Numerical Modeling of Local Penetration of Chloride-Containing Medium into Construction Elements Made of Reinforced Concrete

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Abstract. The task of modeling the kinetics of chloride-containing medium penetration into construction elements out of reinforced concrete that have partially damaged anti-corrosion protective coatings is being discussed. As a result, chlorides penetrate the construction element via local surface areas which leads to irregularities between chloride dispersion volumes. The kinetics of chloride penetration is described by the equation of diffusion to solve which the CONDUCT software complex by professor S. Patankar was used. The methodology used to solve the diffusional equation is described. The results of the evaluation of concentration field in the axial section of a cylindrical construction element, which was centrally reinforced, are given. The chloride diffusion was symmetrical to the axis, the medium was applied through the central ring area equal to one third of the side surface area while the rest of the surface was isolated. It was shown that the methodology of evaluation and its algorithm allow one to evaluate the concentration field of chlorides in reinforced concrete structural elements under local or asymmetrical action of the chloride-containing medium. The example given illustrates that after a certain time interval critical the concentration of chlorides develops even in protected areas which are located far from the initial damaged area. This means that the corrosion destruction of reinforced elements develops not only in the immediate damage area, but also further away from it.

Elements of reinforced concrete structures are subjected to combined action of duress, temperatures and aggressive environmental mediums during their service. One of widespread mediums is chloride-containing one, which degrades the concrete and reinforcements upon its penetration. As a result, load-bearing ability is decreased, deformability is increased and longevity of construction elements also decreases. While the theory of evaluation of reinforced concrete structures under temperature and load-bearing stress is well-researched, such evaluation under the influence of aggressive (especially chloride-containing) environment is at a starting stage.

In articles [1-4] it is noted that the main factor in the destruction of reinforced concrete transport structures is the corrosion of the reinforcement, initiated and accelerated by the use of chloride salts,
deicers. And in [4], data are given that chloride corrosion in 66% of cases is the cause of the
destruction of reinforced concrete bridges. In [5] it is noted that damage due to chloride corrosion
around the world is the main reason for reducing the durability and integrity of reinforced concrete
structures. And although measures of primary and secondary protection are applied to protect concrete
and reinforced concrete [6,7], but chloride corrosion still occurs, and therefore it is of interest to
develop methods for predicting the behavior of reinforced concrete structures under conditions of
chloride corrosion. Various approaches to the evaluation of the service life of concrete structures
under operating conditions are considered in [8-10]. In the paper [11], it is proposed to use the
diffusion equation as a model for the effect of a medium to calculate the stress-strain state of
reinforced concrete structures under the influence of corrosive media, and as an example, the problem
of determining the stress-strain state of a reinforced concrete curved beam of a rectangular cross-
section under the conditions of a liquid aggressive Environment. In [12], data are presented on
modeling the behavior of a reinforced concrete bridge beam exposed to chlorides. The equation of
one-dimensional diffusion is used as a model of the medium's influence, from the solution of which
the time of the beginning of corrosion wear of the armature (incubation period) is determined. In the
paper [13] Dan M. Frangopol and co-authors consider the problem of modeling the penetration of
chlorides into reinforced concrete structures, the process of diffusion penetration being considered as a
diffusion process. In the works of V.I. Solomatova and V.P. Selyaeva [14,15], the change in the
mechanical characteristics of a concrete element is accounted for by the degradation functions of
rigidity and bearing capacity, which are obtained from an analysis of phenomenological models of
cross-sectional degradation. V.M. Bondarenko [16] proposed a technique for assessing the strength
resistance of reinforced concrete structures exposed to corrosive influences, and the non-force
(medium) resistance of concrete depends on the composition and manufacturing technology, on the
nature and mode of environmental influences, structure-forming and destructive processes, and the
temperature and hygrometric characteristics of the medium. N.V. Klyueva [17] constructed a
computational model of the force resistance of the exploited reinforced concrete, taking into account
the simultaneously occurring corrosion processes of the change in the strength and deformation
characteristics of materials in loaded structural elements and additional dynamic improvements from
structural changes in the structural system. In articles [18, 19], the behavior of reinforced concrete
structural elements under the influence of a load and a chloride-containing medium is investigated,
experimental data are presented on the kinetics of penetration of the medium into reinforced concrete,
according to their influence on the mechanical characteristics of concrete and reinforcement. The
models of deformation of compressible and bent ferro-concrete elements exposed to the aggressive
medium are constructed. As can be seen, to date, there is a certain amount of work on modeling the
behavior of reinforced concrete structures under conditions of chloride aggression. However, in these
works constructive elements of a fairly simple form are considered, and the effect of the medium is
taken into account using the frontal corrosion models, or using analytical solutions of the one-
dimensional diffusion equation for simple types of boundary conditions. Under actual conditions, the
structural elements are often subjected to a local asymmetric medium. The calculation schemes used
do not take into account the effects of local and asymmetric effects of chloride-containing media;
therefore, the consideration of cases when these media act on a part of the surface of a structural
element or asymmetrically affect the reinforced structural element is not only theoretical but also of
practical interest.

The process of interaction of a chloride-containing medium with structural elements is represented
as consisting of stages: the penetration of the chloride-containing medium into the volume of the
element, interaction with the material, leading to a change in the mechanical characteristics,
deformation and destruction, taking into account the ongoing process of destruction. The penetration
stage is very important, since the law of distribution of the components of the chloride-containing
medium over the volume of the structural element is formed on it, which then determines the law of
distribution of the mechanical characteristics. Since the concentration of the medium at a point varies
with time and depends on the position of the point with respect to the surface of the structural element,
the equation describing the change in concentration has the form of the mass transfer equation. The kinetics of the penetration of the medium into the material of the prestressed structural element is described by the diffusion equation:

$$\frac{\partial C}{\partial t} = \text{div}(D \text{grad} C)$$

(1)

where $D$ is the diffusion coefficient, which, as shown by experiments, can depend on stress, deformation and the level of material damage.

To find the concentration distribution $C$ over the volume of the structural element, it is necessary to solve equation (1) with the initial and boundary conditions corresponding to the problem under consideration. We confine ourselves to the problem of determining the concentration field $C$ over the cross-section of the constructive element, and we consider the hypotheses: the plane problem is considered; the pores of concrete are saturated with water, and the process of chlorides transfer has a diffusion character; only chlorine ions are considered as an aggressor, the influence of other ions is not taken into account; since the penetration of chlorides into the concrete is very slow ($D = 9 \times 10^{-12} \text{ m}^2/\text{c}$), the chemical composition of the concrete pore substance is considered to be equilibrium throughout the entire diffusion process; the process of diffusion of chlorides is considered to be two-dimensional; the value of the effective diffusion coefficient is assumed to be the same in both directions; the effective diffusion coefficient of chlorides does not depend on their concentration, the position of the considered body point and temperature. The initial condition is determined by specifying the distribution law of the concentration field of the chlorides at the initial instant of time:

$$C(x, y, z, 0) = f(x, y, z)$$

(2)

where $x$, $y$, $z$ are the coordinates of the points.

The boundary condition can be specified in various ways [20]. It is of interest to study the concentration field of chlorides in reinforced concrete structural elements whose penetration kinetics is described by an equation of the form (1) in the case of a local or asymmetric action of a chloride-containing medium.

For this class of problems, obtaining an analytical solution in most cases is not possible. Therefore, the diffusion problem is solved with the help of the CONDUCT software complex, developed by Professor S. Patankar from the University of Minnesota, USA [20].

Let's consider the basic methods and techniques used to obtain a solution. The diffusion equation can be written in the form:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i} \left( D \frac{\partial C}{\partial x_i} \right) + S = -\frac{\partial J_i}{\partial x_i} + S$$

(3)

where $J_i = -D \frac{\partial C}{\partial x_i}$ – is the diffusion flux in the direction of the coordinate $x_i$.

To obtain a numerical solution, the area under investigation is discretized by coordinates and time. The calculation grid is constructed as follows. The calculation area is divided into control volumes, the boundaries of which coincide with the discontinuities in the properties of materials, source members, etc. The grid points are placed in the geometric centers of the control volumes. The grid point at the boundary is placed at the center of the vertex face. The control volume associated with the boundary point is conveniently considered to have an infinitesimal thickness. Then the angular points have infinitesimal sizes of control volumes in both directions, and their influence on the concentration distribution is neglected. It is assumed that the value of the variable at the grid point prevails in the entire control volume surrounding it. Then, according to the known initial distribution and boundary conditions, the concentration distribution is calculated for all subsequent instants of time, with some time step $\Delta t$. 

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There are several ways of obtaining a discrete analogue of equation (3), but a completely implicit scheme is the only scheme that allows physically reasonable results for any $\Delta t$.

Equation (3) is a conservation law that is valid for any subdomain, including for a control volume. Integrating equation (3) over the control volume of an arbitrary internal point, we obtain:

$$\frac{\Delta V}{\Delta t} (C - C^0) = J_{ib}A_{ib} - J_{rb}A_{rb} + J_{ab}A_{ab} - J_{ab}A_{ab} + \bar{S} \Delta V$$

(4)

Where $C^0$ – is the value of $C$ in the previous time layer, $J$ – is the diffusion flux through the corresponding faces of the reference volume, $S$ – is the averaged source member averaged over the control volume, $\Delta V$ – is the volume of the reference volume, and $A$ – is the area of the corresponding face of the reference volume.

The diffusion flux on the right side is calculated as follows:

$$J_{rb}K_{rb} = K_{rb}(C - C_{rb})$$

where $K_{rb}$ – is the diffusion conductivity through the face.

$$K_{rb} = A_{rb}\left(\frac{\Delta x}{2D} + \frac{\Delta x}{2D_{rb}}\right)^{-1}$$

$\Delta x$ – is the size of the corresponding reference volume in the x direction. Diffusion flows on the other faces are defined similarly.

The discrete equation (4) is completely implicit, i.e. new, unknown values of concentration are considered as predominant throughout the time step $\Delta t$. For each nearest inner boundary point of the grid, the corresponding boundary point acts as one of the neighbors. Therefore, for each $C$, a value (boundary condition of the first kind) or an equation (a boundary condition of the second or third kind) must be given at the node on the boundary.

In view of the foregoing, equation (4) can be rewritten as:

$$aC = \sum a_{near} C_{near} + b$$

(5)

where $a_{near}$, $K_{near}$, $b = S \Delta V + a^0 C^0$; $a^0 = S \Delta V + a^0 C^0$ $a = a_{ib} + a_{rb} + a_{ab} + a_{ab} + a^0 - S \Delta V$; $a^0 = \Delta V / \Delta t$.

Algebraic equations (5) are nominally linear and there are as many as unknowns. To solve these equations, the variable direction method (or "line by line") and the block-correction scheme [20] are applied.

With the application of the described numerical algorithm and the modernized software complex CONDUCT, a diffusion problem was solved for calculating the concentration field in the axial section of a cylindrical centrally reinforced structural element, with axisymmetric diffusion of chlorides through a central annular zone equal to one third of the lateral surface, the remaining surface is isolated. The dimensions of the structural element and the scheme of the action of the chloride-containing medium are shown in Figure 1, a. It was believed that as soon as the concentration of chlorides at a certain point on the boundary of the material (concrete) - the reinforcement reaches a critical value, the process of activated corrosion of the metal begins. Initial and boundary conditions:

$$C_a = \text{const} (t = 0, 0 < r < R, 0 < z < L);$$

$$J_{cl} = K(C_h - C_a, r = R, \frac{1}{3L} < z < \frac{2}{3L});$$
\[ J_{cl} = 0 \left( r = R, 0 < z < \frac{1}{3L}, \frac{2}{3L} < z < L \right); \]
\[ J_{cl} = 0 \left( C_b < C_c, r = 0, 0 < z < L \right); \]
\[ J_{cl} = \text{const} \left( C_b \geq C_c \right); \]
\[ J_{cl} = 0 \left( z = 0, 0 < r < R \right). \]

The value \( r = 0 \) corresponds to the interface of the material (concrete) - reinforcement. \( R \) – is the thickness of the protective layer of concrete. The initial data for the calculation are given in Table 1.

| Parameter                                         | Value     |
|---------------------------------------------------|-----------|
| Concentration of chlorides in the surrounding concrete environment, mol / m³ | 642.88    |
| Initial concentration of chlorides in concrete, mol / m³ | 0.045     |
| Critical concentration of chlorides, mol / m³      | 0.18      |
| Outflow of chlorides from the surface of the material-reinforcement with corrosion, mol / m² | 6×10⁻¹⁰    |
| Mass transfer coefficient \( K \), m / s           | 1.73×10⁻¹²|
| The effective diffusion coefficient \( D \), m² / s | 9×10⁻¹²    |

The calculation is performed in an axisymmetric cylindrical coordinate system, and the convergence of the results of the numerical solution on the sequence of embedded grids was previously studied. Calculations of the concentration of the chloride-containing medium at the points \( A(z=0.075; \ r=0.165) \) and \( B(z=0.0417; \ r=0.0275) \), obtained with a time step 5×10⁻³ years on three different uniform grids 27x81, 9x27, 3x9 showed that reliable results are obtained even on rather coarse grids. In Figure 1, b shows the distribution of the concentration field of chlorides in the protective layer of concrete at different times (\( C \) is measured in mol / m³).

**Figure 1.** Central reinforced rod element with partially broken protective coating.

**Conclusions**

The methodology and algorithm which are presented allow to evaluate the concentration field of chlorides in reinforced concrete structures under local or asymmetrical application of chloride-containing medium.
The calculations show that after a certain time interval the higher-than-critical concentration of chlorides develops even in distant areas of construction element, which means that corrosion deterioration of reinforcements occurs not only in the immediate vicinity of chloride application, but also in distant areas.

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