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A robust model of material degradation within a corrosive environment

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Abstract

This paper is a proposition of implementation an amendment to the existing classic definition of degradation described the by Kachanov-Robotnov model. The proposed model allows to determine the rate of degradation the material structure in an independent verified corrosive environment and determining the redistribution of three-dimensional stress fields taking into account the progressive degradation. According to that purpose, the computational solid dynamics (CSD) numerical simulation of corrosion degradation performed with the mathematical model which was calibrated on the basis of an experiment has been performed by Mrowiec and Werber.

Keywords: Corrosion; Material degradation; CSD simulation

Nomenclature

A, c, k	–	constant of model
c, c_g	–	concentration of products of corrosion and ultimate concentration

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D_0, D –   diffusion coefficient, and modified coefficient
E, E^* –   Young's modulus and modified modulus
F   –   tensile force
l_0 –   initial gouge length
l –   final length
R_m –   ultimate rate of material
T –   temperature
t –   time experiment

Greek symbols

δ –   Kronecker delta
ε_{ef}^{cr} –   effective creep strain tensor
ε_{ef}^{el} –   effective elastic strain tensor
ε_{ef}^{pl} –   effective plastic strain tensor
ν, ν^* –   Piosson constants, modified constants
λ, μ –   Lama'e constants
σ_{HMH} –   von Huber-Misses-Hencky stress tensor
$\omega, \dot{\omega}$ –   damage parameter and rate of damage.

Subscripts and superscript

$*$ –   value of the modified
0 –   initial state
$oxides$ –   product of corrosion process

1   Introduction

Operating of the machines and devices in the extremely corrosive environment leads to premature degradation of their elements. Responsible for this phenomenon are highly damaging components found in the work environment of such a device [1–4]. Classifying this phenomenon, the material corrosion can be divided into individual cases in accordance with [3, 4]:

- stay corrosion – which is characterized by the growth of the oxide layer on the material surface, as a result of the oxidation of its surface layers,

- electrochemical corrosion – which is characterized by an implicit increase of the difference in electrochemical potential between the material layer and the flowing factor.

In this case the destruction occurs as a result of the flow of electric charge in the local cells formed on the material surface [9].

One can also distinguish the stress corrosion, where the diffusion rate of

factors into the material is strictly determined by the level of stress, especially, in the top layer of the material [10]. This type of phenomenon most commonly occurs in environment with strong hydrogen concentration, such as: the boiler combustion chambers or glow pipes of steam turbines. Further information about this topic has been collected in [3, 10, 13].

The effect the degradation of the capacitors tubes walls installed in the steam circulation systems of the nuclear power plants was considered in [5]. The installation has been used in one of the professional power plants. The important conclusion, which was published in this paper, was to pay attention to the need for introduction the degradation rate monitoring and to focus on very dangerous nature of the failure having its origin in the degradation of the wall material.

In the work by Kucharski [11] the computational solid dynamics (CSD) calculation methodology was developed to conduct the numerical simulation of a concrete construction element immersed in the highly corrosive environment. The Fick's law has also been used for the description of the mechanism of the corrosion factor diffusion.

The hydrogen and thermocorrosion destruction phenomenon were addressed in Badur *et al.* [1]. This paper describes the influence of the total thermal stress effects connected with the propagation of stress corrosion cracks and consideres the failure of the silos combustion chamber which has been used during the operation of one of the professional working gas turbines. For this purpose, it has been dealt with the strong influence of the hydrogen concentration in the combustion products of fuel which is supplied as fuel to the turbine.

The influence of the various corrosion types on the construction elements viability was considered by Kucharski [13]. In this paper the attempts mathematical description of the destruction caused by various mechanisms has been discussed. Also the outline of the monitoring system has been shown, whose task is supposed to be one-line monitoring and estimated the lifetime of highly intensive locations on the device. It appears that the considered corrosive part played a significant role in this.

2 Calculation model

The proposed model which is taken from the [9, 10] does not work in the case when it is dealing with a pure chemical stay corrosion caused only by environmental factors (weather), and construction element was not loaded

by external forces, temperature gradients or if there is no residual stresses inside the element.

Our proposed is a complete modification of the equation describing the destruction based on Kachanov-Robotnov hypothesis [2]:

$$\dot{\omega} = \frac{\partial}{\partial x_i}\left(D^* \frac{\partial}{\partial x_i}\omega\right) + \left[\frac{\sigma_{HMH}\left(1 - \lambda(\varepsilon_{ef}^{el} + \varepsilon_{ef}^{pl} + \varepsilon_{ef}^{cr} + \text{other})\right)}{(1-\omega)R_m}\right]^{n(T)}, \quad (1)$$
$$i = x,\, y,\, z\,.$$

In case when the equivalent stress $\sigma_{HMH} = 0$, the whole expression is zero and there is no possibility to calculate degradation of the material. This is the case, when the construction is located before the first operation cycle.

Due to not taking into account by the model Eq. (1) a destruction produced by a corrosion degradation resulting from stress-free oxidation of the top layers of the material, some amendment is here proposed for introducing evolution mechanism of the destruction parameter.

Science, the oxides produced on the metal surface are products of the electrochemical corrosion. These oxides have the porous ceramic structure, then according to [8], the equation was proposed which defines change of the Lamé constants depending on the parameter ω:

$$\begin{cases} \lambda = \frac{\nu^* E^*}{(1+\nu^*)} \\ \mu = \frac{E^*}{2(1+\nu^*)} \\ E^* = E(1-\omega) \\ \nu^* = \nu(1-\omega)\,. \end{cases}, \quad (2)$$

where: E^*, ν^* are the modified material parameters, Young modulus and Poisson ratio, respectively.

Ultimately, substituting for $E^* = 100$ GPa and for $E = 200$ GPa obtain the maximum value of the destruction parameter which is $\omega_{max} = 0.2$ for the electrochemical corrosion. The first aforementioned value corresponds to – the average Young modulus for oxides, whereas the second – Young modulus of noncorroded steel. On this basis, it may be written an equation describing dependence the destruction parameter from the concentration of the atmospheric corrosion c and c_g products [3]

$$\omega_{max} = \frac{c}{c_g} = 0.2\,. \quad (3)$$

The constitutive equation for elastic stress in a function of elastic strains is obtained in accordance with [2, 13]:

$$\sigma = 2\mu\varepsilon_{ij} + \lambda\varepsilon_{kk}\delta_{ij} \,. \tag{4}$$

This allows to get symmetrical deformation tensor for small deformations and also with respect to the design as far as corresponds to the definition and the second Piola-Kirchhoff stress tensor.

Additionally, we adopt proposed in [8, 9] the expression for evolution of the diffusion coefficient

$$D_i^* = D\big(A_1\varepsilon_{ii}^{el} + A_2\varepsilon_{ii}^{pl} + A_3\varepsilon_{ii}^{cr} + \text{other}\big) + \omega D_{oxides} \,. \tag{5}$$

The dependence of the diffusion coefficient in the function of temperature was described in the standard relationship proposed by Arrhenius [13] as

$$D = D_0 e^{kT} \,. \tag{6}$$

The factor it is the diffusion coefficient of the aggressive factor in the products of corrosion. The value of the factor should be determined on an experimental basis. In practice it is difficult to arrangement. The approximate value can be obtained calculating the average diffusion coefficient of the aggressive factor in the corrosion products averaged diffusion coefficients of the individual compounds included in the composition of the corrosion products with the weight function [3]. The measure of this function is volume contribution of the individual compounds in the whole volume of the formed chemical compounds.

Introduced new diffusion coefficient in the oxide it is still in function of temperature, T. The size of the new coefficient and its evolution can be saved as expression Eq. (5):

$$D_{oxides} = D_{(0)oxides} e^{k_1 T} \,. \tag{7}$$

Data describing the diffusion coefficients of the corrosion factor is taken from [12].

3 Model geometry and material characteristics

Two geometries used to perform CSD simulations presents in Fig. 1. On the left side – Fig. 1a – a nozzle geometry which was used in the proper CSD

simulation. For this simulation, the robust model was prepared previously and validation with experimental results was conducted.

The calibration and validation of the robust model equation, Eq. (1) is performed basing on the experiment contained in Fan *et al.* [9]. The quasi-static tensile test is performed by using plate with the standard dimensions. The geometry of the sample presents in Fig. 1b.
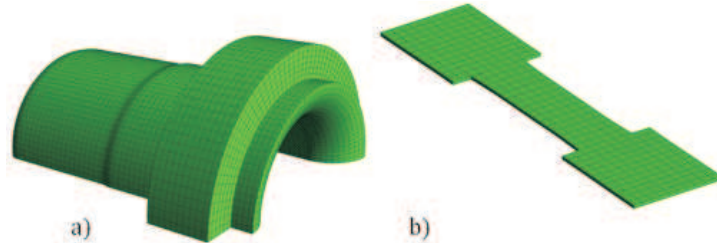

Figure 1: The geometry after discretization: a) the nozzle used in the CSD simulation b) dimensions normalized plate used in the uniaxial tensile trial and in the numerical model validation.

After having the model verification, based on experiment consisting in the axial tensile, the subsequent calibration has been performed for the data of the sample placed in a corrosive environment. The experimental results were taken from [9, 12]. Then CSD simulation of the real geometry in a chemical installation started.

The ST12 steel was adopted as the material of the analysed plate and measuring nozzle. The properties of this material associated at temperatures of levels of around 20 ºC to 600 ºC.

$E = -8 \times 10^{-8} \, T^4 + 0.0005 \, T^3 + 0.2656 \, T^2 - 105.09 \, T + 220583 \, [\text{MPa}]$

$\nu = -9 \times 10^{-14} \, T^4 + 1 \times 10^{-10} \, T^3 - 3 \times 10^{-8} \, T^2 + 5 \times 10^{-5} \, T + 0.2839 \, [–]$

$R_m = -1957 \, \varepsilon^2 + 1186 \, \varepsilon + 187 \, [\text{MPa}]$

$\alpha = -5 \times 10^{-18} \, T^4 + 4 \times 10^{-15} \, T^3 - 1 \times 10^{-12} \, T^2 + 4 \times 10^{-9} \, T + 1 \times 10^{-5} \, [\text{1/K}]$

$\lambda = -5 \times 10^{-11} \, T^4 + 6 \times 10^{-3} \, T^3 - 2 \times 10^{-5} \, T^2 + 0.0074 \times T + 23.852 \, [\text{mW/mmK}]$

$\rho = 7.760 \, E - 9 \, [\text{t/mm}^3]$

4   The model calibration

Firstly, the uniaxial quasi-static tensile test, performed on the standard dimensions plate, has been used to verify the analysis model robust. The

validation results shows in Fig. 2. The presented curve corresponds to the measuring values (points), which were obtained in the analogously performed experiment on a test stand using the tensile machine. The results are posted in [8].
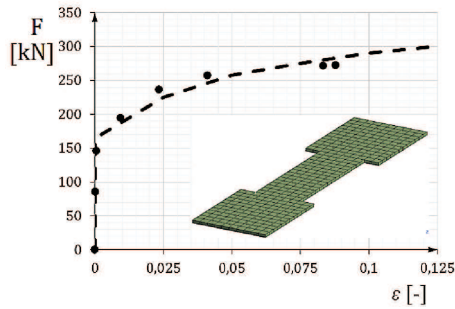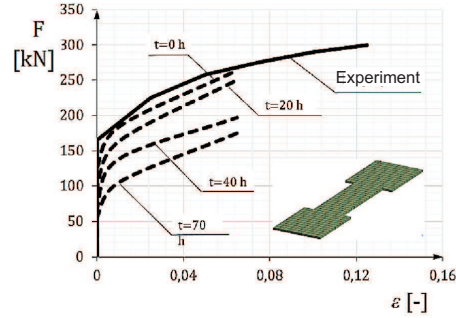

Figure 2: One-axial quasi-static tensil experiment [8].

Figure 3: One-axial tensile which take into account $\varepsilon = \Delta l / l_0$.

Next, having the static tensile test curve of the sample, the simulation, which implements to the model the procedure which calculate displacement obtained for the different stages of the sample corrosion, was repeated.

Standing on the literature data, and Kucharski's results [14] we proposed to take the following values for the coefficients in the robust model Eq. (1) as well in Eqs. (5)–(6) [12]:

$$n(T) = 1.2 \ ,$$

$$A_1, \ A_2, \ A_3 = 0 \ ,$$

$$D_0 = 3.5 \times 10^{-12} [\mathrm{m}^2/\mathrm{s}] \ ,$$

$$k = 5500 \ \mathrm{K} \ ,$$

$$k_1 = 1500 \ \mathrm{K} \ .$$

It is worth to noted that effective equivalent stress σ_{HMH} and strains are defined to be the square of second invariant of an appropriate tensor.

The simulations were consisted on the adoption of the diffusion factor according to the experiment results contained in [12]. The different waveforms of static tensile test curves were obtained for different hold time of the sample in the corrosive environment. The results are consistent with those obtained in [9].

The decreasing stress values for the individual curves (Fig. 3) correspond

to the longer residence time of the sample in the corrosive environment. This means larger and deeper penetration of the corrosion factor into the material. Increased penetration of corrosive factor in the material, depletes volume of 'healthy – native' material capable for the design load transfer. The consequence the application of this model is reduction of a force which is necessary for the plastic deformation of the sample.

In the robust model, the procedure of change the ownership of the Young modulus was used for these elements, which at the time were temporary corrosion. The value of the Young modulus was 100 GPa and the constitutive equations evolution defining stress were consistent with the second Piola-Kirchhoff stress put on the displacement symmetric tensor, describing the slight displacements. The evolution of the material constants proceeded according to Eq. (2) developed in [6, 7]. The displacement curves obtained in accordance with the results from [8–11].

5   The CSD simulation results presentation

On the basis of the verified numerical model, numerical simulations of the real geometry was performed. For this purpose, the 3D model of the measuring nozzle mounted in a chemical installation was used. This installation was transferred very corrosive working medium. The results of the simulation are presented in Figs. 4 and 5.

Figure 4 presents spatial stress fields obtained for different time of the element working in a corrosive environment. The figure label as 'a)' responds to the material in the initial state – noncorroded. Other drawings show changes of the stress fields obtained for the next time steps described in the legend of the figure. According to Eq. (2) with the material properties change, the stress size obtained in relation to the unchanged volume of the facility element was reduced. It is in accordance with Eq. (4) described the second stress tensor Piola-Kirchhoff after conversion to the Lame's constant. The estimated stress value was $\sigma_{HMH} = 121$ MPa for the initial case. After 1400 h facility presence in a highly corrosive environment, the stresses were decreased to 320 MPa in the most intensive areas. This situation is a result of aforementioned changes in material properties by introducing addition of Eq. (2) which describes development of the destruction parameter defined by classical theory of Kachanov-Robotnov Eq. (1) during development of the stress noncorroded. This kind of corrosion is characterized by a development of the oxide on the material surface at the time when the construction
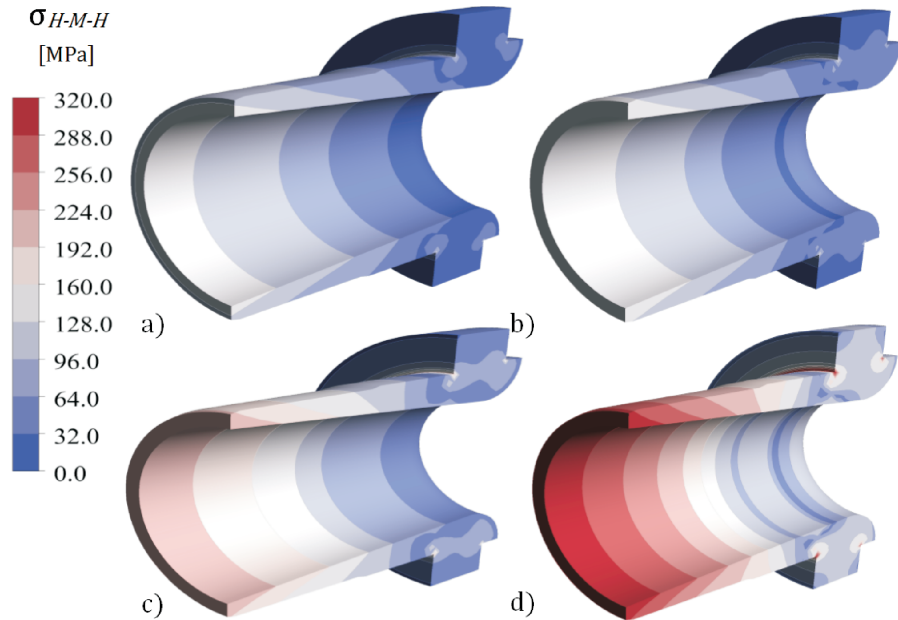
Figure 4: Spatial fields of the reduced stress for the measuring nozzle obtained for: a) the native material and after b) 40 hours in a corrosive environment, c) 700 hours in a corrosive environment, d) 1400 hours in a corrosive environment.

is not subjected of stress, it is 0. In such situations classic definition (1) is not able to take account the development of the destruction parameter. The proposed amendment continues the development of material degradation independent him only from the passage of time, load history load and the unit cut-off.

The Figure 5 presents the fields of the degradation factor changed under the corrosive environments influence. The factor is defined as the last term in Eq. (5). The values are shown for selected time step. This time corresponds to diffusion of the corrosive factor into the material and thus also for the change of the stress field.

6   Conclusions

In this paper review of the literature about corrosive destruction of the materials was conducted. Next we propose the robust model which is an extension of to the classic model of damage described by Kachanov and
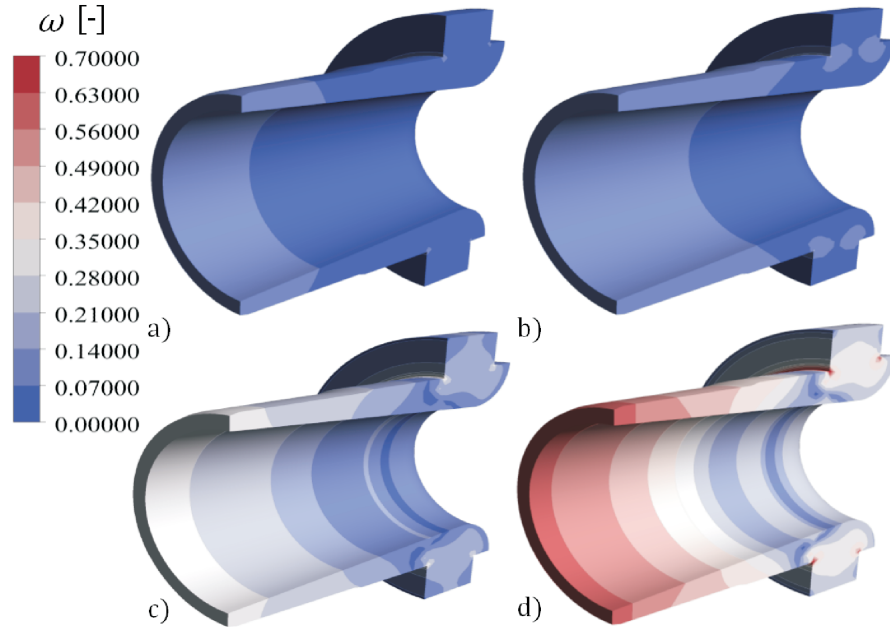
Figure 5: Rate of degradation coefficient for the step time: a) the native material and
after b) 40 h in a corrosive environment, c) 700 h in a corrosive environment,
d) 1400 h in a corrosive environment.

Robotnov. This amendment model, by amending the values of material
constant, allows to maintenance of the evolution of the destruction param-
eter at time intervals in which stress value in the facility is equal to zero.

Next, the proposed model was verified on the basis of tensile test results
for an input sample and presence of the sample in highly corrosive environ-
ment. After receiving the compatibility with the results of the experiments,
CSD simulation on the real geometry of the device, worked in a chemical
installation, was conducted.

The obtained results for corrosive degradation is presented in the spatial
fields which show the change of the facility effort with progressive stress free
corrosion.
The results obtained support the proposed amendment correctness and con-
formity with the physics of the phenomenon and the measurements obtained
during the experiment.

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