of brittle fracture [4,5], the model taking into account the internal pressure of hydrogen

[6], and the bi-continuum model [7,8], which takes into account the influence of hydrogen with different binding energies on the mechanical characteristics of the material.

It is known that even extremely low concentrations of hydrogen lead to a deterioration in the mechanical properties of the material. If the limiting concentrations of hydrogen are not exceeded, the laws of diffusion formulated by Fick [9] are fulfilled. Generalizing Fick's Second Law to the three-dimensional case, we obtain the diffusion equation for material in an elastic body. And the hydrogen diffusion equation in the field of elastic stresses [10] makes it possible to describe the distribution of hydrogen in a metal due to its diffusion under the action of external loads.

In the present work, the hydrogen diffusion equation in a rotating cylindrical elastic body subjected to compression by distributed forces is investigated. This equation includes the hydrostatic component of the stress field, which must be determined at the first step of solving this problem. Its determination is based on the solution of the theory of elasticity problem of loading a body by external forces. This statement simulates the diffusion of hydrogen in the rolling elements of roller bearings during their operation.

This problem has great importance for understanding how the distribution of hydrogen affects the mechanical properties of the material when it leads to premature failure of bearings, and how to prevent it.

2. Determination of the stress state of a cylindrical elastic body

To find the stress state of a considered body, it is reasonable to turn to the solution of the Hertz contact problem of the compression of two cylinders initially touching along the line. The complete solution to this problem is presented in the book by N.M. Belyaev [11]. It is assumed that the cylindrical bodies have an infinite length, along which the compressive load p is distributed perpendicular to the line of contact. When the bodies are compressed, the line of contact, as a result of elastic strains, turns into a pressure area in the form of a strip of width 2b. During the solution, it was found that the half-width b of the pressure strip for two contacting cylinders of radii R_1 and R_2 is equal to

$$b = \sqrt{4p(\theta_1 + \theta_1)/(1/R_1 + 1/R_2)},\tag{1}$$

where ϑ defines the material parameters of both cylinders as

$$\vartheta_{1,2} = (1 - \nu_{1,2}^2) / \pi E_{1,2},\tag{2}$$

here ν is a Poisson's ratio, and E is Young's modulus.

To calculate stresses, elliptical coordinates α and β are entered

$$\begin{cases}
y = b \operatorname{ch} \alpha \operatorname{cos} \beta, \\
z = b \operatorname{sh} \alpha \operatorname{sin} \beta.
\end{cases}$$
(3)

The reference point of the Cartesian coordinates is associated with the point of initial contact of two cylinders, while the x-axis is directed along the axes of the cylinders, the positive direction of the z-axis for each cylinder is directed inside the considered cylinder.

In the introduced elliptical coordinates, the stresses along the areas perpendicular to the Cartesian coordinate axes in the contacting bodies have the form:

$$\begin{cases} \sigma_{x} = -\frac{2p}{\pi b} \frac{\lambda}{\lambda + \mu} e^{-\alpha} \sin\beta, \\ \sigma_{y} = -\frac{2p}{\pi b} e^{-\alpha} \sin\beta + \frac{2P}{\pi b} \sin\beta \sin\alpha \left(1 - \frac{\sin2\alpha}{\cosh2\alpha - \cos2\beta} \right), \\ \sigma_{z} = -\frac{2p}{\pi b} e^{-\alpha} \sin\beta - \frac{2P}{\pi b} \sin\beta \sin\alpha \left(1 - \frac{\sin2\alpha}{\cosh2\alpha - \cos2\beta} \right), \\ \tau_{yz} = -\frac{2p}{\pi b} \sin\beta \sin\alpha \frac{\sin2\beta}{\cosh2\alpha - \cos2\beta}, \\ \tau_{xy} = \tau_{zx} = 0. \end{cases}$$

$$(4)$$

However, using it in the diffusion equation turns out to be difficult, since explicit analytical expressions that convert elliptic coordinates back to Cartesian or polar ones do not exist.

The next way of solution is an attempt to use the theory of functions of a complex variable to find the stresses in the whole body from the known stress vector on the surface [12]. Since at the contact zone the stresses from the Hertz contact problem have an analytical form in polar coordinates

$$\begin{cases} \sigma_{r} = -\frac{2p}{\pi b} \sqrt{1 - \frac{R_{1}^{2} \sin^{2} \varphi}{b^{2}}}, \\ \sigma_{\varphi} = -\frac{2p}{\pi b} \sqrt{1 - \frac{R_{1}^{2} \sin^{2} \varphi}{b^{2}}}, \\ \tau_{r\varphi} = 0. \end{cases}$$
 (5)

In the complex analysis, according to the Goursat formulas, the mean normal stress σ is defined as

$$\sigma = 2Re\Phi(z),\tag{6}$$

where $\Phi(z)$ is a complex potential that is defined by an expression

$$\Phi(\zeta) = \frac{1}{2\pi i} \oint \frac{F(\varphi)ds}{s - \zeta} - \frac{1}{4\pi} \int_0^{2\pi} F(\varphi)d\varphi, \tag{7}$$

where ζ is a variable of coordinates of points of the unit circle on the complex plane, which was entered, when we use a conformal mapping to map the considered area to the inner of the unit circle on the complex plane, s is a boundary of the unit circle. The function $F(\varphi)$ is the stress vector of external loads on the outer surface of the considered body (Fig. 1).

The analytical calculation of the complex potential was considered for three types of external load $F(\varphi)$: in the form of an exact solution of the Hertz contact problem, in the form of an approximate cosine distribution, and in the form of a constant uniform distribution. The considered distributions are illustrated in Fig. 2. Since here we are dealing with the calculation of an improper integral, the solution of the integral could only be found for the case when the stress vector is represented as a constant.

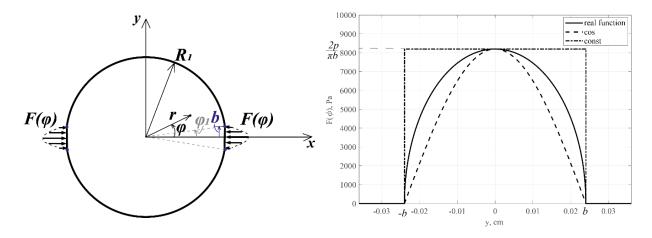


Fig. 1. Action of the stress vector on the outer boundary of the body

Fig. 2. Three considered options for setting an external load

For the points inside the body, the stresses have such a complicated form

$$\sigma(r,\varphi) = -\frac{p}{\pi R_1} + \frac{p}{\pi b} \arctan\left(\frac{\left(\left(\frac{r}{R_1}\right)^2 + \frac{2r}{R_1}\cos\varphi + 1\right) \operatorname{tg}\frac{b}{2R_1} - \frac{2r}{R_1}\sin\varphi}{\left(\frac{r}{R_1}\right)^2 - 1}\right) - \frac{p}{2\pi b} \arctan\left(\frac{\left(\left(\frac{r}{R_1}\right)^2 + \frac{2r}{R_1}\cos\varphi + 1\right) \operatorname{ctg}\frac{2b}{R_1} + \frac{2r}{R_1}\sin\varphi}{\left(\frac{r}{R_1}\right)^2 - 1}\right) - \frac{p}{2\pi b} \arctan\left(\frac{\left(\left(\frac{r}{R_1}\right)^2 + \frac{2r}{R_1}\cos\varphi + 1\right) \operatorname{ctg}\frac{2b}{R_1} - \frac{2r}{R_1}\sin\varphi}{\left(\frac{r}{R_1}\right)^2 - 1}\right).$$

$$(8)$$

And at the boundary, where the integrand function tends to infinity, we can use the Sokhotsky-Plemelj formulas [12]. This solution also turns out to be too complicated and cannot be used further in the hydrogen diffusion equation. As a result, the solution of the stress field obtained by the theory of functions of a complex variable also turns out to be too complicated and may not be used in a hydrogen diffusion equation.

To find analytical expressions of the stress state of the loaded cylindrical elastic body it was decided to use a graphical representation of the solution of the Hertz problem in elliptic coordinates (4), reconstructed in polar coordinates using the MATLAB application package [13], shown in Fig. 3. And according to the graphical representation of the dependences of mean stresses on polar coordinates, we can find the approximating functions f(r) and $g(\varphi)$, shown in Fig. 4. The found functions approximate the stress field from the Hertz contact problem with sufficient accuracy

$$f(r) = \frac{\alpha}{\sqrt{1 + \frac{(R_1 - r)^2}{b^2}}}, \qquad g(\varphi) = \frac{\beta}{(\varphi - \pi/2)^2 + \beta^2}, \tag{9}$$

where α and β are the parameters of approximation.

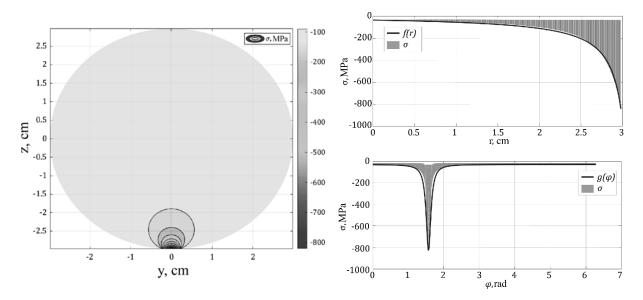


Fig. 3. The mean normal stress field σ from the contact problem

Fig. 4. Dependences of σ and functions f(r) and $g(\varphi)$ on polar coordinates r and φ

Based on the found dependencies (9), we can obtain an analytical expression of the mean normal stresses in a cylindrical body compressed by two symmetrical distributed loads applied at two diametrically opposite points of a cylindrical surface in a horizontal plane

$$\sigma(r,\varphi) = -\frac{2p}{\pi b} \frac{\alpha}{\sqrt{1 + \frac{(R_1 - r)^2}{b^2}}} \left(\frac{\beta}{\varphi^2 + \beta^2} + \frac{\beta}{(\varphi - \pi)^2 + \beta^2} \right). \tag{10}$$

The found stress state of a body was graphically represented in Fig. 5.

3. Analytical expression of the hydrogen diffusion equation in the field of elastic stresses

To determine the nature of the distribution of hydrogen concentration in rolling bearings, the equation of hydrogen diffusion in the field of elastic stresses is considered. It was obtained taking into account a number of assumptions: all properties of the metal are isotropic, the contribution from the magnetic and gravitational fields to the process of hydrogen diffusion is negligibly small, the diffusion coefficient of hydrogen and stresses in the body do not depend on the hydrogen concentration. As a result, the equation of hydrogen diffusion in the field of elastic stresses has the following form [10]

$$\frac{\partial C}{\partial t} = D\Delta C - \frac{DV_H}{RT} \nabla C \cdot \nabla \sigma - \frac{DV_H}{RT} C\Delta \sigma,\tag{11}$$

where C – hydrogen concentration, D – hydrogen diffusion coefficient, V_H – partial molar volume of hydrogen, σ – mean normal stress, R – gas constant, T – absolute temperature.

Since considered body rotates with a constant angular velocity ω , the transition to a rotating coordinate system can help to reduce the dynamic problem to a quasi-static one, and the equation turns to the form

$$\Delta C - \frac{V_H}{RT} \left[\frac{\partial C}{\partial r} \frac{\partial \sigma}{\partial r} + \frac{1}{r^2} \frac{\partial C}{\partial \varphi} \frac{\partial \sigma}{\partial \varphi} \right] - \frac{\omega}{D} \frac{\partial C}{\partial \varphi} - \frac{V_H}{RT} C \Delta \sigma = 0.$$
 (12)

Substituting the found hydrostatic component of the stress state of the body (10) into this hydrogen diffusion equation written in a rotating coordinate system (12), we obtain the analytical form of the hydrogen diffusion equation in the field of elastic stresses found on the basis of approximation of the graphical representation of the Hertz contact problem solution

$$\Delta C + \frac{2p}{\pi b} \frac{V_H}{RT} \left[\frac{\alpha b (R_1 - r)}{(b^2 + (R_1 - r)^2)^{\frac{3}{2}}} \left(\frac{\beta}{\varphi^2 + \beta^2} + \frac{\beta}{(\varphi - \pi)^2 + \beta^2} \right) \frac{\partial C}{\partial r} - \frac{2\beta \alpha}{r^2 \sqrt{1 + \frac{(R_1 - r)^2}{b^2}}} \left(\frac{\varphi}{(\varphi^2 + \beta^2)^2} + \frac{\varphi - \pi}{(\varphi^2 + \beta^2)^2} \right) \frac{\partial C}{\partial \varphi} \right] - \frac{\omega}{D} \frac{\partial C}{\partial \varphi} = 0.$$
(13)

The resulting equation (13) has a complicated form, so the exact analytical solution of the equation cannot be found. Only approximate analytical or numerical methods may be used. In this paper, we will present the numerical solution to this equation. To implement a numerical solution of the hydrogen diffusion equation the finite difference method is used.

4. Analytical description of the numerical solution realization

For a numerical solution, the hydrogen diffusion equation in rotating cylindrical elastic bodies under compression by distributed forces is rewritten in the following dimensionless form:

$$\frac{1}{\xi} \frac{\partial}{\partial \xi} \left(\xi \frac{\partial C}{\partial \xi} \right) + \frac{1}{\xi^2} \frac{\partial^2 C}{\partial \varphi^2} - V_1 \frac{\partial C}{\partial \xi} - V_2 \frac{\partial C}{\partial \varphi} = 0, \tag{14}$$

$$\xi = \frac{r}{R_1}, \qquad V_1 = AK_1, \qquad V_2 = AK_2 \frac{1}{\xi^2} + W, \qquad A = \frac{V_H P}{RT}, \qquad W = \frac{\omega R_1^2}{D},$$

$$K_1 = \frac{\partial \sigma}{\partial \xi}, \qquad K_2 = \frac{\partial \sigma}{\partial \varphi}, \qquad 0 \le \xi \le 1, \qquad 0 \le \varphi \le 2\pi.$$
(15)

A uniform difference mesh along the coordinates ξ and φ of size $N \times M$ (N = 100, M = 200) was constructed to solve equation (14). The partial derivatives in equation (14) were replaced by the following approximate difference relations [14], as an approximation of the first derivative with respect to ξ and φ , the right or left difference derivative is used, it depends on the sign of the coefficients in V_1 and V_2 :

derivative is used, it depends on the sign of the coefficients in
$$V_1$$
 and V_2 :
$$\frac{1}{\xi} \frac{\partial}{\partial \xi} \left(\xi \frac{\partial C}{\partial \xi} \right) = \frac{(\xi_{i+1} + \xi_i)C_{i+1,j} - (\xi_{i+1} + 2\xi_i + \xi_{i-1})C_{i,j} + (\xi_i + \xi_{i-1})C_{i-1,j}}{2\xi \Delta \xi^2},$$

$$\frac{\partial^2 C}{\partial \varphi^2} = \frac{C_{i,j+1} - 2C_{i,j} + C_{i,j-1}}{\Delta \varphi^2}, \quad \frac{\partial C}{\partial \xi} = \begin{cases} \frac{C_{i+1,j} - C_{i,j}}{\Delta \xi}, V_1 > 0 \\ \frac{C_{i-1,j} - C_{i,j}}{\Delta \xi}, V_1 < 0 \end{cases}$$

$$(16)$$

$$\frac{\partial C}{\partial \varphi} = \begin{cases} \frac{C_{i,j+1} - C_{i,j}}{\Delta \varphi}, V_2 > 0\\ \frac{C_{i,j-1} - C_{i,j}}{\Delta \varphi}, V_2 < 0 \end{cases}$$

where $0 \le i \le N - 1$, $0 \le j \le M - 1$.

Thus, the considered equation can be written in the form:

$$\left(\frac{2\xi_{i+\frac{1}{2}}}{\xi_{i}\Delta\xi_{i}(\Delta\xi_{i}+\Delta\xi_{i-1})} + \frac{|V_{1}|-V_{1}}{2\Delta\xi_{i}}\right) \left(C_{i+1,j}-C_{i,j}\right) + \\
+ \left(\frac{2\xi_{i-\frac{1}{2}}}{\xi_{i}\Delta\xi_{i-1}(\Delta\xi_{i}+\Delta\xi_{i-1})} + \frac{|V_{1}|+V_{1}}{2\Delta\xi_{i-1}}\right) \left(C_{i-1,j}-C_{i,j}\right) + \\
+ \left(\frac{2}{\xi_{i}^{2}\Delta\varphi_{j}(\Delta\varphi_{j}+\Delta\varphi_{j-1})} + \frac{|V_{2}|-V_{2}}{2\Delta\varphi_{j}}\right) \left(C_{i,j+1}-C_{i,j}\right) + \\$$
(17)

$$\begin{split} &+ \bigg(\frac{2}{\xi_i^2 \Delta \varphi_{j-1} \Big(\Delta \varphi_j + \Delta \varphi_{j-1} \Big)} + \frac{|V_2| + V_2}{2 \Delta \varphi_{j-1}} \bigg) \Big(C_{i,j-1} - C_{i,j} \Big) = 0. \\ &\text{where } \xi_{i+\frac{1}{2}} = \frac{\xi_{i+1} + \xi_i}{2}, \ \xi_{i-\frac{1}{2}} = \frac{\xi_i + \xi_{i-1}}{2}. \end{split}$$

Difference scheme can be written as

$$a_{i,j} C_{i,j-1} + b_{i,j} C_{i,j+1} + d_{i,j} C_{i-1,j} + e_{i,j} C_{i+1,j} - c_{i,j} C_{i,j} = -f_{i,j},$$
 where

$$\begin{split} a_{i,j} &= \frac{2}{\xi_i^2 \Delta \varphi_{j-1} \left(\Delta \varphi_j + \Delta \varphi_{j-1} \right)} + \frac{|V_2| + V_2}{2 \Delta \varphi_{j-1}}, b_{i,j} = \frac{2}{\xi_i^2 \Delta \varphi_j \left(\Delta \varphi_j + \Delta \varphi_{j-1} \right)} + \frac{|V_2| - V_2}{2 \Delta \varphi_j}, \\ d_{i,j} &= \frac{2 \xi_{i-\frac{1}{2}}}{\xi_i \Delta \xi_{i-1} \left(\Delta \xi_i + \Delta \xi_{i-1} \right)} + \frac{|V_1| + V_1}{2 \Delta \xi_{i-1}}, \qquad e_{i,j} &= \frac{2 \xi_{i+\frac{1}{2}}}{\xi_i \Delta \xi_i \left(\Delta \xi_i + \Delta \xi_{i-1} \right)} + \frac{|V_1| - V_1}{2 \Delta \xi_i}, \\ c_{i,j} &= a_{i,j} + b_{i,j} + d_{i,j} + e_{i,j}, \qquad f_{i,j} &= 0. \end{split}$$

Next, the difference scheme (18) was rewritten in matrix form

$$A_j Y_{j-1} - C_j Y_j + B_j Y_{j+1} = -F_j,$$
 where

To solve the resulting difference scheme (19), the tridiagonal matrix algorithm (or, otherwise, Thomas algorithm) [14] was used.

In our case average normal stresses (10) have the following form $\sigma = -Pf(\xi)g(\varphi), \tag{20}$

where
$$P = \frac{2p}{\pi b}, \qquad f(\xi) = \frac{\alpha}{\sqrt{1 + \frac{(1 - \xi)^2}{b^2}}},$$
$$g(\varphi) = \left(\frac{\beta}{\varphi^2 + \beta^2} + \frac{\beta}{(\varphi - \pi)^2 + \beta^2} + \frac{\beta}{(\varphi - 2\pi)^2 + \beta^2}\right),$$
then

$$\begin{split} A &= \frac{V_H P}{RT} = \frac{2V_H p}{\pi RT b}, \qquad W = \frac{\omega R_1^2}{D}, \\ K_1 &= \frac{\partial \sigma}{\partial \xi} = -\alpha \beta b \frac{(1 - \xi)}{\sqrt{(b^2 + (1 - \xi)^2)^3}} \left(\frac{1}{\varphi^2 + \beta^2} + \frac{1}{(\varphi - \pi)^2 + \beta^2} + \frac{1}{(\varphi - 2\pi)^2 + \beta^2} \right), \\ K_2 &= \frac{\partial \sigma}{\partial \varphi} = 2\alpha \beta b \frac{1}{\sqrt{b^2 + (1 - \xi)^2}} \left(\frac{\varphi}{(\varphi^2 + \beta^2)^2} + \frac{\varphi - \pi}{((\varphi - \pi)^2 + \beta^2)^2} + \frac{\varphi - \pi}{((\varphi - \pi)^2 + \beta^2)^2} + \frac{\varphi - \pi}{((\varphi - \pi)^2 + \beta^2)^2} \right). \end{split}$$

$$+ \frac{\varphi - 2\pi}{((\varphi - 2\pi)^2 + \beta^2)^2},$$

$$V_1 = AK_1 = -\frac{2V_H p}{\pi R T} \alpha \beta \frac{(1 - \xi)}{\sqrt{(b^2 + (1 - \xi)^2)^3}} \left(\frac{1}{\varphi^2 + \beta^2} + \frac{1}{(\varphi - \pi)^2 + \beta^2} + \frac{1}{(\varphi - \pi)^2 + \beta^2} + \frac{1}{(\varphi - 2\pi)^2 + \beta^2}\right),$$

$$V_2 = AK_2 \frac{1}{\xi^2} + W = \frac{4V_H p}{\pi R T} \alpha \beta \frac{1}{\xi^2} \frac{1}{\sqrt{b^2 + (1 - \xi)^2}} \left(\frac{\varphi}{(\varphi^2 + \beta^2)^2} + \frac{\varphi - 2\pi}{((\varphi - 2\pi)^2 + \beta^2)^2} + \frac{\omega R_1^2}{D}\right).$$
(21)

5. Numerical results of the solution of the hydrogen diffusion equation

The program code developed to implement the described procedure of the numerical method was written in the C++ programming language. The distribution fields of hydrogen concentration in the body and plots of the dependence of concentration on polar coordinates for the boundary conditions of the first kind and the third kind are represented in Figs. 5- 8. The developed program allows us to set various input parameters for the rotation speed, geometry sizes, finite difference mesh sizes, and various boundary conditions. It is also allowed to construct a non-uniform mesh with thickening near the surface and load application points.

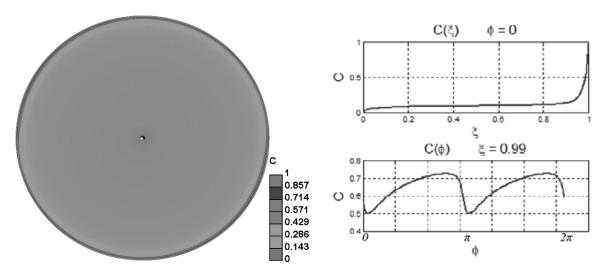


Fig. 5. Concentration field for the boundary conditions of the first kind

Fig. 6. Concentration plots for the boundary conditions of the first kind

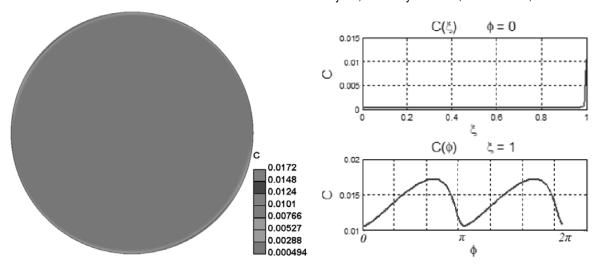


Fig. 7. Concentration field for the boundary conditions of the third kind

Fig. 8. Concentration plots for the boundary conditions of the third kind

On these plots, a sharp increase in hydrogen concentration in the subsurface layer is observed. This result is consistent with experimental studies of the distribution of hydrogen concentration in roller bearings. In addition, the distribution of hydrogen concentration over the angles φ shows that near the points of load application ($\varphi=0$ and $\varphi=\pi$), the hydrogen concentration takes the smallest values. This effect is explained by the fact that diffusing hydrogen atoms tend to the region of the material where tensile stresses are distributed.

6. Conclusions

In the framework of this paper, the stress state of the rotating elastic body loaded by two distributed forces was obtained. An analytical form of the equation of the hydrogen diffusion in the rotating body under the field of elastic stresses was written. This equation was solved using numerical methods. A numerical solution of the diffusion equation made it possible to detect the effect of localization of the hydrogen concentration near the outer surface of the body. This result is consistent with experimental research on the hydrogen concentration distribution in roller bearings. The results obtained in this work can help in describing the hydrogen impact on the mechanical properties of rolling bearing materials. This problem requires further research in order to construct the description of the influence of the hydrogen distribution field on the mechanical properties of the material.

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