Application of the Monte Carlo Method to Evaluate the Impact of Uncertainty of Model Parameters on the Time of Concrete Cover Damage

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Abstract. The work concerns the evaluation of the cover cracking time in corrosion conditions of reinforcement. The simulation approach using the Monte Carlo method was used to determine the limit values of corrosive volumetric strains that can be created as the result of corrosion. The calculations were made using the ATENA package, taking into account the effect of concrete curing on the cracking propagation of the test sample.

1. Introduction

Computer-aided modelling of damage propagation resulting from corrosion of reinforcement in reinforced concrete elements is an important aspect of research [1], [2]. Problems on the adequate representation of behavior of reinforced concrete elements are related not only to the adequate simulation of the material [3], but also the evaluation of uncertainty of the model parameters [4]. The available literature describes many models that represent corrosion of reinforcement in reinforced concrete elements. The majority of them simulate the effect of reinforcement corrosion by introducing the equivalent coefficient of corrosive expansion of a rebar [5]. Some of them additionally allow for product penetration into pore voids of the interfacial transition zone [6] at the initial stage of the process or their expansion to deeper layers of concrete [2], [7], [8]. The main problem is that the mentioned models generally assume parameters defining constants of the model as strictly determined which is not true.

This paper describes the application of the simulation Monte Carlo method [9] and the FEM method to evaluate the time of concrete cover damage. Parameters of the model describing the impact on the environment and the corrosion process were assumed to be random variables that could be partially correlated and depend on moisture content, temperature and concrete creeping. The issues described in this paper broaden the scope of the previous papers [10], [11]. The simulation approach was used to determine critical coordinates for the tensor of volumetric strains, which was the effect of the deposition of corrosion products in the steel-concrete interface. $\min(\varepsilon_{ij}^v)$ and $\max(\varepsilon_{ij}^v)$ interfacial transition zone. Boundary values of volumetric strains were determined using the M-C method and the code written in the MATLAB software. The ATENA software was used to simulate the process of concrete cover cracking for the extreme values of corrosion volumetric strains.
2. Computational model

The analysis of reinforcement corrosion is closely related to the microstructure of steel-concrete contact zone (so called ITZ layer). The process of reinforcement corrosion can be divided into three stages:

- First stage - deposition of corrosion products in pore voids in the interfacial transition layer surrounding the rebar, \( t \leq t_0 \), \( t \) – time, \( t_0 \) – time required to fill pore voids in the ITZ.
- Second stage - expansion of corrosion products, gradual increase in pressure related to the impact of corrosion products on cover concrete, the formation of micro-cracks in the ITZ and pushing some of the corrosion products to deeper layers of concrete, \( t_0 \leq t \leq t_{cr} \), \( t_{cr} \) – time required for cover expansion.
- Third stage - development of corrosion damage, begins after time \( t = t_{cr} \), all corrosion products have the mechanical impact on the cover (tightened ITZ structure).

The visualizations of the impact of corrosion products on the structure of pores in concrete is shown in Figure 1. Figure 1a illustrates the rebar with the surrounding cover. The inspected area containing a fragment of the interfacial transition zone is shown in Figure 1b and the simplified model describing corrosion process in the cover is presented in Figure 1c. Numbers marked in Figure 1 refer to:
1) cement grout, 2) products from reinforcement corrosion 3) pore voids (with air and pore solution), 4) steel rebar, 5) corrosion pit filled with products from reinforcement corrosion.

![Figure 1. The model of corrosion products deposition in concrete pores](image-url)

In the cases of corrosion process, the resulting products penetrate into the contact zone and the structure of pores in the ITZ. No interaction between corrosion products and the cover structure occurs in the initial phase. Filling of pore structure in the transition zone induces the mechanical interaction. Each change in the mass of corrosion products in the analyzed area \( \Delta m_{ew} \) is accompanied by changes related to the transfer of corrosion products to deeper layers of concrete \( \Delta m_{tran} \) and to areas of micro-damage developed in the transition zone \( \Delta m_{por} \). The effective mass balance in the analysed area of the interfacial transition zone can be expressed as:
where: $m_{\text{eff}}$ is the effective change in the mass of corrosion products, $\dot{m}_R$ is the source of the mass of corrosion products – accumulation rate of corrosion products in the analyzed area, $\dot{m}_{R,Fe^{2+}}$ is the rate of change of the mass of corrosion products as the result of their deposition in the corrosion pit in the rebar (proportional to the formation of this loss in accordance with Faraday’s law), $\dot{m}_{\text{tran}}$ is the rate of change in the mass of corrosion products as the result of their migration to deeper layers of concrete, $\dot{m}_{\text{por}}$ is the rate of change in the mass of corrosion products as the result of their migration to pore space and micro-cracks formed in the interfacial transition zone - ITZ. As thickness of the transition zone is relatively low, the model representing changes in this zone can be simplified as shown in Figure 1c. Assuming the constant density of corrosion products $\rho_R$, the equation (1) can be represented with the volume change rate for relevant components of the relationship (1):

$$
\dot{V}_{\text{eff}} = \dot{V}_{ekw} - \dot{V}_{\text{por}} - \dot{V}_{\text{tran}}, \quad \dot{V}_{ekw} = \dot{V}_R - \dot{V}_{Fe^{2+}}, 
$$

(2)

$$
\dot{V}_{Fe^{2+}} = \dot{V}_{R,Fe^{2+}}, \quad \dot{V}_{R,Fe^{2+}} = \frac{\dot{m}_{R,Fe^{2+}}}{\rho_R}, \quad \dot{V}_{Fe^{2+}} = \frac{\dot{m}_{Fe^{2+}}}{\rho_{Fe^{2+}}}, \quad \dot{m}_{Fe^{2+}} = kI, \quad (3)
$$

where: $\dot{V}_{\text{eff}}$ is the rate of change of effective volume of corrosion products having mass of $m_{\text{eff}}$, $\dot{V}_R$ is the rate of change in mass of products from reinforcement corrosion having mass of $m_R$, $\dot{V}_{Fe^{2+}}$ is the rate of change in volume of corrosion loss having mass of $m_{Fe^{2+}}$ (Faraday’s law) tightly filled with corrosion products with volume $V_{R,Fe^{2+}} = V_{Fe^{2+}}$ and mass $m_{R,Fe^{2+}}$, $\dot{V}_{\text{por}}$ is the rate of change in volume of corrosion products brought into pore spaces and micro-cracks formed in ITZ, while $\dot{V}_{\text{tran}}$ is the rate of change in volume of corrosion products brought into deeper layers of concrete. Introducing into this discussion the parameter $\beta$, which is the quantity defining the intensity at which developing corrosion affects the cover structure [2], [8] the following equations (2) and (3) can be expressed in the modified form:

$$
\dot{V}_{\text{eff}} = (1 - \beta)\dot{V}_{ekw}, \quad \dot{V}_{ekw} = \Phi I, \quad I = A_0i, \quad \beta \dot{V}_{ekw} = \dot{V}_{\text{por}} + \dot{V}_{\text{tran}}, \quad (4)
$$

$$
\Phi = \frac{(\alpha^{-1}\vartheta - 1)k}{q_{Fe^{2+}}}, \quad \alpha = m_{Fe^{2+}}m_R^{-1}, \quad \vartheta = q_{Fe^{2+}}q_R^{-1}. \quad (5)
$$

In the equations (4), (5) $\beta$ is the function describing the impact of corrosion products on the concrete cover, $\alpha$ and $\vartheta$ are parameters dependent on chemical composition of corrosion products, $q_{Fe^{2+}}$ is density of Fe ions, $q_R$ is density of corrosion products, $k$ is electrochemical equivalent of Fe, $I$ is intensity of corrosion current, $A_0$ is area of rebar side surface, $i$ is density of corrosion current.

Coordinates of the tensor of volumetric strains can be defined depending on the phase, in which corrosion occurs [8], [10].

- Initial and intermediate stages, $t \leq t_{cr}$

$$
\varepsilon = \varepsilon^\gamma = \frac{\lambda(1 - \beta)\dot{V}_{ekw}}{V_0} \delta_{\gamma\delta}, \quad \gamma, \delta = 1,2, \quad \varepsilon^\gamma_{33} = \beta \varepsilon^\gamma, \quad \eta = 3\beta + 2(1 - \beta), \quad (6)
$$
- **Active state of corrosion, \( t \geq t_{cr} \)**

\[
\varepsilon^V = \frac{\lambda}{2 V_0} \epsilon_{\gamma \delta}, \quad \varepsilon^V_{33} = 0. 
\] (7)

When modeling the process of corrosion it was assumed that the impact of corrosion products is only in the plane perpendicular to the rebar axis.

In the equations (6), (7) \( V_0 \) is initial volume of the examined region, for which an increment in corrosion products is observed, and \( \lambda \) is the function allowing for describing additional loss related to migration of corrosion products beyond the contact area between steel and concrete, which can occur after cover cracking. The parameter \( \beta \) is the linear function that modifies the impact of corrosion products depending on the phase of their impact on concrete [8] (similar relationship has been already applied in the paper [2]).

\[
\beta = \begin{cases} 
1, & t < t_0 \ (V_{ekw} < V_{por.in}), \\
(t_{cr} - t) / (t_{cr} - t_a), & t_0 \leq t \leq t_{cr} \ (V_{por.in} \leq V_{ekw} \leq V_{cr} = V_{ekw}(t_{cr})), \\
0, & t > t_{cr} \ (V_{ekw} > V_{ekw}(t_{cr}) = V_{cr}). 
\end{cases} 
\] (8)

where \( V_{por.in} \) is the initial volume of the pore space in ITZ, \( V_{cr} \) is the critical volume of corrosion products (the tight layer of corrosion products is created in the transition layer after time \( t = t_{cr} \) )

**3. Numerical example**
The reinforced concrete element with dimensions of 800 x 100 x 160 mm, reinforced with steel rebar \( \phi 20 \) was subjected to the numerical analysis. The analyzed fragment of the structure and the FEM model are shown in Figure 2.

![Figure 2](image_url)

**Figure 2.** Test reinforced concrete elements and the FEM model: a) FEM model, b) diagram of test element.

The element was assumed to be exposed to chloride ions (of the defined concentration ) and the effects of temperature \( T \) and relative humidity \( h \) variable over time (the functions were simplified [12], [13]).

\[
h = 0.5(h_{min} + h_{max}) - 0.5(h_{min} - h_{max}) \sin(2\pi t), 
\] (9)
\[ T = 0.5(T_{\min} + T_{\max}) + 0.5(T_{\min} - T_{\max}) \sin(2\pi t), \]  

(10)

where \( T_{\max}, T_{\min} \) are random variables defining the maximum and minimum, \( h_{\max} \) and \( h_{\min} \) are random variables defining the maximum and minimum values of relative humidity. The functions of corrosion current density \( i \) and electrical resistance of concrete \( R \) were determined using the modified empirical functions \([12], [13], [14]\) (i = \( t(s) \) for \( t \leq 14 \, \text{dni}, t_s = 14 \, \text{dni}\))

\[ i = 0.9259(8.37 + 0.618 \ln(1.69C_{mc} - 3034T^{-1} - 105^{-6}R_{c, res} + 2.25t^{-0.215})) \]  

\[ R = 90.537h^{-7.2548}(1 + \exp(5 - 50(1 - h))) \]  

(11)

(12)

where: \( i \) is corrosion current density \( \mu A/cm^2 \), \( C_{Fe} \) is chloride concentration on the reinforcement surface \( kg/m^3 \) \( (C_{mc} = m_{cem}C_{Cl^-}) \), \( m_{cem} \) is cement content in concrete, \( C_{Cl^-} \) is concentration of chloride ions on the reinforcement surface, \( T \) is the temperature at the reinforcement surface \( K \), \( R \) is the electrical resistance of concrete \( \Omega \), \( t \) is the exposure time, \( year \), \( h \) is relative humidity, \( l \).

Boundary curves of volumetric strains caused by the impact of corrosion products on cover concrete were determined during the first stage of calculations. The calculations were made using the M. C. method taking account of the correlation with random variables of the model (the algorithm was introduced in the paper \([4]\)). Due to the lack of experimentally obtained data, expected values and standard deviations of parameters characterized by the normal Gauss distribution were arbitrary assumed as equal to similar values obtained for numerical intervals assuming the uniform distribution \( X \in (X^-, X^+) \), mean value \( X_0 = 0.5(X^+ + X^-) \), variability range \( \Delta X = X^+ - X^- \), deviation from mean value \( \eta = 5\% \) (A), 15\% (B) in accordance with the relationships

\[ X^- = X_0 - 0.5\Delta X, \quad X^+ = X_0 + 0.5\Delta X, \quad \Delta X = \eta X_0 \]  

\[ \mu_{X_i} = \frac{X_{\max} + X_{\min}}{2}, \quad \sigma_{X_i} = \sqrt{\frac{(X_{\max} - X_{\min})^2}{12}}, \]  

(13)

(14)

where \( \mu_{X_i} \) is expected value (average value), \( \sigma_{X_i} \) is standard deviation. Additionally, random values with the normal Gauss distribution were assumed to be limited to intervals \( (R^-, R^+) \), \( R^- = \mu_{X_i} - 2\sigma_{X_i}, \quad R^+ = \mu_{X_i} + 2\sigma_{X_i} (95.4\% \text{ of observations}) \). The expected values \( \mu_x \) and \( \mu_y \) (1) of corrosion products were assumed as mean values for the mixture \( Fe(OH)_2 \) and \( Fe(OH)_3 \) \([15]\). Mean values and standard deviations of random variables are compared in table 1.

These random variables describing the parameters \( X_1 \equiv \alpha, \quad X_2 \equiv \theta \quad X_3 \equiv \psi, \quad X_4 \equiv w_{wp} \) were assumed to be correlated. The matrix of correlations between random variables \([4]\) with elements \( \rho_{XX} = 1, \quad \rho_{12} = \rho_{21} = 0.5, \quad \rho_{34} = \rho_{43} = 0.5 \) were arbitrary assumed (other values were equal to zero). The calculations were made for \( N = 500 \) randomly selected numbers to obtain the general approximated solution.

As a result of calculations made using the M. C. method to assess the impact of uncertainty of the model parameters, lower and upper bounds of the function of corrosion current density \( min(i) \), \( max(i) \) and electrical resistance of concrete \( min(R), \, max(R) \) were determined. The results taken account of uncertainty of the model parameters 5\% case A and 15\% case B are shown in Figure 1:

a) Figure 1a for deviation A, b) Figure 1b for deviation B. Changes in the volume of corrosion products in a function of corrosion current density were determined using the M. C. method for uncertainty of the model parameters assumed in the calculations, cases A and B are shown in figure 2:
a) figure 2a, equivalent volume $V_{ekw}$, b) figure 2b, effective volume $V_{eff}$. Similarly, figure 3 presents lower \( \min \) and upper \( \max \) bounds that were determined using the M. C. method and applied for increments in volume strains caused by the presence of corrosion products in the plane perpendicular to the rebar axis, \( \min (\Delta e^V) \) and \( \max (\Delta e^V) \). 

Cracking of the element cover was analyzed to conduct loading program within 5 years, which is illustrated in figure 5. The performed calculations took into account the contact at the interface between steel and concrete (interface elements) and the process of concrete creep [16]. The load was applied only in the plane perpendicular to the rebar axis to simplify the calculation algorithm.

**Table 1.** Expected values and standard deviations of random variables for analyzed cases A and B

| Material parameters | Expected values (A) | Standard deviat. (A) | Expected values (B) | Standard deviat. (B) |
|---------------------|---------------------|----------------------|---------------------|----------------------|
| \( X_1 \equiv \alpha \cdot 10^3, l \) | \( \mu_X \), 573 | \( \sigma_X \), 8.263 | \( \mu_X \), 573 | \( \sigma_X \), 24.790 |
| \( X_2 \equiv \theta \cdot 10^3, l \) | \( \mu_X \), 216.5 | \( \sigma_X \), 31.249 | \( \mu_X \), 216.5 | \( \sigma_X \), 93.747 |
| Porosity of transition zone, \( X_3 \equiv \psi \cdot 10^3, l \) | \( \mu_X \), 550 | \( \sigma_X \), 7.939 | \( \mu_X \), 550 | \( \sigma_X \), 23.816 |
| Width of transition zone, \( X_4 \equiv w_{wp} \cdot 10^3, cm \) | \( \mu_X \), 7.5 | \( \sigma_X \), 0.108 | \( \mu_X \), 7.5 | \( \sigma_X \), 0.325 |
| Electrochemical equivalent of Fe, \( X_5 \equiv k \cdot 10^3 g/\mu A r o k \) | \( \mu_X \), 9.122 | \( \sigma_X \), 0.132 | \( \mu_X \), 9.122 | \( \sigma_X \), 0.395 |
| Concentration of chloride ions on reinforcement surface, \( X_6 \equiv C_{Cl^-}, \% m. c. \) | \( \mu_X \), 0.4 | \( \sigma_X \), 0.0058 | \( \mu_X \), 0.4 | \( \sigma_X \), 0.017 |
| Max. temperature \( X_7 \equiv T_{\max}, K \) | \( \mu_X \), 298.15 | \( \sigma_X \), 0.253 | \( \mu_X \), 298.15 | \( \sigma_X \), 0.758 |
| Min. temperature \( X_8 \equiv T_{\min}, K \) | \( \mu_X \), 283.15 | \( \sigma_X \), 0.253 | \( \mu_X \), 283.15 | \( \sigma_X \), 0.758 |
| Max. relative humidity \( X_9 \equiv h_{\max}, l \) | \( \mu_X \), 0.8 | \( \sigma_X \), 0.010 | \( \mu_X \), 0.8 | \( \sigma_X \), 0.030 |
| Min. relative humidity \( X_{10} \equiv h_{\min}, l \) | \( \mu_X \), 0.6 | \( \sigma_X \), 0.010 | \( \mu_X \), 0.6 | \( \sigma_X \), 0.030 |
| Critical time \( X_{11} \equiv t_{kryt}, year \) | \( \mu_X \), 0.685 | \( \sigma_X \), 0.0099 | \( \mu_X \), 0.685 | \( \sigma_X \), 0.0297 |

**Figure 3.** Changes in density of corrosion current \( i \) and electrical resistance of cover \( R \) (lower \( \min \) and upper \( \max \) bounds, the Monte Carlo method): a) case A, b) case B – description in the text.
The critical time was assumed to be equal to $t_{cr} \approx 8.2$ months, parameter $\lambda = 1$ and cement content $m_{cwm} = 350 \text{ kg/m}^3$. The values of crack width in the reinforced concrete specimens were determined using the Monterey-Willam and Rankine models [16]. The following parameters of concrete [10] were used in the calculations: Young’s modulus, $E = 38.28 \text{ GPa}$, Poisson’s ratio, $\nu = 0.2$, average compressive strength of concrete $f_{cm} = 56.4 \text{ MPa}$, average tensile strength, $f_{ctm} = 3.99 \text{ MPa}$, cracking energy $G_F = 0.151 \text{ kN/m}$, maximum diameter of aggregate grains $d_{max} = 8 \text{ mm}$. Material parameters of the contact zone (the role of interface was stabilization of numerical computations) between steel and concrete: stiffness in normal direction $k_{nn} = 2 \cdot 10^8 \text{ MN/m}^3$, stiffness in tangential direction $k_{tt} = 2 \cdot 10^6 \text{ MN/m}^3$, cohesion coefficient $c = 1 \text{ MPa}$, friction coefficient $\phi=0.1$, tensile strength $f_t = 3 \text{ MPa}$. The elastic-plastic Huber–Misses–Hencky model was assumed for steel: Young’s modulus $E = 200 \text{ GPa}$, Poisson’s ratio $\nu = 0.3$, tensile strength of steel, $f_y=235 \text{ N/mm}^2$. Creep was calculated for the model FIB MC2010. The following were assumed: curing time of concrete - 10 days, cement class 42.5N, ratio $V_{\text{specimen}}/A_{\text{extern}} = 2.35 \text{ m}$, average relative humidity $h_{\text{avg}} = 0.7$, concrete density $\rho_{\text{concrete}} = 2300 \text{ kg/m}^3$. First loading of the specimen was applied after two months. Changes in the width of cracks in the specimen were calculated for lower $\text{min} (\Delta\varepsilon^V)$ and upper $\text{max} (\Delta\varepsilon^V)$ bounds of increments in the volume of corrosion products. The

![Figure 4](image1)

**Figure 4.** Changes in volume of corrosion products in a function of corrosion current density (the Monte Carlo method, lower $\text{min}$ and upper $\text{max}$ bounds, cases A and B): a) equivalent volume $V_{\text{ekw}}$, b) effective volume $V_{\text{eff}}$ – description in the text.

![Figure 5](image2)

**Figure 5.** Ultimate increments in volume deformations caused by products of reinforcement corrosion $\Delta\varepsilon^V = \Delta\varepsilon^V_{YY}$ (the Monte Carlo method, lower $\text{min}$ and upper $\text{max}$ bounds, cases A and B) – description in the text.
width of cracks was calculated at Gauss points of finite elements (at the Gauss point closest to the point, at which crack width is measured, point A, figure 2). The results calculated for both analyzed cases of loading with and without creeping, and the graphical image illustrating the mode of the specimen cracking at the assumed criterion for crack visibility $w_{\text{min}} \geq 0.1 \, \text{mm}$ are presented in figure 6. Limit values of time, at which cracks were developed in the assumed material models and the records of specimen loading (with and without creeping - p index) are compared in table 2 and table 3.

**Figure 6.** Limit width of cracks in the test reinforced concrete element for limit increments in volume strains determined using the Monte Carlo method $\min(\Delta e^V)$ and $\max(\Delta e^V)$, and the map of cracks (schemes A and B).

**Table 2.** Approximated predicted limit times for reaching characteristic width of cracks in the element for analyzed variants (loading schemes A and B, no creep)

| Time of test element damage | Approximated time of reaching the ultimate width of cracks month |
|-----------------------------|---------------------------------------------------------------|
|                             | $w = 0.1 \, \text{mm}$ | $w = 0.3 \, \text{mm}$ | $w = 0.6 \, \text{mm}$ |
| $t_{\text{min}}$ (A)       | 9                         | 17                        | 33                      |
| $t_{\text{max}}$ (A)       | 10                        | 21                        | 43                      |
| $t_{\text{min}}$ (B)       | 7                         | 13                        | 25                      |
| $t_{\text{max}}$ (B)       | 12                        | 25                        | 52                      |

**Table 3** Approximated predicted limit times for reaching characteristic width of cracks in the element for analyzed variants (loading schemes A and B, with creep)

| Time of test element damage | Approximated time of reaching the ultimate width of cracks month |
|-----------------------------|---------------------------------------------------------------|
|                             | $w = 0.1 \, \text{mm}$ | $w = 0.3 \, \text{mm}$ | $w = 0.6 \, \text{mm}$ |
| $t_{\text{min, creep}}$ (A) | 9                         | 18                        | 35                      |
| $t_{\text{max, creep}}$ (A) | 10                        | 22                        | 46                      |
| $t_{\text{min, creep}}$ (B) | 7                         | 13                        | 25                      |
| $t_{\text{max, creep}}$ (B) | 12                        | 25                        | 52                      |
4. Result and discussion
The proposed calculation approach is useful in estimating intervals, within which damage to reinforced concrete elements in structures are observed under the corrosion of reinforcement. The performed computer simulations clearly indicated a very high effect of the uncertainty of the model parameters on the propagation time of damage in the cover (the difference in extreme damage time could be even 100%). Propagation times of damage should be regarded as the approximate ones. It is very likely that the possible deposition of corrosion products in the cracks delays propagation of damage (the parameter $\lambda = 1$ was assumed in the analysed case). The suggested scheme of procedure should be regarded as the indicative approach. The function of distribution of probability density, which should be experimentally determined, is crucial for such calculations.

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