Modeling of the reinforced concrete structure performance at joint influence of mechanical and chemical loads

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Abstract. The present work offers formation principles of reinforced concrete structures design models that are used in the environment with joint influence of mechanical loads and chemically aggressive media. The model is proposed to be described with an equations system of mechanics and physics and chemical kinetics which includes: static equations (L. Navier); geometric equations (A. Cauchy); physical equations (R. Hooke, etc.); kinetic equations of aggressive medium transfer (A. Fick); kinetic equation of substances interaction (K. Guldberg – P. Waage); sorption equation (I. Langmuir). Practical methods for assessing the kinetics of estimated parameters change were developed. Methods for assessing a service life of reinforced concrete structures used in the joint conditions influence of mechanical loads and chemically aggressive media allowing predicting the service life of a structure at different stages - from design to physical wear - were developed.

1. Introduction
The use of reinforced concrete structures at joint influence of force factors and aggressive media is accompanied with changes, usually deterioration of strength, deformation, and geometric properties of a product over time.

In the normative calculation methods for considering the environmental influence, it is suggested to multiply the initial modulus value of elasticity, design resistance of concrete and concrete reinforcement by operation $\gamma_{bi}$ conditions ratio $\gamma_{si}$. However, this method is based on the use of safety factors and does not allow estimating the structure state evolution over time and providing a reliable prediction of its elements service life.

In the works of V.V. Bolotin, A.R. Rzhanitsin, V. D. Raiser, V. P. Chirkov, probabilistic methods for calculating a building structures service life [1 - 4] were suggested.

The works of the scientists C. A. Apostolopoulos, M. A. Baltasar Zamora, T. Saito, Yu. M. Bazhenov, P. G. Komkhov, A. F. Polak suggest to evaluate the concrete structures performance in aggressive media by the change of chemical composition and properties of concrete and reinforcement in the corrosion process [5 - 11].

Methods for prediction of concrete structures durability on the basis of the materials strength theory and thermodynamic approach to description of destruction kinetics were developed in the works of V.M. Bondarenko, V.I. Kolchunov, A.Aktinson, P.S. Mangat, B.Mohebimoghadam [12 -15].

The present level of knowledge and materials and structures interaction with the environment create objective preconditions for the unified theory development of materials strength to mechanical, chemical, and physical interactions. In the process of the materials strength models design, products,
and structures to mechanical loads are explored well enough and their reliability is proven by centuries-long experience of using the buildings and construction, the models of material resistance to chemical influence of aggressive media are still at development stage [16 - 18].

This work aims to provide experimental and theoretical substantiation of principles for drawing up design models of reinforced concrete structure elements that are used in the conditions of joint influence of mechanical factors and reactive media.

2. Mathematical model
The principles for drawing up a design model of reinforced concrete structure force resistance are known and based on the fundamental laws of deformable solids theory.

The classical model of reinforced concrete resistance to mechanical loads is presented in the form of equation system: equilibrium differential equation (L. Navier), geometrical equations (A. Cauchy ratio) and physical equations connecting stress and strain.

Engineering model for calculating reinforced concrete structures are based on the method of limit states taking into account conditions of the limit state occurrence in a certain point or in a cross section.

A design model of concrete product resistance to chemically active medium will be drawn up on the basis of experimental and theoretical data analysis on kinetics of concrete and reinforcement degradation contacting liquid aggressive media.

Experimental studies of cement interaction and polymer composites with aggressive media have brought the following conclusion: strength ($\sigma_{\text{mod}}$) modulus of elasticity ($E_0$) reduces under the influence of aggressive media; in some cases, a temporary increase of strength caused by colmatation effect followed by destruction of the concrete structure progressive and decrease of strength properties to zero was observed. Change of the strength properties occurs unevenly over the product volume, it has the greatest extent on the surface, which can be explained by uneven distribution of aggressive media at its penetration from the surface to the inside of a body and it is experimentally confirmed by measuring the strength and the material hardness in the cross a sample sectional area.

Dimensions and weight of a product may increase (sorption, swelling) or decrease (shrinkage, dissolution, washing-out) under the influence of aggressive media [16].

We suggest describing the degradation process kinetics with equation system: kinetic equation of liquid mass transfer (A. Fick); sorption (I. Langmuir); kinetic equation of substances interaction (law of K. Guldberg – P. Waage).

A phenomenological theory of diffusion processes, transfer and distribution of a substance mass are described by the second equation of A. Fick that, if the value of mass transfer ratio (diffusion) $D$ does not depend on coordinate $x$ and concentration $C$, has the following form:

$$\frac{dc}{dt} = D \frac{d^2c}{dx^2}.$$  \hspace{1cm} (1)

Solving the bilateral diffusion problem of aggressive fluids into the concrete plate with thickness of $2h$ and with limit conditions of the first kind ($C = C_0$ if $x = \pm h$ and $t \geq 0$, where $C = C_u$ at $t = 0$ and $-h \leq x \leq h$, where $C_u$ and $C_0$ are initial and equilibrium concentration values has the following form [15]:

$$\frac{C(t, x) - C_u}{C_0 - C_u} = 1 - \frac{4}{\pi} \exp \left(\frac{\pi^2}{4} \cdot \frac{D t}{h^2}\right) \cos \frac{\pi x}{2h}$$ \hspace{1cm} (2)

$$\omega(t) = \omega_m \left[1 - \frac{8}{\pi^2} \exp \left(\frac{\pi^2}{4} \cdot \frac{D t}{h^2}\right)\right]$$ \hspace{1cm} (3)

where $\omega(t)$ is the amount of fluid in the volume of the sample in time $t$; $\omega_m$ is the ultimate sorption capacity of the sample.
We offer to analytically describe the saturation kinetics of the composites with liquid which is graphically presented as sorption curves with the equation of 1. Langmuir:

\[ \omega(t) = \omega_m/(t_{0.5} + t) \]

(4)

where \( t_{0.5} \) is kinetic property of sorption processes rate.

The process kinetics of the corrosive liquid transfer can be analytically described with a system of equations (2) - (4) if kinetic constants \( \omega_m, t_{0.5}, D \) are known. Equation (3) allows defining \( D \) as a function:

\[ D = 4R^2 \pi t \left[ \ln \frac{8}{\pi^2} - \ln \frac{\omega_m - \omega(t)}{\omega_m} \right]. \]

(5)

If \( t \) is expressed from equation (4) through \( \omega_m \) and \( t_{0.5} \) and then put into equation (5), then we get:

\[ D = 0.4 A \frac{R^2}{B} = k_\tau \frac{R^2}{t_{0.5}}, \]

(6)

where

\[ 0.4 = \frac{4}{\pi^2}; A = \left[ \ln \frac{8}{\pi^2} - \ln \frac{\omega_m - \omega(t)}{\omega_m} \right]; B = \frac{\omega(t)/\omega_m}{1 - \omega(t)/\omega_m}. \]

The diagram drawn up on axes \( k_\tau = \omega(t)/\omega_m \) shows that the maximum value \( k_\tau = 0.17 \) if \( \omega(t)/\omega_m = 0.5 \).

We offer the following measures for diffusion ratio determination: take \( k_\tau = 0.17 \) in the formula (6); determine \( t_{0.5} \) constant by sorption curves [17].

Solving the equation (1) for the model of semi-infinite space allows determining coordinate of the front "\( \alpha \)" of diffusion zone with the following function:

\[ \alpha = k(\zeta)\sqrt{D t} \]

(7)

where

\[ k(\zeta) = 1 - \frac{C(a) - C_u}{C_0 - C_u}. \]

Ratio \( k(\zeta) \) is determined by experimental data obtained by measuring the microhardness, provided that \( \alpha \) is considered as coordinate of the front of composite structure destruction by aggressive medium (depth index).

We suggest describing the kinetics of material structure destruction on the kinetic equations basis of substances interaction (law of K. Guldberg – P. Waage). We suggest considering mono-, bi-, trimolecular interactions, depending on the number of substance types that are involved in the elementary reaction [16, 17]:

\[ V_1 = k_1[x]^n; \ V_2 = k_2[x]^m[y]^m; \ V_3 = k_3[x]^n[y]^m[z]^0 \]

(8)

where \( V_i \) is the rate of elementary reaction which is proportional to concentrations of \( x, y, z \) of reacting molecules; \( n, m, 0 \) – order of reactions.

All reactions of first order are described by monomolecular model as a differential equation:

\[ V_1 = -\frac{dc}{dt} = k_1C. \]

(9)

Solution of the equation is known: \( C = C_0 \exp[-k_1t]. \)

For bi- and tri-molecular reactions under assumption of equal concentrations of \( x, y, z \) reagents, the corresponding differential equations of second and third order are recorded:

\[ V_2 = -\frac{dc}{dt} = k_2C, \quad V_3 = -\frac{dc}{dt} = k_3C^3. \]

Solving the equations provides us with the following data:

\[ C = \frac{C_0}{k_2C_0t + 1}; \quad C = \sqrt[2]{\frac{1}{2k_2C_0t + 1}} \cdot C_0 \]

(10)
Assuming that \( C = C_k \) is a specific content or concentration of healthy bonds in the composite we can write as:

\[
\sigma(t) = C_k \cdot \sigma_0, \quad \text{where} \quad \sigma(t) = \frac{\sigma_0 \cdot \alpha \cdot n(t)}{A}
\]

where \( \sigma_0 \) is the bond strength; \( \alpha \) is the cross section area of a bond; \( n(t) \) is a number of healthy bonds; \( A \) is a cross section area of the product.

Then the change of relative strength, modulus of elasticity, or chemical resistance ratio \( k_{si} \) will be determined by the corresponding functions:

\[
k_{si} = \frac{\sigma(t)}{\sigma(0)} = C_0 \exp(-k_1t); \quad k_{s2} = \frac{C_0}{k_2C_n^e + 1}; \quad k_{s3} = C_0\sqrt{\frac{1}{2k_3C_n^e t + 1}}.
\]  

(11)

Experimental data processing of the cement composite strength kinetics under the influence of aggressive medium taking into account obtained formulas enables to determine the proper model for describing the process of chemical interaction between reactive masses.

It is determined that: monomolecular model should be used at high chemical reaction rates; bimolecular model at colmatation mechanism of mass interaction. Kinetics of the degradation processes in the concrete products that are used in the conditions of aggressive media can be described with degradation functions obtained from analysis of the corresponding models [15].

For the bending elements, the degradation function of hardness, bearing capacity has the following form:

\[
D(\sigma_n) = \iiint_{F(t)} E(t, x, y) y^2 dxdy / \iiint_{F(t)} E(t_0, x, y) y^2 dxdy
\]

(12)

\[
D(M) = \iiint_{F(t)} \varepsilon(t, x, y) E(t, x, y) dxdy / \iiint_{F(t)} \varepsilon(t_0, x, y) E(t_0, x, y) dxdy.
\]  

(13)

We suggest drawing up the degradation model graphically in the form of isochrone degradation showing properties destructive changes over the height of the product’s cross section [16].

In the first approximation, we take the following key parameters of the model degradation: depth indicator – \( a(t, y) \) defined by the formula (7); chemical resistance ratio \( k(t) \) describing the change of elasticity and strength properties of material on the product surface.

Since cement composites nonlinearly deformable, special attention should be paid to selection of a function for analytical description of the strain diagram. The following selection criteria are determined after analyzing over thirty functional dependencies between stress \( \sigma \) and deformation \( \varepsilon \):

- dependence should be a continuous differentiable function on diagram zone under consideration “\( \sigma - \varepsilon \)”, i.e. it should have the extremum at \( \varepsilon = \varepsilon_{bu} \);
- parameters of functional dependence of \( \alpha \) and \( \beta \) should be chosen from the limit conditions and expressed through rated elastic properties of material: \( E_0 \) - modulus of elasticity; \( \sigma_{bu} \) - ultimate strength; \( \varepsilon_{bu} \) - deformation corresponding to stress \( \sigma_{bu} \).

These criteria correspond to the functions of the F. I. Gerstner, A. Saint-Venant, ECB.

Taking into account the obtained results, we have got the following degradation function of the flexible element bearing capacity with a rectangular cross section, single reinforcement, linear isochrones of degradation in compressed area based on the limiting states method:

\[
D(M) = 1 - \frac{0.5 \cdot \frac{D(t)}{k} \left(1 - \exp(-k_1 t)\right)}{1 - 0.5 \mu \left(\frac{R_y}{R_{y_0}}\right)}.
\]  

(14)

Diagrams of flexible element changes bearing capacity with normal cross section that are used in the conditions of sulfate corrosion allow to determine service life of the product with known admissible reduction of the bearing capacity (in 20, 30, 40% at \( D=0.8; 0.7; 0.6 \)). Numerical values of \( D, k \) ratios are determined from the experimental data.

The problems on plates bending made of nonlinear deformable material that are loaded with unevenly distributed load and used in corrosive media were studied.
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