

Random hydrogen-induced stresses and effects on cracking

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THE PAPER PRESENTS a method for quantitative characterization of random hydrogen-induced stresses. The method is based on randomized diffusion-elasticity equations. Also a stochastic parametric model, suitable for representing relevant empirical data, is outlined. The general considerations are illustrated by two particular examples. The first one concerns the effect of random hydrogen concentration on material failure time in a half-space, whereas the second one shows its effect on the Mode-I stress intensity factor for a crack in a circular cylinder.

1. Introduction

THERE ARE A VARIETY of engineering/technological situations in which various microstructural stresses play an important role; they have to be carefully taken into account if the material reliability is to be properly estimated. Since a long time it has been evident that hydrogen-induced stress may significantly influence the structural integrity of materials; e.g. the associated cracking is a phenomenon that affects high-strength steels as well as aluminium and titanium alloys.

It is known that in such materials, when they are exposed to hydrogen, sub-critical crack growth can occur at loads far below those which are required for crack growth in the absence of hydrogen (cf. UNGER [1]; GŁOWACKA, ŚWIĄT-NICKI [2]). A well known phenomenon is the hydrogen embrittlement which manifests itself in various parameters used in the evaluation of materials such as e.g. tensile strength, fracture toughness, time to failure. It may also change the mode of fracture from ductile coalescence to brittle intergranular failure (cf. SOFRONIS, MCMEEKING [3]).

Exposure to hydrogen can take different “physical” forms. Direct exposure to hydrogen gas occurs in pressure vessels and in pipelines. Indirect exposure can occur from physical contact with water or water vapor (in this situation chemical reactions between the metal and water produce hydrogen gas, which then enters the metal structure and embrittles it). Hydrogen can also be introduced into a material (cf. [1]) during the manufacturing process. The problems how hydrogen penetrates the metal structure at micro-level (e.g. atomic lattice diffusion,

transport by mobile dislocations, diffusion along grain boundaries) will not be discussed here. Our analysis relies on a continuum (macroscopic) description.

There is no single mechanism causing hydrogen embrittlement. The existing literature indicates that rather different mechanisms govern different situations. But it was recognized that the damaging effect of hydrogen is due to its interaction with the atomic lattice and defects in the vicinity of the major crack. For example, in the paper [1] by Unger, a decohesion mechanism of hydrogen embrittlement is assumed (which means that high hydrogen concentrations reduce the cohesive bonding forces between the metal atoms) and the crack opening displacement is used for the characterization of material degradation. Earlier ORIANI and JOSEPHIC [4] related the threshold stress intensity factor for crack initiation to a critical hydrogen concentration using experimental data. Other papers (cf. ANDERSON [5]) deal with hydrogen-induced cracking in a heat-affected zone of steel weldments. In this case the diffusion of hydrogen increases essentially with the increase of temperature. More general thermodynamical analyses of hydrogen-induced embrittlement are presented by WANG in [6]. In all these papers hydrogen concentration is assumed to be deterministic.

Although the existing analyses provide interesting insight into the problem of hydrogen-assisted degradation and cracking, it seems that there is still a need for further and more systematic approach to this important problem. In this paper we provide a systematic analytical derivation of the diffusive microstresses in elastic materials, taking into account the randomness of the hydrogen concentration. Afterwards, we use the random stresses obtained for a quantitative evaluation of the material failure time and stress intensity factors, generated by the hydrogen diffusion stresses. The analysis is illustrated by calculations of specific exemplary problems.

2. Formulation of the problem

Let us assume, in general, that we have an elastic body which constitutes a region B in \mathbb{R}_3 ; the boundary of B will be denoted by ∂B . As it is customary in elasticity theory – this body, depending on the physical situations, can be subjected to body forces as well as to the surface actions. Here we are primarily concerned with the situation when the surface of the body is exposed to the action of an aggressive hydrogen environment. Therefore, we assume that on the surface ∂B hydrogen concentration is prescribed as a random function $C^*(\mathbf{r}, t, \gamma)$, $\mathbf{r} \in \partial B$, $t \in [0, \infty)$, $\mathbf{r} = (x_1, x_2, x_3)$, whereas γ is a variable indicating randomness; more exactly, $\gamma \in \gamma$, where γ is the space of elementary events in the basic scheme of probability theory (cf. SOB CZYK, KIRKNER [7]). The boundary concentration function is positive-valued, i.e. $C^*(\mathbf{r}, t, \gamma) \geq 0$ for all \mathbf{r}, t, γ in their domains of definition. For each fixed $\gamma \in \gamma$, $C^*(\mathbf{r}, t, \gamma)$ becomes

an ordinary (deterministic) function of (\mathbf{r}, t) ; it describes a particular realization of the concentration field in space and time.

The concentration $C^*(\mathbf{r}, t, \gamma)$, $\mathbf{r} \in \partial B$, induces hydrogen diffusion through the material. The resultant hydrogen concentration $C(\mathbf{r}, t, \gamma)$ in the body B ($\mathbf{r} \in B$) generates a random microstructural stress field $\boldsymbol{\sigma}^h(\mathbf{r}, t, \gamma) \equiv \sigma_{ij}^h(\mathbf{r}, t, \gamma)$. In many situations (when some critical conditions are exceeded) these stresses may produce considerable cracking along the grain boundaries. In order to predict quantitatively the hydrogen stress effects on crack initiation and growth, the random stress field $\boldsymbol{\sigma}^h(\mathbf{r}, t, \gamma)$ has to be properly characterized. Under a simplifying assumption of linear diffusion-elasticity, we present an effective approach to the problem. In what follows we tacitly assume that the prescribed random concentration field $C^*(\mathbf{r}, t, \gamma)$ as well as the initial conditions are sufficiently regular to assure regular (with probability one) probabilistic solutions of the stochastic differential equations under consideration (cf. SOBCZYK [8]).

3. Characterization of random hydrogen induced stresses

3.1. Randomized diffusion-elasticity problem

It is clear that the characterization of the diffusion process in solids and the induced stress analysis can be approached at various levels of sophistication (e.g. nonlinear diffusion, inhomogeneity of the material). Since our main focus here is on the randomness in the hydrogen action, and on the probabilistic effects on the degradation of the material, we perform the analysis within the following standard linear model.

Diffusion equation

$$(3.1) \quad \frac{\partial C}{\partial t} = D \Delta C,$$

$$C(\mathbf{r}, t, \gamma) = C^*(\mathbf{r}, t, \gamma), \quad \mathbf{r} \in \partial B$$

where D is the diffusion constant of the material, $C^*(\mathbf{r}, t, \gamma)$ is the given random field characterizing hydrogen concentration on the surface of the body, and Δ is the Laplace operator; we assume for simplicity that the initial condition (at $t = t_0$) is zero.

Elasticity theory equations with diffusion

$$(3.2) \quad \mu U_{i,jj} + (\lambda + \mu) U_{j,ji} + X_i = \beta C_{,i}$$

where U_i and X_i , $i = 1, 2, 3$, are the components of displacements and mechanical body forces respectively, μ and λ are the Lamé parameters of the elastic material in question, β is a coefficient of coupling between diffusion and elastic deformation, $U_{i,jj} = \sum_{j=1}^3 \partial^2 U_i / \partial x_j^2$, $U_{j,ji} = \sum_{j=1}^3 \partial^2 U_j / \partial x_j \partial x_i$, and $C_{,i} = \partial C / \partial x_i$.

It is seen that in the model adopted here, the diffusion-elasticity equations are in a separated form, i.e. the effect of elastic deformation on the diffusion process is neglected. Therefore, in order to evaluate the random hydrogen-induced stresses, the following steps should be taken.

1. Collect empirical data concerning the random hydrogen stream on the surface of the body (for variable \mathbf{r} and t , or – to simplify the problem – for fixed \mathbf{r} ; then C^* depends only on time), and perform statistical inference on C^* to obtain its basic probabilistic characteristics, e.g. mean value, correlation function and possibly higher-order probabilistic moments.

2. Solve the diffusion Eq. (3.1) with the random boundary condition C^* . Since the equation is linear, the solution – random concentration field $C(\mathbf{r}, t, \gamma)$ in the body – is the integral of the product of the Green's function of Eq. (3.1) and the surface random field $C^*(\mathbf{r}, t, \gamma)$. This integral and its statistics can be calculated exactly in some simple cases (e.g. in the 1-dimensional case, or when C^* depends on time only) or via numerics. Sometimes the boundary concentration of hydrogen can be approximately modelled as a Gaussian random field (with such values of parameters that its probability of becoming negative is sufficiently low). If the probability distribution of the boundary concentration field is Gaussian then also the random hydrogen concentration in the body B will be Gaussian. However, one should keep in mind that when there is some other random uncertainty hidden in the problem (e.g. the material contains “some” random inhomogeneity) and not accounted for in the model (3.1), empirical data on C in the body may indicate a significant departure from normality (i.e. from Gaussian distribution) – cf. SOBCZYK *et al.* [9].

3. Having characterized the random hydrogen concentration field C in the body considered, find the probabilistic characteristics of its derivatives with respect to spatial coordinates x_1, x_2, x_3 (which define the right-hand side of the elasticity theory equations (3.2)). As it is known, the means and correlation functions of $C_{,i}(\mathbf{r}, t, \gamma)$ are expressed in terms of derivatives of the mean and correlation function of $C(\mathbf{r}, t, \gamma)$. It should be noticed that in order to improve the effectiveness of calculations it is beneficial to approximate $C(\mathbf{r}, t, \gamma)$, after solving the diffusion equation (3.1), by a possibly simple random field.

4. Solve the elasticity theory Eqs. (3.2), when $X_i \equiv 0$; the term $\beta C_{,i}(\mathbf{r}, t, \gamma)$ plays the role of the “body” forces. The solution of (3.2) yields the random displacement field \mathbf{U} generated by the concentration field $C(\mathbf{r}, t, \gamma)$, whereas the hydrogen-induced stresses are characterized by the formulae

$$(3.3) \quad \sigma_{ij}^h(\mathbf{r}, t, \gamma) = 2\mu\varepsilon_{ij} + (\lambda\varepsilon_{kk} - \beta C(\mathbf{r}, t, \gamma))\delta_{ij},$$

$$(3.4) \quad \varepsilon_{ij} = \frac{1}{2}(U_{i,j} + U_{j,i})$$

where $i, j = 1, 2, 3$, δ_{ij} is the Kronecker delta, $\varepsilon_{kk} = \varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33}$, and $U_{i,j} = \partial U_i / \partial x_j$.

5. Another approach to the characterization of σ_{ij}^h consists in the usage of the stress equations of elasticity (with a diffusion term) and the Green's function $G_{ij}(\mathbf{r}, t; \boldsymbol{\xi}, \tau)$ for the diffusion-elasticity equations (for the stress formulation of elasticity problems – see: HETNARSKI, IGNACZAK [10] and references therein). In both approaches (via the displacement or stress formulation) one comes to the representation of the random hydrogen-induced stress field which, in general, can be written as

$$(3.5) \quad \sigma_{ij}^h(\mathbf{r}, t, \gamma) = A_{ij} [C^*(\boldsymbol{\xi}, \tau, \gamma), \mathbf{r}, t]$$

where A_{ij} are integral operators with the Green's function $G_{ij}(\mathbf{r}, t; \boldsymbol{\xi}, \tau)$ as the kernel. Formula (3.5) constitutes the general basis for the probabilistic characterization of $\sigma_{ij}^h(\mathbf{r}, t, \gamma)$ via numerical calculations.

The algorithm for probabilistic characterization of hydrogen-induced stresses presented above for the general 3-dimensional case and for a quite general space-time random variability of hydrogen action is computationally quite involved. However, it can be simplified in various specific situations (e.g. plane stress problem, specific invariance properties of the prescribed hydrogen field $C^*(\mathbf{r}, t, \gamma)$ like spatial homogeneity and isotropy, dependence of C^* on time only, etc.).

3.2. Stochastic parametric model

In many practical situations one needs a simple model of a phenomenon, which captures both the basic regularity of empirical data and their statistical scatter. In fact this is a situation in which one is looking for a statistical-empirical model. The problem which arises is: what class of random functions has the features which are especially adequate to the properties of the real phenomenon in question, and – at the same time – whether the random functions introduced are simple enough to make further analysis effective. In the context of residual stresses, such a model was indicated in paper [11] by Sobczyk and Trębicki.

Let us assume here that the real residual hydrogen-induced stress $\boldsymbol{\sigma}^h$ in the body is characterized by a random function $\boldsymbol{\sigma}^h = \mathbf{S}_h(\mathbf{r}, t, \gamma)$. Probabilistic properties of $\mathbf{S}_h(\mathbf{r}, t, \gamma)$ are determined (not as in Sec. 3.1. via a diffusion-elasticity model) by elaboration of empirical data. A useful class of random functions capable to model the random variability contained in data can be represented in the form of a deterministic function of its argument, say $\boldsymbol{\xi}$, with random variables as parameters, i.e.

$$(3.6) \quad \mathbf{S}_h(\boldsymbol{\xi}, \gamma) = \mathbf{g}(\boldsymbol{\xi}; \mathbf{Z}(\gamma)) = \mathbf{g}(\boldsymbol{\xi}; Z_0(\gamma), \dots, Z_n(\gamma))$$

where the argument $\boldsymbol{\xi}$ denotes \mathbf{r} , or t , or both (\mathbf{r}, t) . The functional form of \mathbf{g} is given and random variables $Z_k(\gamma)$, $k = 0, \dots, n$, have specified probabilistic

properties. For example, in the uniaxial case when $\boldsymbol{\xi} = \mathbf{r} = (x, 0, 0)$, a random polynomial of degree n is a special case of (3.6); namely

$$(3.7) \quad S_h(x, \gamma) = \sum_{k=0}^n Z_k(\gamma) x^k$$

There is a theorem (cf. ONICESCU and ISTRATESCU [12]) which asserts that if $S(x, \gamma)$ is any random function continuous in probability in the interval $I \in \mathbb{R}_1$, then there exists a family of random polynomials $\{S_n(x, \gamma)\}$ converging uniformly in probability to $S(x, \gamma)$, as $n \rightarrow \infty$. This is a stochastic counterpart of the known Weierstrass theorem on polynomial approximation of continuous deterministic functions.

Another special case of (3.6) which has the power to capture a variety of random empirical variations, and particularly – random hydrogen-induced stresses, is

$$(3.8) \quad S_h(\boldsymbol{\xi}, \gamma) = \sigma^h(x, \gamma) = g(x; \mathbf{Z}(\gamma)) = Z_0(\gamma) p_1(x; Z_1(\gamma)) p_2(x/L; Z_2(\gamma)),$$

where $Z_0(\gamma)$, $Z_1(\gamma)$, $Z_2(\gamma)$ are independent random variables with known probability distributions, and $p_1(x; \zeta)$ and $p_2(x; \zeta)$ are suitable empirical functions representing the shape of the stress variability in x -direction (e.g. polynomials, trigonometric functions, exponentials etc.). Function $p_2(x; \zeta)$ may characterize a dependence of the hydrogen stress on the microstructural length scale L (e.g. grain size).

The empirical-type probabilistic models (3.6)–(3.8) may be very handy in the analysis of cracking due to the hydrogen stress distribution (cf. Example 2).

4. Hydrogen-induced microcracking

4.1. Poissonian approximation of random failure time

When the hydrogen-induced stress outcrosses the boundary, say ∂G , of its “safety domain”, microcrack nucleation occurs. More generally, one can assume that the nucleation takes place if the local limiting condition

$$(4.1) \quad \varphi(\sigma_{ij}^h) < \sigma_{\text{cr}}$$

does not hold any longer, where φ is, most often, an empirically motivated relationship for a specific material and σ_{cr} is its limiting value. Our purpose here is to determine the probability of the failure time at a fixed “critical” point \mathbf{r} of the material. When \mathbf{r} is fixed, random function σ_{ij}^h reduces to a tensor-valued stochastic process $\sigma_{ij}^h(t, \gamma)$, so the variable \mathbf{r} will be omitted. Criterion (4.1) can be interpreted as a condition on all the components of the tensor

$\sigma^h = \{\sigma_{ij}^h(t, \gamma)\}$, or – on some “representative” values of σ^h , e.g. on the invariants of the stress field σ^h . In what follows we will deal with a stochastic process $\sigma_{ij}^h(t, \gamma)$, $i, j = 1, 2, 3$.

Let us denote by G the set of those values of σ_{ij}^h , for which condition (4.1) holds, i.e.

$$(4.2) \quad G = \{\sigma_{ij}^h : \varphi(\sigma_{ij}^h) < \sigma_{cr}\}.$$

Therefore the problem of estimation of the random failure time (due to a random time-varying hydrogen stress) consists in finding the probability of the first “excursion” of the process $\sigma_{ij}^h(t, \gamma)$ from the domain G .

In order to obtain an effective solution of the problem, we assume that our stress process is such a stochastic process $\sigma_{ij}^h(t, \gamma)$, for each fixed (i, j) , which – in general – has the “potential” to cross the boundary ∂G of G many times. We will denote by $N_G(t)$ the random number of its excursions in the time interval $(0, t]$.

As in other problems of reliability (cf. MADSEN *et al.* [13]), we will assume that the excursions occur independently of each other with $\lambda(t)$ denoting the intensity, i.e. the mean number of outcrossings in a time unit. We assume also that the ∂G -outcrossings of $\sigma_{ij}^h(t, \gamma)$ are characterized by the Poisson random process, i.e.

$$P\{N_G(t) = k\} = \frac{\Lambda(t)^k}{k!} e^{-\Lambda(t)}, \quad \Lambda(t) = \int_0^t \lambda(\tau) d\tau$$

where $k = 0, 1, \dots$. The probability that the stress process will not outcross ∂G in the time interval $(0, t]$ is equal to the probability that its initial value $\sigma_{ij}^h(0, \gamma)$ belongs to G and the process $\sigma_{ij}^h(t, \gamma)$ does not show any ∂G -outcrossing within the time interval $(0, t]$, i.e.

$$P_G(t) = P\{[\sigma_{ij}^h(0, \gamma) \in G] \cap [N_G(t) = 0]\}.$$

This probability can be approximated by the product, i.e.

$$(4.3) \quad P_G(t) = P_0 P\{N_G(t) = 0\} = P_0 e^{-\Lambda(t)},$$

where $P_0 = P\{\sigma_{ij}^h(0, \gamma) \in G\}$. Therefore, the probability $P_F(t)$ of the material failure in the interval $(0, t]$ is

$$(4.4) \quad P_F(t) = 1 - P_G(t) = 1 - P_0 e^{-\Lambda(t)}.$$

If the process $\sigma_{ij}^h(t, \gamma)$ can be represented by a stationary random process, then the associated stream of outcrossings is a homogeneous Poisson process,

i.e. $\lambda(t) = \lambda_0 = \text{const}$. In this case formulae (4.3), (4.4) take a simple form. For example, the probability distribution function of the material failure in the time interval $(0, t]$ is

$$(4.5) \quad P_F(t) = 1 - P_0 e^{-\lambda_0 t}.$$

The derivative of $P_F(t)$ yields the probability density $f_T(t)$ of the random variable T characterizing the random failure time.

To make use of the formulae above one has to express $\lambda(t)$ or λ_0 in terms of probabilistic characteristics of the underlying random stress process $\boldsymbol{\sigma}^h(t, \gamma)$. This can be done in two ways. The first approach is based on retaining the multi-dimensional character of the stress tensor and investigating the rate, at which $\boldsymbol{\sigma}^h(t, \gamma)$, treated as a process with values in \mathbb{R}_6 (its components are $\sigma_{11}^h, \sigma_{22}^h, \sigma_{33}^h, \sigma_{12}^h = \sigma_{21}^h, \sigma_{13}^h = \sigma_{31}^h, \sigma_{23}^h = \sigma_{32}^h$), outcrosses ∂G . The value of $\lambda(t)$ can then be obtained from the Belayev formula (cf. BELAYEV [14]). The second approach is based on definition (4.2) of the set G and the observation that $\boldsymbol{\sigma}^h(t, \gamma)$ outcrosses ∂G exactly when $\varphi(\boldsymbol{\sigma}^h(t, \gamma))$, treated as a scalar stochastic process, upcrosses the level σ_{cr} . This auxiliary scalar process will be further denoted by $\sigma(t, \gamma)$, i.e.

$$(4.6) \quad \sigma(t, \gamma) = \varphi(\boldsymbol{\sigma}^h(t, \gamma)).$$

It follows that the mean number of outcrossings of ∂G by $\boldsymbol{\sigma}^h(t, \gamma)$ equals the mean number of upcrossings of the level σ_{cr} by $\sigma(t, \gamma)$. The latter can be obtained from the Rice formula (cf. SOONG, GRIGORIU [15]), which is a scalar version of the Belayev formula for multi-dimensional processes. The Rice formula gives

$$(4.7) \quad \lambda(t) = \int_0^\infty v p(\sigma_{cr}, v, t) dv$$

where $p(u, v, t)$ is the joint probability density function of the process $\sigma(t, \gamma)$ and its time derivative $\dot{\sigma}(t, \gamma)$ at time t . The second, scalar approach is followed in the first numerical example given below.

4.2. Example 1. A half-space under random time-varying hydrogen action; effect on failure time

As an exemplary problem we will show how to estimate the hydrogen-induced failure time, using the theoretical approach described in the previous sections.

Assume that the elastic body B constitutes a half-space $B = \{\mathbf{r} = (x_1, x_2, x_3) : x_3 \geq 0\}$ with the boundary $\partial B = \{\mathbf{r} : x_3 = 0\}$; the initial hydrogen concentration $C_0(\mathbf{r}) \equiv 0$, $\mathbf{r} \in B$, whereas the boundary ∂B is subjected to a constant in (x_1, x_2) , time-varying random concentration of hydrogen: $C^*(t, \gamma)$. It is assumed

that $C^*(t, \gamma)$ is a stationary Gaussian stochastic process with the following mean and correlation function:

$$(4.8) \quad m(t) = m_0, \quad K(t_1, t_2) = s^2 e^{-\alpha^2(t_1 - t_2)^2},$$

where m_0 is constant, s denotes the standard deviation of $C^*(t, \gamma)$, whereas α is a correlation parameter characterizing the dependence between hydrogen concentration at time instants t_1 and t_2 . All Gaussian probability distributions (for all possible $\{t_1, t_2, \dots, t_n\}$) are expressed in the known way in terms of m_0 and the elements of the correlation matrix $\{K(t_i, t_j)\}$, $i, j = 1, 2, \dots, n$; (see e.g. SOBCZYK, SPENCER [16]). It should be underlined here that although the Gaussian distribution is theoretically extended over the entire real line $(-\infty, +\infty)$ it can, nevertheless, be assumed in practice as a model of non-negative quantities; as it is known, there is a "three sigma" rule which asserts that the probability that the possible values of a Gaussian variable, say X , depart from their mean m by more than 3σ is very small (i.e. $P\{|X - m| \geq 3\sigma\} \approx 0.003$); σ is the standard deviation which in (4.8) is denoted by s . Therefore, we assume here that $m_0 \geq 3s$.

It may further be observed that since hydrogen stresses are expressed as linear transformations of the boundary concentration of hydrogen (relation (3.5)) and since, in the present case, $C^*(t, \gamma)$ is Gaussian, the resulting stress field is also Gaussian (cf. [8]). To obtain a full stochastic description of $\sigma_{ij}^h(\mathbf{r}, t, \gamma)$ one therefore only needs to find the integral operators A_{ij} and apply them to the mean and correlation function of $C^*(t, \gamma)$.

Because of the symmetry properties of the present problem, the concentration of hydrogen $C(\mathbf{r}, t, \gamma)$ and stresses $\sigma_{ij}^h(\mathbf{r}, t, \gamma)$ depend only on coordinate x_3 and time. For simplicity, we further write x instead of x_3 . The solution of the diffusion equation (3.1) in the considered case is

$$(4.9) \quad C(x, t, \gamma) = \int_0^t \frac{x C^*(\tau, \gamma)}{2\sqrt{\pi D(t - \tau)^3}} e^{-x^2/(4D(t - \tau))} d\tau,$$

where $C^*(t, \gamma)$ is the given random boundary concentration field and the integral is understood as a sample function integral. The solution of the elasticity problem (3.2)–(3.4) yields

$$(4.10) \quad \sigma_{11}^h(x, t, \gamma) = \sigma_{22}^h(x, t, \gamma) = -\frac{2\mu\beta}{2\mu + \lambda} C(x, t, \gamma)$$

and other components $\sigma_{ij}^h = 0$. After combining (4.9) and (4.10), and performing

simple transformations, one can express the operators A_{11} and A_{22} as

$$(4.11) \quad A_{11}[g(\circ), x, t] = A_{22}[g(\circ), x, t] = -b \int_0^t g(t-\tau) z \tau^{-3/2} e^{-z^2/\tau} d\tau,$$

where $b = 2\mu\beta/((2\mu + \lambda)\sqrt{\pi})$, $z = x/(2\sqrt{D})$, and $g(\circ)$ stands for any particular function on which the operator acts. Thus, the entire stress field in the body is essentially described by one scalar field given by (4.10) and its integral operator in (4.11). Since the stress field in (4.10) is always non-positive, one can define a new non-negative field $\sigma(x, t, \gamma) = -\sigma_{11}^h(x, t, \gamma) = -\sigma_{22}^h(x, t, \gamma)$ and the corresponding new integral operator $A = -A_{11} = -A_{22}$. It can now be observed that many local stress-based damage criteria, like the von Mises or Tresca yield criteria, or the Mohr brittle fracture criterion (cf. PAUL [17]), reduce in the present case to the following safety condition

$$(4.12) \quad \sigma(x, t, \gamma) < \sigma_{cr}$$

where σ_{cr} is a material-dependent critical value. Condition (4.12) will therefore be of our concern in the subsequent analysis of time-to-failure. It can be seen that $\sigma(x, t, \gamma)$, as defined above, is just the auxiliary scalar process introduced in (4.6) under the same name. Therefore it remains to determine the crossing properties of $\sigma(x, t, \gamma)$ with respect to the level σ_{cr} .

As remarked above $\sigma(x, t, \gamma)$, being a linear transform of the Gaussian $C^*(t, \gamma)$, is itself Gaussian. Its mean and correlation function are obtained by applying A to the mean and correlation function of $C^*(t, \gamma)$ respectively (as defined in (4.8)), which gives

$$(4.13) \quad m_\sigma(x, t) = A[m(\circ), x, t] \\ = b m_0 \int_0^t z \tau^{-3/2} e^{-z^2/\tau} d\tau = b m_0 \left[\sqrt{\pi} - 2 \int_0^{z/\sqrt{t}} e^{-u^2} du \right],$$

$$(4.14) \quad K_\sigma(x', t_1, x'', t_2) = A[A[K(\circ, \circ), x'', t_2], x', t_1] \\ = b^2 s^2 \int_0^{t_1} \int_0^{t_2} z_1 z_2 (\tau_1 \tau_2)^{-3/2} e^{-\alpha^2(t_1 - \tau_1 - t_2 + \tau_2)^2 - z_1^2/\tau_1 - z_2^2/\tau_2} d\tau_2 d\tau_1,$$

where in (4.14) the outer A acts with respect to the first, and the inner A with respect to the second argument of $K(\circ, \circ)$. Above, x' and x'' are two possible

values of x , $z_1 = x'/(2\sqrt{D})$, and $z_2 = x''/(2\sqrt{D})$. Because of the symmetry of the correlation function one may assume, without loss of generality, that $t_2 \geq t_1$, and accordingly set $t_1 = t$, $t_2 = t + \delta$, where $\delta \geq 0$. It can now be observed that both m_σ (for fixed x) and K_σ (for fixed x' and x'') tend to well-defined limits as $t \rightarrow \infty$, and moreover K_σ tends to its limit function uniformly in δ . Therefore it will be assumed, as an approximation, that $\sigma(x, t, \gamma)$ is a stationary Gaussian process, whose mean and correlation function are

$$(4.15) \quad \bar{m}_\sigma(x) = \lim_{t \rightarrow \infty} m_\sigma(x, t) = b m_0 \sqrt{\pi} = \frac{2\mu\beta m_0}{2\mu + \lambda},$$

$$(4.16) \quad \begin{aligned} \bar{K}_\sigma(x', x'', \delta) &= \lim_{t \rightarrow \infty} K_\sigma(x', t, x'', t + \delta) \\ &= \lim_{t \rightarrow \infty} b^2 s^2 \int_0^t \int_0^{t+\delta} z_1 z_2 (\tau_1 \tau_2)^{-3/2} e^{-\alpha^2(\tau_1 - \tau_2 + \delta)^2 - z_1^2/\tau_1 - z_2^2/\tau_2} d\tau_2 d\tau_1. \end{aligned}$$

As in Sec. 4.1 we assume here that x is a fixed "critical" point and we treat $\sigma(x, t, \gamma)$ as a stochastic process in t only, with x being a fixed parameter. We therefore further write $\sigma(t, \gamma)$.

In order to exploit expressions (4.5) and (4.7) and calculate $P_F(t)$ at x , probabilistic characteristics of the joint vector process $\{\sigma(t, \gamma), \dot{\sigma}(t, \gamma)\}$ must be computed. Since $\sigma(t, \gamma)$ is stationary Gaussian, $\dot{\sigma}(t, \gamma)$ is also stationary Gaussian, and they are independent for each fixed t (cf. [8]). The mean and correlation function of $\sigma(t, \gamma)$ are given by (4.15) and (4.16) respectively, with $x = x' = x''$. In particular, the variance has the form

$$(4.17) \quad \begin{aligned} V_\sigma &= \bar{K}_\sigma(x, x, 0) \\ &= \lim_{t \rightarrow \infty} b^2 s^2 \int_0^t \int_0^t z^2 (\tau_1 \tau_2)^{-3/2} e^{-\alpha^2(\tau_1 - \tau_2)^2 - z^2/\tau_1 - z^2/\tau_2} d\tau_2 d\tau_1. \end{aligned}$$

The corresponding quantities for $\dot{\sigma}(t, \gamma)$ are

$$\bar{m}_{\dot{\sigma}} = \frac{d}{dt} \bar{m}_\sigma = 0,$$

$$\bar{K}_{\dot{\sigma}}(\delta) = \bar{K}_{\dot{\sigma}}(t_2 - t_1) = \frac{\partial^2 \bar{K}_\sigma(x, x, t_2 - t_1)}{\partial t_1 \partial t_2} = -\frac{\partial^2 \bar{K}_\sigma(x, x, \delta)}{\partial \delta^2}$$

and the variance (after certain transformations) takes the form

$$(4.18) \quad V_{\dot{\sigma}} = \bar{K}_{\dot{\sigma}}(0) \\ = -\lim_{t \rightarrow \infty} b^2 s^2 z^2 \int_0^t \int_0^t \frac{15\tau_1^2 - 20z^2\tau_1 + 4z^4}{4\sqrt{\tau_1^{11}\tau_2^3}} e^{-\alpha^2(\tau_1 - \tau_2)^2 - z^2/\tau_1 - z^2/\tau_2} d\tau_2 d\tau_1.$$

The variances in (4.17) and (4.18) have to be computed numerically.

The joint one-dimensional probability density function of $\sigma(t, \gamma)$ and $\dot{\sigma}(t, \gamma)$ can be written as

$$p(u, v, t) = p_{\sigma}(u) p_{\dot{\sigma}}(v),$$

where $p_{\sigma}(u)$ and $p_{\dot{\sigma}}(v)$ are the one-dimensional Gaussian probability density functions of the individual processes, given by

$$p_{\sigma}(u) = \frac{1}{\sqrt{2\pi V_{\sigma}}} e^{-(u - \bar{m}_{\sigma})^2 / (2V_{\sigma})}, \\ p_{\dot{\sigma}}(v) = \frac{1}{\sqrt{2\pi V_{\dot{\sigma}}}} e^{-v^2 / (2V_{\dot{\sigma}})}.$$

The Rice formula (4.7) now yields the mean number of upcrossings of the level σ_{cr} by the process $\sigma(t, \gamma)$ in unit time as

$$(4.19) \quad \lambda_0 = \int_0^{\infty} v p_{\sigma}(\sigma_{\text{cr}}) p_{\dot{\sigma}}(v) dv = \frac{1}{2\pi} \sqrt{\frac{V_{\dot{\sigma}}}{V_{\sigma}}} e^{-(\sigma_{\text{cr}} - \bar{m}_{\sigma})^2 / (2V_{\sigma})}.$$

Also the probability of safety at $t = 0$ can now be computed as

$$(4.20) \quad P_0 = P\{\sigma(0, \gamma) < \sigma_{\text{cr}}\} \\ = \int_{-\infty}^{\sigma_{\text{cr}}} p_{\sigma}(u) du = \int_{-\infty}^{\sigma_{\text{cr}}} \frac{1}{\sqrt{2\pi V_{\sigma}}} e^{-(u - \bar{m}_{\sigma})^2 / (2V_{\sigma})} du.$$

The values of λ_0 and P_0 , given by (4.19) and (4.20), may eventually be substituted into formula (4.5). This yields the probability $P_F(t)$ of material failure at the point x until time t . Finally, the expectation and variance of the time to failure at x are computed from the known formulae as

$$(4.21) \quad E_F = \int_0^{\infty} t \dot{P}_F(t) dt = \int_0^{\infty} t \lambda_0 P_0 e^{-\lambda_0 t} dt = \frac{P_0}{\lambda_0},$$

$$(4.22) \quad V_F = E_F^2(1 - P_0) + \int_0^\infty (t - E_F)^2 \dot{P}_F(t) dt = \frac{P_0}{\lambda_0^2}(2 - P_0).$$

To summarize the procedure: first, \bar{m}_σ , V_σ and $V_{\hat{\sigma}}$ are computed with (4.15), (4.17) and (4.18) respectively, from the supplied values of parameters; then, \bar{m}_σ , V_σ and $V_{\hat{\sigma}}$ are substituted into (4.19) and (4.20), to obtain λ_0 and P_0 respectively; finally, λ_0 and P_0 are used in (4.5), (4.21) and (4.22) to calculate respectively $P_F(t)$, E_F and V_F .

Below are presented the results of numerical calculations, intended to show the character of typical solutions. The chosen material is a low-alloyed, low-strength steel with a Young modulus $E = 205$ [GPa], Poisson coefficient $\nu = 0.3$, and yield stress $\sigma_{cr} = 250$ [MPa]. The corresponding Lamé constants are $\lambda = 118$ [GPa] and $\mu = 78.8$ [GPa]. The diffusion coefficient is taken as $D = 10^{-9}$ [m²/s] (cf. BOELLINGHAUS *et al.* [18]). The coupling coefficient is $\beta = 332$ [kJ/mol], a value based on assuming the partial molar volume of hydrogen in steel to be 2 [cm³/mol] (cf. HIRTH [19]). The mean concentration of hydrogen on the boundary is chosen as $m_0 = 900$ [mol/m³], which is a possible equilibrium concentration in high pressure vessels (cf. SAN MARCHI *et al.* [20]).

Figure 1 shows the dependence of $P_F(t)$ on the correlation coefficient α of the random hydrogen concentration. It can be seen that, for the chosen data, stronger correlation of the values of $C^*(t, \gamma)$ results in a smaller probability of failure. (Smaller α corresponds to higher correlation.) In the case shown in Fig. 1 x is close enough to the boundary, so that higher frequencies in the spectrum of $C^*(t, \gamma)$ are not filtered out by the operator A (in the given range of α). Therefore

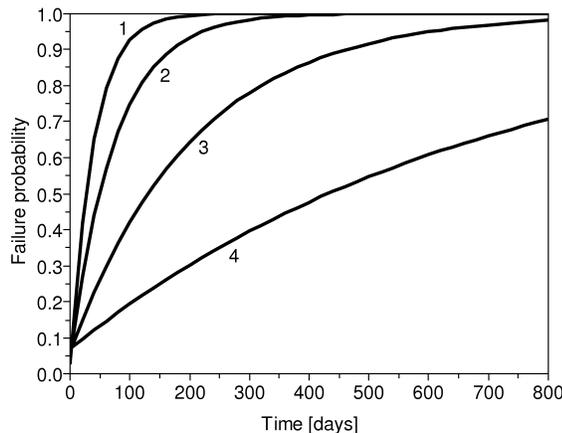


FIG. 1. Probability of failure P_F vs. time, for $x = 5$ [mm] and $s = 300$ [mol/m³]. Curve 1 corresponds to $\alpha = 10^{-5}$, curve 2 to $\alpha = 10^{-5.5}$, curve 3 to $\alpha = 10^{-6}$, and curve 4 to $\alpha = 10^{-6.5}$ [s⁻¹].

higher variability of $C^*(t, \gamma)$ transfers to $\sigma(x, t, \gamma)$, which increases its probability of reaching the critical value. The nonzero probability of instantaneous failure at $t = 0$, visible in Fig. 1, is due to the stationary approximation of $\sigma(x, t, \gamma)$ made in calculations.

Figure 2 illustrates how failure probability diminishes with depth x , and Fig. 3 shows how $P_F(t)$ may grow with the growth of the intensity of scatter (standard deviation s) of $C^*(t, \gamma)$.

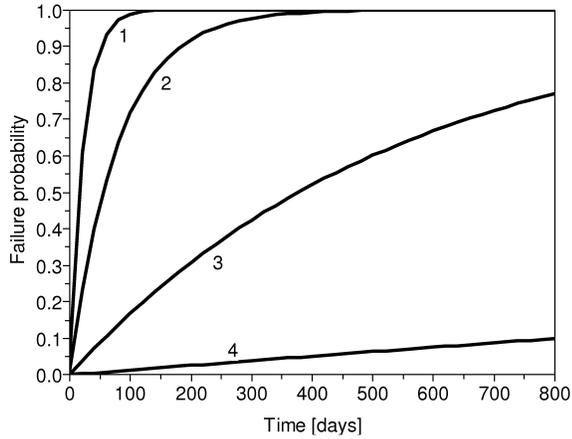


FIG. 2. Probability of failure P_F vs. time, for $s = 300$ [mol/m³] and $\alpha = 10^{-5}$ [s⁻¹]. Curve 1 corresponds to $x = 2.5$, curve 2 to $x = 7.5$, curve 3 to $x = 12.5$, and curve 4 to $x = 17.5$ [mm].

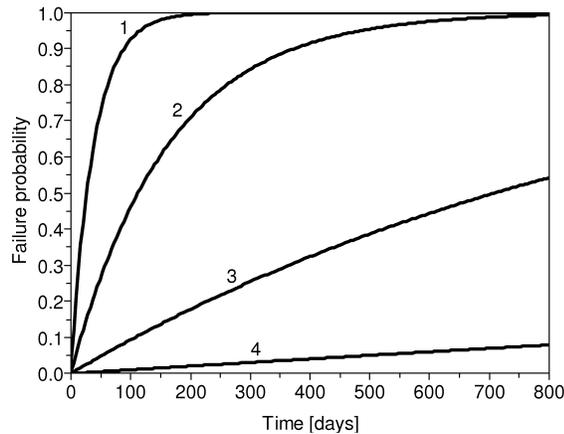


FIG. 3. Probability of failure P_F vs. time, for $x = 5$ [mm] and $\alpha = 10^{-5}$ [s⁻¹]. Curve 1 corresponds to $s = m_0/3 = 300$, curve 2 to $s = m_0/4 = 225$, curve 3 to $s = m_0/5 = 180$, and curve 4 to $s = m_0/6 = 150$ [mol/m³].

The explicit dependence of failure probability on x is visualized in Fig. 4. At points near the boundary, higher correlation of the values of $C^*(t, \gamma)$ involves longer expected time to failure. However, for deeper points in the half-space the relation turns out to be reversed, with higher correlation entailing shorter expectation times. Thus for deeper points, the operator A is a low-pass filter: the influences of quick variations of a realization of $C^*(t, \gamma)$ average out, making failure less probable.

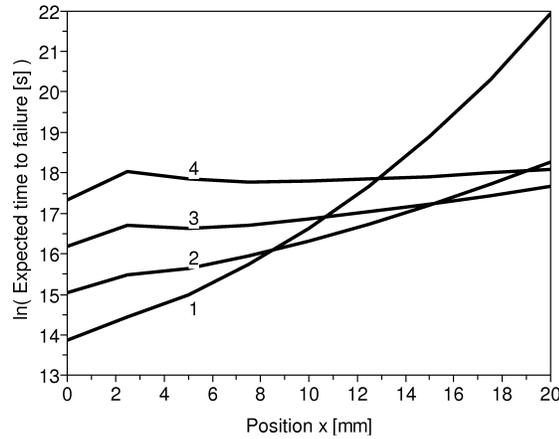


FIG. 4. Expected time to failure E_F vs. position x , for $s = 300$ [mol/m³]. Curve 1 corresponds to $\alpha = 10^{-5}$, curve 2 to $\alpha = 10^{-5.5}$, curve 3 to $\alpha = 10^{-6}$, and curve 4 to $\alpha = 10^{-6.5}$ [s⁻¹].

4.3. Example 2. Infinite cylinder under random time-varying hydrogen action; effect on stress intensity factor

As the second example, we consider an infinite circular cylinder of radius b : $B = \{\mathbf{r} = (r, \theta, z) : 0 \leq r \leq b\}$ (cylindrical coordinate system is used), exposed to the action of a random hydrogen concentration $C^*(t, \gamma)$ on its boundary. It is thus assumed, as in the preceding example, that C^* varies in time but is constant on ∂B at any given moment. The initial condition for hydrogen concentration is homogeneous: $C_0(\mathbf{r}) = 0$, $\mathbf{r} \in B$, and the boundary ∂B is free of tractions, i.e. surface loading on the boundary is zero for all t . Therefore, at $t = 0$, the cylinder is in a stress-free state. For further stress calculations, plane state of strain is assumed in z direction.

The cylinder contains a radially oriented crack of rectilinear cross-section and length a (Fig. 5), extended indefinitely along the z axis. As a result of the boundary hydrogen concentration $C^*(t, \gamma)$, hydrogen diffuses through the cylinder and residual stresses are induced in the material, giving rise to nonzero stress

intensity factors at the edges of the crack. In the following, we determine approximate probabilistic characteristics of the corresponding Mode-I stress intensity factors K_I^1 (at r_1) and K_I^2 (at $r_2 = r_1 + a$).

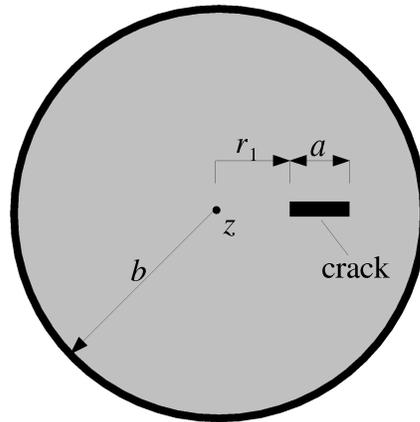


FIG. 5. Geometry of the crack (cross-section of the cylinder).

In the considered case, the resultant hydrogen concentration $C(\mathbf{r}, t, \gamma)$ in the cylinder, and hydrogen-induced stresses $\sigma_{ij}^h(\mathbf{r}, t, \gamma)$, $\mathbf{r} \in B$, $t \in [0, \infty)$, $i, j = r, \theta, z$, are independent of θ and z . Therefore we can simply write $C(r, t, \gamma)$ and $\sigma_{ij}^h(r, t, \gamma)$. The solution of the diffusion equation (3.1) for the cylinder with a zero initial condition and a constant boundary condition $C^*(t, \gamma) = 1$, expressed in cylindrical coordinates, is (cf. NOWACKI, OLESIAK [21])

$$(4.23) \quad C_1(r, t) = 1 - 2b^{-1} \sum_{n=1}^{\infty} e^{-Dt\alpha_n^2} \frac{J_0(\alpha_n r)}{\alpha_n J_1(\alpha_n b)},$$

where J_0 and J_1 are the Bessel functions of the first kind of orders 0 and 1 respectively, and the sum is taken over all positive roots of equation $J_0(\alpha_n b) = 0$. For a differentiable boundary concentration function $C^*(t, \gamma)$ one therefore obtains

$$(4.24) \quad C(r, t, \gamma) = C^*(0, \gamma)C_1(r, t) + \int_0^t \dot{C}^*(\tau, \gamma)C_1(r, t - \tau) d\tau,$$

where $\dot{C}^*(t, \gamma) = \partial C^*(t, \gamma)/\partial t$. The random hydrogen-induced stresses are

(based on [21])

$$\begin{aligned}
 \sigma_{rr}(r, t, \gamma) &= m \left[r^{-2} \int_0^r C(\rho, t, \gamma) \rho \, d\rho - b^{-2} \int_0^b C(\rho, t, \gamma) \rho \, d\rho \right], \\
 (4.25) \quad \sigma_{\theta\theta}(r, t, \gamma) &= m \left[C(r, t, \gamma) - r^{-2} \int_0^r C(\rho, t, \gamma) \rho \, d\rho - b^{-2} \int_0^b C(\rho, t, \gamma) \rho \, d\rho \right], \\
 \sigma_{zz}(r, t, \gamma) &= m \left[C(r, t, \gamma) - \frac{\lambda}{(\lambda + \mu)b^2} \int_0^b C(\rho, t, \gamma) \rho \, d\rho \right].
 \end{aligned}$$

where $m = -2\mu\beta/(\lambda + 2\mu)$. All other components of the stress tensor are zero. In the sequel, to effectively characterize the stress intensity factors K_I^1 and K_I^2 , we make the following two simplifications. First, we disregard the multiaxial character of the stress field and consider only the component $\sigma_{\theta\theta}$ which is perpendicular to the crack surface. Second, for present considerations, we assume the crack to be suitably small and distant from the boundary of the cylinder to be treated as if it were placed in an infinite medium. (This second condition can be avoided by using more specialized weight functions than we do below.) We thus consider the crack as a rectilinear through crack in an infinite space, under uniaxial state of stress perpendicular to the crack surface. The stress intensity factors for this case can be expressed as (based on SIH [22])

$$(4.26) \quad K_I^1(t, \gamma) = R \int_{r_1}^{r_2} \sigma_{\theta\theta}(r, t, \gamma) \sqrt{\frac{r_2 - r}{r - r_1}} \, dr,$$

$$(4.27) \quad K_I^2(t, \gamma) = R \int_{r_1}^{r_2} \sigma_{\theta\theta}(r, t, \gamma) \sqrt{\frac{r - r_1}{r_2 - r}} \, dr,$$

where $R = \sqrt{2/(\pi a)}$. By combining Eqs. (4.23)–(4.27), the following expressions for the stress intensity factors are obtained:

$$(4.28) \quad K_I^i(t, \gamma) = \sum_{n=1}^{\infty} A_n^i (e^{b_n t} C_n^*(0, \gamma) + C_n^*(t, \gamma)), \quad i = 1, 2$$

where

$$A_n^1 = R \int_{r_1}^{r_2} a_n(r) \sqrt{\frac{r_2 - r}{r - r_1}} \, dr, \quad A_n^2 = R \int_{r_1}^{r_2} a_n(r) \sqrt{\frac{r - r_1}{r_2 - r}} \, dr,$$

$$C_n^*(t, \gamma) = \int_0^t \dot{C}^*(\tau, \gamma) e^{b_n(t-\tau)} d\tau,$$

$$a_n(r) = -\frac{4\mu\beta}{b(\lambda + 2\mu)\alpha_n^2} \left(\frac{J_1(\alpha_n r) - \alpha_n r J_0(\alpha_n r)}{r J_1(\alpha_n b)} + \frac{1}{b} \right), \quad b_n = -D\alpha_n^2.$$

We next consider the case, when the boundary concentration $C^*(t, \gamma)$ is given by a stochastic parametric model (cf. Sec. 3.2.) of the particular form of a sum of deterministic base functions with random coefficients

$$(4.29) \quad C^*(t, \gamma) = \sum_{j=1}^N Z_j(\gamma) f_j(t).$$

Because of the linearity of Eqs. (4.28) in $C^*(t, \gamma)$, the resultant stress intensity factors can likewise be written as sums of deterministic functions with random coefficients

$$(4.30) \quad K_I^i(t, \gamma) = \sum_{j=1}^N Z_j(\gamma) K_I^{ij}(t), \quad i = 1, 2$$

where $K_I^{ij}(t)$, $i = 1, 2$, are the solutions of (4.28), with $f_j(t)$ taken as the boundary concentration function. The relevant probabilistic moments are easily computed. The mean values are

$$(4.31) \quad M_I^i(t) = E\{K_I^i(t, \gamma)\} = \sum_{j=1}^N M_j K_I^{ij}(t), \quad i = 1, 2$$

where $M_j = E\{Z_j(\gamma)\}$ is the mean of the random variable $Z_j(\gamma)$. The variances are given by

$$(4.32) \quad V_I^i(t) = E\{(K_I^i(t, \gamma) - M_I^i(t))^2\} = \sum_{j,k=1}^N V_{jk} K_I^{ij}(t) K_I^{ik}(t), \quad i = 1, 2$$

where $V_{jk} = E\{(Z_j(\gamma) - M_j)(Z_k(\gamma) - M_k)\}$ is the covariance of $Z_j(\gamma)$ and $Z_k(\gamma)$. In particular, when $Z_j(\gamma)$, $j = 1, 2, \dots, N$, are independent, formula (4.32) reduces to

$$(4.33) \quad V_I^i(t) = \sum_{j=1}^N V_{jj} K_I^{ij}(t)^2, \quad i = 1, 2$$

with V_{jj} being the variance of $Z_j(\gamma)$.

For numerical calculations we consider a cylinder of radius $b = 0.1$ [m] made of low-strength steel, with material parameters as in Example 1. The crack is of length $a = 2$ [mm]. The boundary concentration is assumed in the form (4.29) with $N = 3$ and $f_j(t) = \sin(k_j t) + 1$, $j = 1, 2, 3$. The random variables $Z_1(\gamma)$, $Z_2(\gamma)$, $Z_3(\gamma)$ are independent and uniformly distributed between 0 and $\bar{Z} = 500$ [mol/m³]. The means and variances of $Z_j(\gamma)$ are: $M_j = \bar{Z}/2 = 250$ [mol/m³] and $V_{jj} = \bar{Z}^2/12 \approx 20833$ [mol²/m⁶], $j = 1, 2, 3$. The frequencies are assumed to have the following values: $k_1 = 2\pi/7$, $k_2 = 2\pi/16$, and $k_3 = 2\pi/60$ [day⁻¹].

In Figures 6 and 7 only the results for the crack edge at r_1 are shown, because the corresponding values for the two edges differ only slightly (owing to the short chosen crack length). It can be seen that under the action of a cyclic boundary

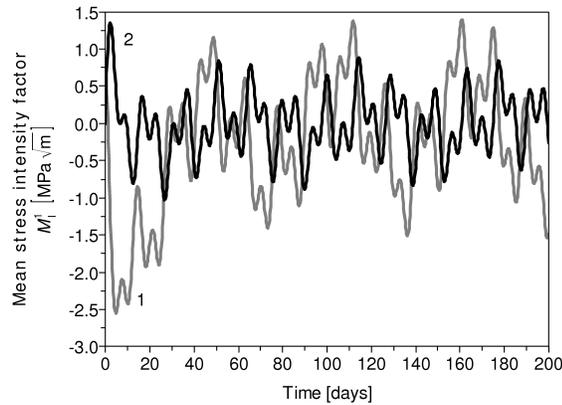


FIG. 6. Mean stress intensity factor at the inner edge of the crack, M_I^1 , vs. time. Curve 1 corresponds to $r_1 = 78$, and curve 2 to $r_1 = 58$ [mm].

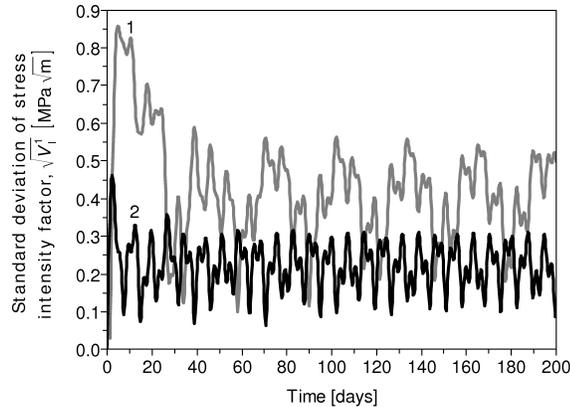


FIG. 7. Standard deviation of the stress intensity factor at the inner edge of the crack, $\sqrt{V_I^1}$, vs. time. Curve 1 corresponds to $r_1 = 78$, and curve 2 to $r_1 = 58$ [mm].

concentration $C^*(t, \gamma)$, the crack undergoes cyclic tension and compression (as presented in Fig. 6 for the case of mean values). The influence of hydrogen is also more attenuated towards the center of the cylinder: cracks closer to the boundary sustain higher stress amplitudes, and are therefore more likely to propagate. Their stress intensity factors also exhibit greater statistical scatter (Fig. 7).

5. Conclusions

In the paper, an effective method for quantitative characterization of random hydrogen-induced stresses has been presented. The method is based on the randomized diffusion-elasticity equations, but also a simpler, stochastic parametric model, based on empirical information on hydrogen stresses, is briefly sketched. The analysis allows to perform specific calculations in a wide range of real situations. The numerical calculations for the examples considered provide quantitative effects of random hydrogen-induced stresses on the random time to material failure and on the stress intensity factors. The graphical visualization exhibits the effects of the basic statistical characteristics of the hydrogen concentration (e.g. its standard deviation and correlation time) on the failure time and on the Mode-I stress intensity factor.

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