



MODELING OF HYDROGEN-INDUCED FRACTURE TOUGHNESS DEGRADATION OF PIPE STEEL

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Abstract. A correction to the existing hydrogen-induced fracture toughness degradation model was introduced. We formulated a new degradation model that simplifies predictions without compromising accuracy, effectively reducing the mean absolute error from 93 N/mm to 1.4 N/mm on experimental data – a reduction of more than 60 times. The fundamental difference between degraded steel and its as-delivered (reserve) state was demonstrated, and two separate models were proposed for each case. It was shown that the difference between using a constant stress value and the solution to the Lamé equation is only 2%, which justified simplifying the chosen diffusion equation to a classical form. An example application of the new model, together with the solution to the diffusion equation, was presented. The developed models were applied to the parameters of real pipes and validated against experimental data.

Key words: steel, mechanical characteristics, hydrogen, degradation, modeling, experimental data, fracture toughness, J-integral, diffusion equation, error reduction.

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1. INTRODUCTION

Green energy is mainstream in the current research activities. One of the promising green energy carriers is hydrogen. However, the widespread adoption of hydrogen is challenged by its interaction with materials, particularly its impact on the mechanical properties of structural steels [1]. As a result, steel structural components affected by hydrogen no longer meet the required operational standards. One critical issue associated with hydrogen exposure is hydrogen embrittlement, which can significantly degrade material performance and compromise the safety and reliability of infrastructure.

Hydrogen can be transported through existing natural gas pipelines, though this requires managing technical challenges like hydrogen embrittlement of steel and operational deterioration of mechanical properties [2–4]. Fracture toughness is widely recognized as a key mechanical property for evaluating the susceptibility of steels to hydrogen embrittlement [4–6]. Accurately assessing the loss of fracture toughness under operational conditions involving mechanical loading and hydrogen exposure is crucial for ensuring the serviceability and safety. The experimental studies of fracture toughness under hydrogen exposure are often complicated and time-consuming. Therefore, it is more efficient to predict the fracture toughness during operation of pipe steels under hydrogen service by methods of machine learning, in particular, neural networks, which show the good results [7, 8]. To do this, it is necessary to know the hydrogen concentration throughout the thickness of the pipe, as hydrogen diffusion plays a decisive role in embrittlement phenomena. This requires solving the diffusion equation while considering factors such as temperature, mechanical loading, and others.

Machine learning methods are widely used to predict the mechanical properties of materials [7–11], considering hydrogen embrittlement phenomenon, as well [7–9]. Over the last decade, phase-field fracture modeling has revolutionized fracture mechanics by providing

a unified variational framework [7, 9]. This approach effectively captures key fracture phenomena such as crack nucleation, propagation, merging, and branching. Due to these advantages, phase-field models have been widely applied and extended to a broad spectrum of fracture problems.

In recent years, significant efforts were devoted to using advances in machine learning to precisely model physical phenomena [8, 12, 13]. Among these efforts, physics-informed neural networks (PINNs) or deep learning techniques have been widely adopted to solve partial differential equations and other problems effectively [8]. These approaches integrate physical laws directly into the neural network training process, enabling data-driven solutions that respect underlying physics, thereby enhancing accuracy and reliability in modeling complex systems.

While the integration of physical models into PINNs represents a promising direction for future research, the current study is primarily dedicated to developing and improving models for fracture toughness degradation in pipeline steels under hydrogen exposure and operational conditions. These advancements will lay the groundwork for future incorporation into PINNs, ultimately aiming to create robust predictive frameworks for assessing and mitigating hydrogen-induced degradation in structural materials.

2. MATERIALS AND METHODS

The research object was the 17H1S pipe steel in different states, as-delivered and after 38 years of operation on gas transit pipeline. The outer diameter is 1220 mm and wall thickness 12 mm. Mechanical characteristics of steels were as follows: 17H1S in the as-delivered state – ultimate strength $\sigma_{UTS} = 568$ MPa, impact toughness $KCV = 129$ J/cm², in the post-operated state – $\sigma_{UTS} = 570$ MPa, $KCV = 103$ J/cm².

Information on pipeline steel properties used for parameter fitting and validation provided below in Table 1.

The parameters J_0 corresponding to the start of the crack and fracture toughness, the critical value of the stress intensity factor K_{Jc} , were determined [4] by standardized testing method using the J -integral method, following the requirements of the ASTM E 1820 standard. Single edge notched bend specimens with dimensions of 4×15×100 mm were used. Before bending loading, they were electrolytically hydrogen-charged in a solution of H₂SO₄ (pH1) + 10 g/l of thiourea at a cathode current density of $i = 0.05$ and 1.0 mA/cm² for 120 hours.

Hydrogen concentration was determined by heat extraction technique using Eltra H-500 Analyser under the temperature of 950°C.

Table 1

Data gathered for parameter fitting and validation purposes to develop a fracture toughness degradation model

Test condition	Hydrogen concentration C_0 , ppm	J_0 , N/mm	Fracture toughness K_{Jc} , MPa·√m
Steel of reserve pipe			
No pre-treatment	0.18	90.2	143.4
Hydrogen pre-charged	1.29	85.4	139.5
Hydrogen pre-charged	3.82	62.0	118.9
Pipe steel after 38 years of operation			
No pre-treatment	0.29	75.0	130.7
Hydrogen pre-charged	1.65	46.5	102.9
Hydrogen pre-charged	5.14	37.9	92.9

3. RESULTS AND DISCUSSION

3.1 Derivation of diffusion equation

The corrected and newly derived model requires hydrogen concentration as an input parameter. These values can be obtained by solving the diffusion equation. At this stage, it is important to consider the underlying physical processes in order to select the most appropriate set of governing equations. In our case, the gas pipeline operates under controlled conditions, meaning that its temperature is carefully regulated by pipeline operators and the system is under pressure. Since there is no temperature gradient, temperature does not affect the diffusion process, and the diffusion coefficient remains constant throughout the depth of the pipe wall. To investigate the influence of stress, we must perform a series of mathematical manipulations.

The parameters of the pipe were selected based on real pipes used for natural gas transportation [4] and are as follows: internal radius $r_1 = 598$ mm, external radius $r_2 = 610$ mm, initial hydrogen concentration $C_0 = 0$ ppm, hydrogen concentration near inner pipe surface $C_1 = 4$ ppm, hydrogen concentration near outer pipe surface $C_2 = 0$ ppm, hydrogen diffusion coefficient $D = 3.2 \cdot 10^{-3}$ mm²/s. The pipe cross-section scheme is presented in Fig. 1.

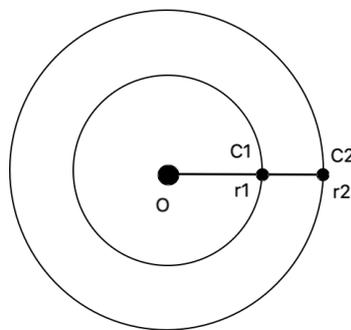


Figure 1. Pipe cross-section

According to Fick's first law, the concentration flux with chemical potential is given by:

$$J = -D\nabla C - \frac{DC}{RT} \nabla v, \quad (1)$$

where J – particle flux density;
 D – diffusion coefficient;
 ∇ – gradient operator;
 C – hydrogen concentration;
 ∇C – gradient of hydrogen concentration;
 R – universal gas constant;
 T – temperature;
 ∇v – gradient of chemical potential/

The chemical potential in presence of stress is expressed as [14]:

$$v = v_0 + V\sigma, \quad (2)$$

where v_0 – chemical potential without stress;
 V – partial molar volume;
 σ – mechanical stress.

Considering the gradient properties and fact that $v_0 = \text{const}$, the equation becomes:

$$J = -D\nabla C - \frac{DC}{RT} V \nabla \sigma \quad (3)$$

This means that in order to apply Fick’s second law and solve it, we need to formally express $\nabla\sigma$ (mechanical stress).

To determine the stress in a pipe under internal pressure, we refer to static mechanics. By analyzing the forces on a hollow cylinder (the pipe model), we use hoop stress, which is twice as large as the radial stress [15]:

$$\sigma_1 = \frac{pr}{t}, \tag{4}$$

where p – internal pressure;
 r – pipe radius;
 t – wall thickness.

This solution is valid for thin-walled pipes, where the ratio of wall thickness to radius is small ($t/r \ll 1$). For the comparison, we also consider the Lamé equation, which is applicable to thick-walled cylinders. The hoop stress is calculated as:

$$\sigma_\theta(r) = A + \frac{B}{r^2}, \tag{5}$$

where

$$A = \frac{p_1 r_1^2 - p_2 r_2^2}{r_2^2 - r_1^2}, \tag{6}$$

$$B = \frac{(p_1 - p_2)r_2^2 r_1^2}{r_2^2 - r_1^2}, \tag{7}$$

p_1 – internal pressure;
 p_2 – external pressure;
 r_1 – inner radius;
 r_2 – outer radius;
 r – radius for calculating stress.

Comparison between them is shown in the graph in Fig. 2.

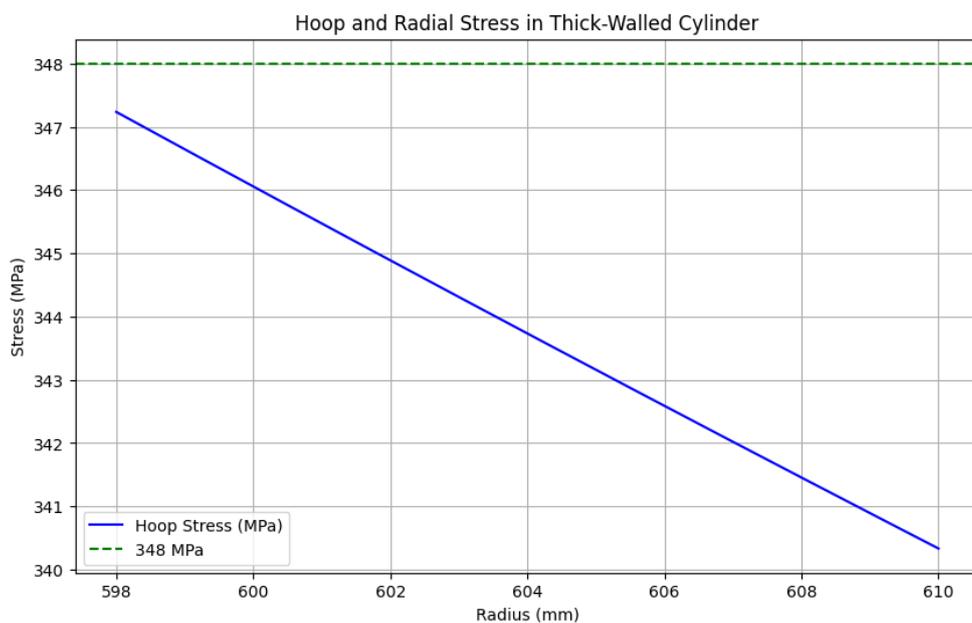


Figure 2. Comparison between constant hoop stress calculation and solution by Lamé equation

The biggest difference between them is 8 MPa at 610 mm of the pipe, which in turn means 2% of deviation. Such small difference isn't influencing diffusion much and can be neglected, ultimately yielding $\sigma = const$. Considering gradient properties that gradient of constant is 0 (zero) equation (3) becomes:

$$J = -D\nabla C \quad (8)$$

One can apply mass conservation law and derived Fick's first law of diffusion

$$\frac{\partial C}{\partial t} = D\nabla^2 C \quad (9)$$

According to Raichenko [14], equation (9) after switching to cylindrical coordinate system becomes:

$$\frac{\partial C_{r,t}}{\partial t} = D \left(\frac{\partial^2 C(r,t)}{\partial r^2} + \frac{1}{r} \frac{\partial C(r,t)}{\partial r} \right), \quad (10)$$

where $\frac{\partial}{\partial t}$ – partial derivative with respect to time;

$\frac{\partial}{\partial r}$ – partial derivative with respect to radius;

$\frac{\partial^2}{\partial r^2}$ – second partial derivative with respect;

D – diffusion coefficient;

$C_{r,t}$ – hydrogen concentration as function of r and t variables.

Analytical solution for equation (10) with initial and boundary conditions $C(r, 0) = 0$ $C(r_1, t) = C_1$ $C(r_2, t) = 0$ is [16]:

$$C(r, t) = C_1 \frac{\ln\left(\frac{r_2}{r}\right)}{\ln\left(\frac{r_2}{r_1}\right)} + \pi \sum \frac{c_1 J_0(\beta_n r_1) J_0(\beta_n r_2) U_0(\beta_n r)}{J_0^2(\beta_n r_1) - J_0^2(\beta_n r_2)} e^{-\beta_n^2 D t}, \quad (11)$$

where $U_0(r) = J_0(r) \cdot r \cdot Y_0(r_2) - J_0(r_2) \cdot Y_0(r) \cdot r$;

J_0 Y_0 – Bessel's functions of first and second orders accordingly;

β_n – roots of equation $U_0(r = r_2) = 0$.

Graph of hydrogen concentration distribution over time at a 2 mm from the inner surface of the pipe is presented in Fig. 3 (cross-section of the pipe at a specific radius).

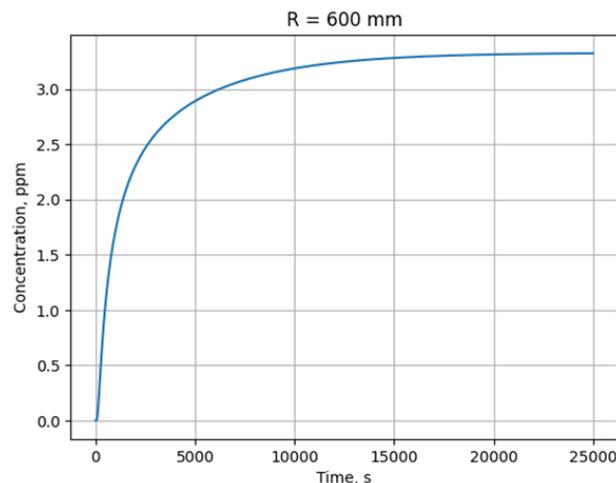


Figure 3. Graph of hydrogen concentration distribution over time at a 2 mm cross-section from the inner surface of the pipe

3.2. Correction of existing fracture toughness model

We consider the existing fracture toughness degradation model [6]:

$$G_c(c) = \begin{cases} (\zeta - 1) \frac{c}{c_0} G_c & G_c(c) > \xi G_c \\ \xi G_c & G_c(c) \leq \xi G_c, \end{cases} \quad (12)$$

where G_c – fracture toughness (critical energy release rate);
 ξ – parameter controlling the reduction of G_c .

In this analysis, we assumed that mechanical parameter cannot decrease more by than half; therefore $\xi = 0.5$ was selected for both analysed steels. The parameters C_0 and G_c were determined from experimental data (Table 1). Specifically, the pairs $C_0 = 0.18$ ppm, $G_c = 75$ N/mm and $C_0 = 0.29$ ppm, $G_c = 90$ N/mm correspond to the as-delivered (reserved) and post-operated steels, respectively. Given these values, function (12) can be expressed as follows:

$$G_c(c) = \begin{cases} (\zeta - 1) \frac{c}{259} & G_c(c) > 37.5 \\ 37.5 & G_c(c) \leq 37.5 \end{cases} \quad (13)$$

To estimate ζ , we employ the method of least squares, comparing the model to experimental data and calculating the prediction error. According to the formulas [2] for calculating the coefficients of a linear function, the model is given by

$$y_0 = \beta_0 + \beta_1 x + \epsilon, \quad (14)$$

where the coefficients are determined as follows:

$$\beta_1 = \frac{S_{xy}}{S_{xx}} \quad (15)$$

with

$$S_{xx} = \sum_{i=1}^n (x_i - \bar{x})^2 \quad (16)$$

$$S_{xy} = \sum_{i=1}^n y_i (x_i - \bar{x}) \quad (17)$$

and

$$\beta_0 = \bar{y} - \beta_1 \bar{x}. \quad (18)$$

Here (x_i, y_i) pairs of observed data and ϵ – represents the error term. Having determined the coefficients, the resulting function (13) is:

$$G_c(c) = \begin{cases} 0.00007c & G_c(c) > 37.5 \\ 37.5 & G_c(c) \leq 37.5 \end{cases} \quad (19)$$

Graph of this function with experimental points is shown in Fig. 4.

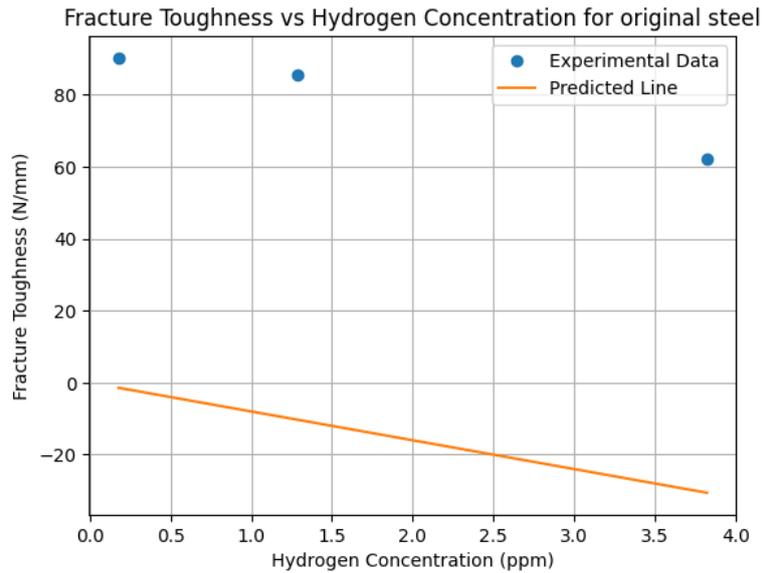


Figure 4. Existing model prediction compared to experimental data

The existing model demonstrates poor performance, as it predicts negative values for fracture toughness, which is not physically meaningful. The mean absolute error for this model is 93 N/mm. The discrepancy suggests a possible typographical error in the formulation. To address this issue, we introduce an additional material parameter η to account for model bias.

$$G_c(c) = \begin{cases} ((\zeta - 1) \frac{c_0}{c} G_c + \eta) & G_c(c) > \xi G_c \\ \xi G_c & G_c(c) \leq \xi G_c \end{cases} \quad (20)$$

By fitting the parameters of model (20) using the same method of least squares we obtain the following function:

$$G_c(c) = \begin{cases} \frac{208.3}{c} + 37.7 & G_c(c) > 37.5 \\ 37.5 & G_c(c) \leq 37.5 \end{cases} \quad (21)$$

A graph of the function is presented in Fig. 5.

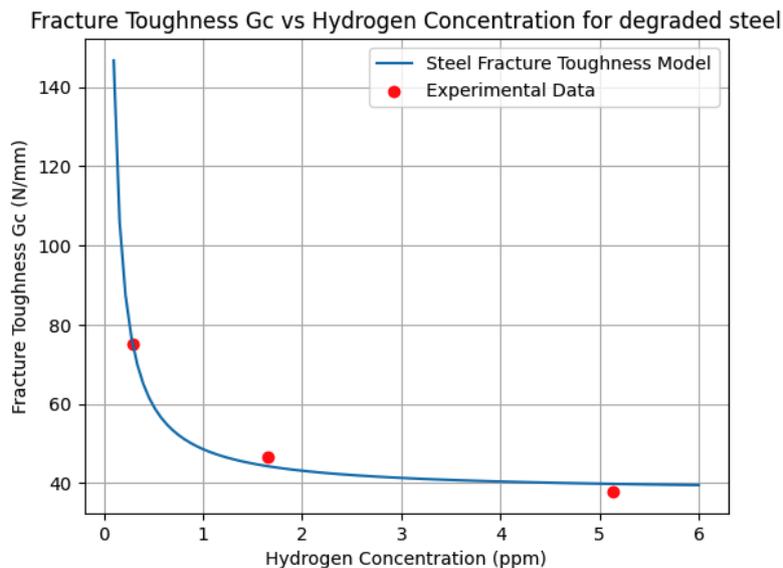


Figure 5. Fracture toughness prediction using the corrected model for the degraded steel depending on hydrogen concentration

The mean absolute error for the corrected model is 1.46 N/mm indicating a significant improvement accuracy.

3.3. Development of simpler model based on relationships between relative values of hydrogen concentration and fracture toughness

For as-delivered steel, we propose an alternative model. This model exploits the relationship between the relative concentration, scaled by its maximum value, and the relative fracture toughness, also scaled by its maximum value. Based on these relationships, the function is defined as:

$$G(c) = G_{max} \left[\frac{c}{c_{max}} k + b \right], \tag{22}$$

where G_{max} – is the maximum value of fracture toughness;
 C_{max} – is the maximum hydrogen concentration, both determined experimentally. The coefficients k and b were fitted using the least square method. Substituting the fitted values, the function becomes:

$$G(c) = G_{max} \left[\frac{c}{c_{max}} (-8) + 83 \right]. \tag{23}$$

A graph of the model is shown in Fig. 6.

The mean absolute error for this function is 1.6 N/mm. Our model shows good agreement with experimental results – for example, [4–6, 17] as well as with other models reported in literature [17]. We differentiate between two types of steel in our analysis: as-delivered (reserve pipe) and degraded (operated pipe). Based on graphs and models, we can conclude that the degradation of fracture toughness differs significantly between these two types. The fracture toughness degradation of the as-delivered steel is well approximated by linear model, whereas that for the degraded steel is better described by a reciprocal function. This difference arises from the physical characteristics of the steels, specifically the presence of vacancies and sites for hydrogen accumulation and trapping. In operated steels, increased damage allows hydrogen to be permeated and trapped more readily, which accelerates hydrogen embrittlement and consequently lead to a more pronounced degradation of fracture toughness.

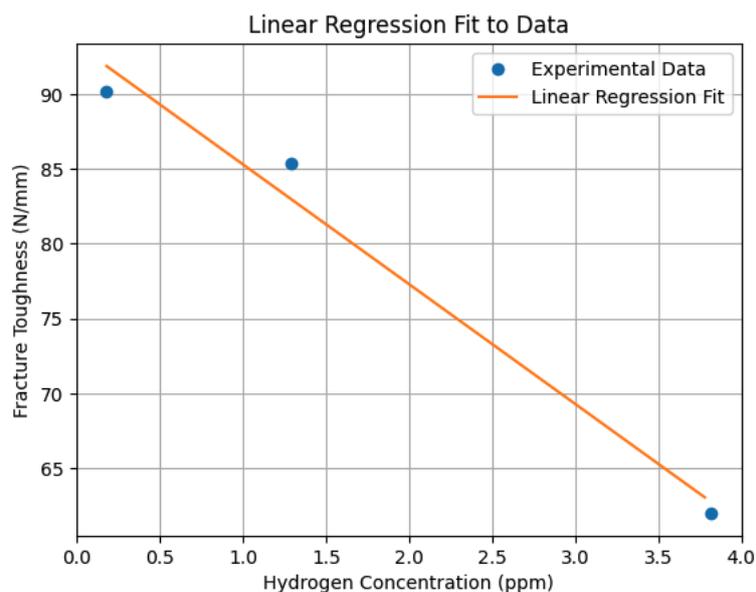


Figure 6. Fracture toughness prediction using the developed model of relative feature for as-delivered steel (reserved pipe) depending on hydrogen concentration

3.4. Modeling using solution of established hydrogen diffusion equation, corrected and our fracture toughness models

The developed models were applied to real pipeline parameters to assess the impact of hydrogen exposure on fracture toughness. By solving the diffusion equation under operational conditions, it was determined that the maximum hydrogen concentration within the pipe wall reaches 4 ppm at a depth of 2 mm from the inner radius after approximately 7 hours of exposure. Utilizing this concentration as input for the corrected fracture toughness degradation model, the predicted reduction in fracture toughness was found to be 10% compared to the initial value.

This result demonstrates the effectiveness of the new model in accurately capturing the degradation process. The model's predictions align closely with experimental data, confirming its reliability for practical applications. The approach also highlights the importance of considering both the physical diffusion process and material-specific parameters when evaluating hydrogen-induced embrittlement in pipeline steels.

Overall, the integration of the analytical solution to the diffusion equation with the improved fracture toughness model provides a robust framework for predicting material performance under hydrogen service. These findings support the use of simplified yet accurate models for operational safety assessments and maintenance planning in hydrogen transport infrastructure.

4. CONCLUSIONS

An analysis of the existing hydrogen-induced fracture toughness degradation model was carried out and its inconsistency with experimental data was established.

New models for fracture toughness degradation in pipeline steels under hydrogen exposure and operational conditions were developed that describes the experimental data more accurately and simply. A Physics-Informed Neural Networks were used for predicting hydrogen diffusion in the wall of a gas pipeline. Physical factors that may influence diffusion were considered, and the use of a simpler classical diffusion model was justified.

Due to a significant difference in fracture toughness degradation depending on hydrogen concentration observed for the pipeline steels in different state (as-delivered and operated one), two separate models were proposed for each case.

An example application of the new model, together with the solution to the diffusion equation, was presented. The developed models were applied to the parameters of real pipelines and validated against experimental data.

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УДК 539.3

МОДЕЛЮВАННЯ ДЕГРАДАЦІЇ ТРІЩИНОСТІЙКОСТІ У ТРУБНІЙ СТАЛІ ПІД ВПЛИВОМ ВОДНЮ

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Резюме. У роботі запропоновано уточнення до існуючої моделі деградації тріщиностійкості трубної сталі під впливом водню шляхом введення додаткового коефіцієнта матеріалу. Сформульовано нову модель деградації, яка дозволяє значно спростити процес прогнозування без втрати точності. Запропонована модель оперує відносними концентраціями водню та тріщиностійкістю, що дало змогу знизити середню абсолютну похибку більш ніж у 60 разів.

Показано фундаментальну різницю між деградованою сталлю після експлуатації та її вихідним станом, для кожного з яких розроблено окремі моделі. Для обох моделей використано метод найменших квадратів для визначення коефіцієнтів на основі експериментальних даних. Виведено рівняння дифузії водню з урахуванням механічного навантаження, що діє на стінку труби. Доведено, що різниця між використанням сталого значення напруження та розв'язком рівняння Ламе становить лише 2%, що дозволяє спростити рівняння дифузії до класичної форми. Наведено приклад застосування нової моделі разом із розв'язком рівняння дифузії для реальних параметрів труб. Розроблені моделі апробовано на експериментальних даних і показано високу точність прогнозування деградації тріщиностійкості сталі. Моделі враховують вплив концентрації водню по товщині стінки труби. Встановлено, що деградація тріщиностійкості у сталі після тривалої експлуатації відбувається значно інтенсивніше, ніж у сталі у вихідному стані. Для резервної сталі деградація добре описується лінійною моделлю, а для деградованої – оберненою функцією. Моделі можуть бути використані для оцінювання технічного стану трубопроводів, що транспортують водень чи водневмісні середовища. Обґрунтовано можливість подальшої інтеграції розроблених моделей у фізично-інформовані нейронні мережі для підвищення точності прогнозування. Отримані результати можна використати для оцінювання залишкового ресурсу водневих трубопроводів та оптимізації планування їхнього обслуговування, що сприятиме підвищенню безпеки їхньої експлуатації.

Ключові слова: сталь, механічні властивості, водень, деградація, моделювання, експериментальні дані, в'язкість руйнування, J-інтеграл, рівняння дифузії, зменшення похибки.