The Influence of Structure Formation Conditions of the Composite on the Mass Transfer Processes

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Abstract. The article describes the phenomenon of moisture transfer in the system "composite non-metallic reinforcement – cement mortar" at the stage of hardening of the composite. The processes of moisture transfer occurring during the structure formation have an impact on the water-cement ratio of the cement mixture. The deformation and operational characteristics of cement concrete, its structural and phase composition, porosity, density and corrosion resistance depend on the water-cement ratio. To obtain a mathematical model of moisture transfer in the formation of the cement matrix, the equations of mathematical physics, the equations of unsteady mass transfer and the differential equations of mass conductivity of parabolic type are used. Mathematical models of mass transfer processes make it possible to predict the change in the characteristics of the composite at the hardening stage and to obtain concretes with specified properties. The presented physical and mathematical model of moisture transfer for the system "cement concrete – composite reinforcement" allows to take into account the change in water-cement ratio at the stage of hardening of the composite and to establish its influence on the structure formation of the composite and its performance characteristics. The formulated physical and mathematical problem can be solved for special cases by the method of microprocesses.

1. Introduction

In modern concrete science, increasing attention is paid to the reinforcement of concrete with non-metallic fibrous materials. The main advantages of composite materials in comparison with metals and their alloys are low density, high specific stiffness and strength, sufficient fatigue strength, durability, high corrosion resistance, good thermal insulation and low thermal expansion. These properties allow us to consider composite materials very attractive.

However, the fibers can absorb moisture from the cement mixture at the hydration stage of the composite, thereby reducing the water-cement ratio. As everyone knew, the water-cement ratio has a huge impact on the deformation and performance characteristics of cement concrete, its porosity, density and corrosion resistance.

With a decrease in the water-cement ratio, the strength and crack resistance of concrete increase [1-4], its porosity decreases [5, 6].
To take into account the effect of changes in the water-cement ratio on the strength characteristics of concrete, dependencies are derived for calculating the composition of concrete of various densities [7], in which the true water-cement ratio is one of the main factors taken into account.

2. Relevance
Equations are derived to describe the strength set of concrete during 28 days of hardening, on the basis of which the strength characteristics of concrete of different compositions depending on the water-cement ratio can be calculated [8-10].

There are equations to establish the degree of hydration and to describe the hardening processes of cement concretes depending on the water-cement ratio [11, 12]. It is established that with increasing water-cement ratio at the stage of hydration, the formation of various structural-phase composition of concrete occurs, the resulting calcium hydroxides have a reduced basicity, which negatively affects the strength of the composite [12-15].

On the basis of significant theoretical and experimental studies, scientists have derived equations describing the effect of water-cement ratio on the processes of self-compaction of concrete and its porosity [16].

A mathematical model is developed that expresses the dependence of the ratio of concrete strength in compression to cement activity on the water-cement ratio [17]. Mathematical models make it possible not only to predict the effect of W/C on the strength characteristics of concrete, but also to design the compositions of cement concrete, establishing the necessary water-cement ratio to produce concrete with the specified characteristics [17, 18].

An algorithm for determining the air entrainment during cement concrete hardening is developed, taking into account the influence of water-cement ratio on the basis of the calculated formulas of concrete strength [19]. The proposed algorithm also allows to design the composition of concrete with normalized compressive strength, tensile bending and frost resistance [20, 21].

3. Problem statement
Since the water-cement ratio is of great importance at the stage of structure formation of the composite, it is necessary to take into account all the factors that can affect the change in the amount of mixing water in the cement mixture during the hardening of concrete. One of these factors is the absorption of water by fiber composite non-metallic reinforcement.

The method of mathematical modeling used in the work is based on the equations of mathematical physics, equations of unsteady mass transfer and differential equations of mass conductivity of parabolic type [20, 21].

4. Results of experimental studies
Mathematical model of moisture transfer in the formation of the cement matrix will include the equation of moisture conductivity in concrete and fiber reinforcement:

$$\frac{\partial U_{\text{con}}(x, \tau)}{\partial \tau} = k_{\text{con}} \frac{\partial^2 U_{\text{con}}(x, \tau)}{\partial x^2} - q_{\text{vm}}(x, \tau) \quad (1)$$

$$\frac{\partial U_{\text{rein}}(x, \tau)}{\partial \tau} = k_{\text{rein}} \left[ \frac{\partial^2 U_{\text{rein}}(x, \tau)}{\partial x^2} + \frac{1}{x} \frac{\partial U_{\text{rein}}(x, \tau)}{\partial x} \right] \quad (2)$$

Equation (2) is written in cylindrical coordinates, since the model is presented for the system "composite reinforcement – cement concrete".

Initial conditions:

$$U_{\text{con}}(x, \tau)|_{\tau=0} = U_{0,\text{con}}; \quad U_{\text{rein}}(x, \tau)|_{\tau=0} = U_{0,\text{rein}}. \quad (3)$$

Here: $k_{\text{con}}, k_{\text{rein}}$ are coefficients of moisture conductivity of concrete and composite reinforcement, respectively, m$^2$/s; $q_{\text{vm}}(x, \tau)$ is mass source, kg/m$^3$.s; $x$ is coordinate, m; $\tau$ is time, s.

The mass source depends on the processes and can be distributed by coordinate and time.
Boundary conditions for problems (1)-(2) at the stage of hydration and structure formation will be written as follows:

1) For the inner layer of concrete:

\[-k_{\text{con}} \cdot \rho_0 \frac{\partial U_{\text{con}}(x, \tau)}{\partial x} \bigg|_{x=\delta_{\text{con}}} = \beta (P_{\text{ex}} - P_{\text{in}})\]  (4)

2) At the interface "concrete – fiber»:

\[j_{m.\text{rein}}(\tau) = j_{m.\text{con}}(\tau)\]  (5)

\[-k_{\text{rein}} \frac{\partial U_{\text{rein}}(x, \tau)}{\partial x} \bigg|_{x=R_{\text{rein}}=0} = -k_{\text{con}} \frac{\partial U_{\text{con}}(x, \tau)}{\partial x} \bigg|_{x=0'}\]  (6)

Here: \(P_{\text{ex}}, P_{\text{in}}\) are external and internal partial pressure; \(\beta\) is the mass transfer coefficient, m/s; \(j\) is density of substance flow, kg/s; \(R_{\text{rein}}\) is radius of composite reinforcement, m; \(\delta_{\text{con}}\) is the thickness of the protective layer of concrete, m.

At the stage of hydration of cement concrete, moisture is bound, and a cement stone is formed. Until the setting is started, moisture can be transferred to the fiber.

Figure 1 describes the processes occurring in reinforced concrete after pouring into a closed form, when moisture evaporation from the surface does not occur.

Figure 2 describes the processes occurring in reinforced concrete after pouring into an open form, that is, moisture evaporation from the surface occurs, and the fiber does not absorb water from the cement mixture.

Figure 3 describes the processes occurring in reinforced concrete after pouring into an open form, while there is a simultaneous evaporation of moisture from the surface and absorption of water by fiber.

When the structure of the cement stone is formed, the diffusion processes occurring in the pores of the composite will be decisive in the transfer of water in the concrete. If the fiber intensely absorbs water from the cement mixture, the water-cement ratio decreases, which affects the formation of the structure of concrete and its strength. This phenomenon is important to consider when producing composites with specified performance characteristics.
Figure 2. Field of moisture contents in concrete with the exposed surface.

Figure 3. Field moisture contents in the concrete with an open surface and sorption of moisture by fibers.

We introduce some assumptions to the model that do not distort the physical representation of the characteristic features of mass transfer phenomena in the system under study. First, we specify that from the point of view of equations of mathematical physics, the boundary problem of mass conductivity in the system "composite reinforcement - protective layer of concrete" is formulated in the problem of non-stationary mass conductivity with boundary conditions of the VI kind, which in itself “accumulates” serious problems for obtaining a solution. In addition, taking into account the dependence of the moisture conductivity coefficients on the moisture content makes the problem significantly nonlinear. Therefore, secondly, to solve the problem, we will use the numerical-analytical
method of "microprocesses" [22], which has proved itself positively in solving the problems of non-stationary heat transfer for heterogeneous systems.

Thirdly, the works of professor S.P. Rudobashta [23] showed that diffusion in non-porous bodies and polymers proceeds at much lower rates than in capillary-porous bodies. Therefore, in the formulation of the problem of moisture diffusion into the fiberglass reinforcement, it can be assumed that the field of moisture content is localized in a narrow zone, not penetrating the axis of the reinforcement. And this, in turn, allows to write the boundary conditions in the corresponding problem of moisture conductivity:

\[ U_{\text{rein}}(x, \tau)|_{x=x_b} = 0. \] (7)

It becomes possible to translate the problem of mass conductivity in a cylindrical coordinate system to the problem in a Cartesian system for an unlimited plate.

At the accepted assumptions for the solution of the considered problem we can use the solution given in the work of professors S.P. Rudobashta and E.M. Kartashov [24]:

- for concrete:

\[
U_{\text{con}}(x, \tau) = \frac{1}{\delta_{\text{con}}} \int_0^{\delta_{\text{con}}} U_{0,\text{con}}(x) \, dx - \frac{1}{\delta_{\text{con}}} (\beta(P_{\text{ex}}(\tau) - P_{\text{in}}) \cdot \tau - j_{\text{ex}}(\tau)) \]

\[ + \frac{2}{\delta_{\text{con}}} \sum_{n=1}^{\infty} \cos \left( \frac{m\pi x}{\delta_{\text{con}}} \right) \exp \left( -\pi^2 n^2 F_{\text{om}} \right) \int_0^{\delta_{\text{con}}} U_{0,\text{con}}(\xi) \cos \left( \frac{m\pi \xi}{\delta_{\text{con}}} \right) \, d\xi \]

\[ - \frac{2}{\delta_{\text{con}}} \sum_{n=1}^{\infty} \cos \left( \frac{m\pi x}{\delta_{\text{con}}} \right) \int_{\tau}^{\delta_{\text{con}}} \exp \left[ -\pi^2 n^2 \frac{D(\tau - \tau')}{\delta_{\text{con}}^2} \right] \cdot j_{\text{ex}}(\tau') \cdot (-1)^n \cdot j_{\text{ex}}(\tau') \, d\tau' \]

\[ + \frac{2}{\delta_{\text{con}}} \sum_{n=1}^{\infty} \cos \left( \frac{m\pi x}{\delta_{\text{con}}} \right) \int_0^{\tau} \int_{0}^{\delta_{\text{con}}} j(\xi, \tau') \cos \left( \frac{\pi n \xi}{\delta_{\text{con}}} \right) \exp \left[ -\pi^2 n^2 \frac{D(\tau - \tau')}{\delta_{\text{con}}^2} \right] \, d\tau' \, d\xi; \] (8)

- for reinforcement:

\[ U_{\text{rein}}(x, \tau) = \frac{1}{x_b} \int_0^{x_b} U_{0,\text{rein}}(x) \, dx - \frac{1}{x_b} \cdot j_{\text{in}}(\tau) \]

\[ + \frac{2}{x_b} \sum_{n=1}^{\infty} \cos \left( \frac{m\pi x}{x_b} \right) \int_0^{x_b} \exp \left[ -\pi^2 n^2 \frac{D(\tau - \tau')}{x_b^2} \right] \cdot j_{\text{in}}(\tau') \, d\tau'. \] (9)

Here: \( F_{\text{om}} \) is Fourier mass transfer criterion, \( \xi \) is integration coordinate in the range \( 0 \leq \xi \leq x_b; n \) is number of row members; \( D \) is diffusion coefficient, m²/s.

Thus, the article contains the theoretical basis of the phenomenon of moisture transfer in the system "composite reinforcement – cement concrete" at the stage of hardening of the composite, including a mathematical apparatus to describe the process of moisture transfer through the thickness of the concrete to the reinforcing fiber, taking into account its water absorption. Obtaining analytical solutions for the mass transfer boundary problem is not included in the scope of this article and will be presented in the following works of the authors.

5. Conclusion
The presented physical and mathematical model of moisture transfer for the system "cement concrete – composite reinforcement" allows to take into account the change in water-cement ratio at the stage of hardening of the composite and to establish its influence on the structure formation of the composite and its performance characteristics. In the future, the formulated physical and mathematical problem can be solved for special cases by the method of microprocesses.

Let's note one more important point. From the standpoint of the fundamentals of the theory of heat and mass transfer at mass transfer across the interface during the process the condition of equality of mass capacities is fulfilled at the point of contact of the phases [25]. It is expressed in the fact that the
mass content of a substance in one phase is equal to the mass content of this substance in another phase multiplied by a certain coefficient. For absorption processes ("liquid – gas" system) this coefficient is called the Henry coefficient [26, 27]. When considering the transfer processes in systems "liquid – solid" it is called an analogue of the Henry coefficient. A certain analogy is observed with the contact of solid phases. This explains, for example, the fact that the filter paper in contact with wood of lower moisture content absorbs moisture from the wood. In accordance with the approach presented in this article, it can also be assumed that a certain equilibrium is established in the "composite – concrete" system at the interface between them. And this topic is also of scientific interest for future research.

References

[1] Sekhar N S and Raghunath P N 2014 Influence of Water Binder Ratio on High Performance Concrete The Open Construction and Building Technology Journal 8 18-21
[2] Kovernichenko L and Shishkin A 2018 Regulation of the influence of the structure of inorganic binders on their properties Technology audit and production reserves 3 1(41) 37-42
[3] Klyuyev S V, Klyuyev A V, Sopin D M, Netrebenko A V and Kazlitin S A 2013 Heavy loaded floors based on finegrained fiber concrete Magazine of Civil Engineering 3(38) 7-14
[4] Haach V G, Vasconcelos G and Loureno P B 2011 Influence of aggregates grading and water/cement ratio in workability and hardened properties of mortars Construction and Building Materials 25 6 2980-2987
[5] Bai Z, Dong Y, Wang Z and Zhu T 2006 Emission of ammonia from indoor concrete wall and assessment of human exposure Environment International 32 3 303-311
[6] Latifee Enamur R, Sen Debasish and Kabir Md Rashedul 2016 Effect of Water to Cement Ratio and Age on Portland Composite Cement Mortar Porosity, Strength and Evaporation Rate American Journal of Engineering Research 5 8 120-127
[7] Elaty M 2014 Compressive strength prediction of Portland cement concrete with age using a new model HBRC Journal 10 2 145-155
[8] Singh S B, Vummadisetty Sudhir and Chawla Himanshu 2018 Influence of curing on the mechanical performance of FRP laminates Journal of Building Engineering 16 1-19
[9] Singh S B, Munjal Pankaj and Thammishetti Nikesh 2015 Role of water/cement ratio on strength development of cement mortar Journal of Building Engineering 4 94-100
[10] Dvorkin L and Dvorkin O 2015 Effective concrete based on composite low water-demand cement Scientific Israel – Technological Advantages 17 2 172-179
[11] ElNemr Amr 2019 Role of water-binder ratio on strength development of cement mortar American Journal of Engineering Research 8 1 172-183
[12] Shuldyakov K, Kramar L, Trofimov B and Ivanov I 2016 Superplasticizer Effect on Cement Paste Structure and Concrete Freeze-Thaw Resistance AIP Conference Proceedings 1698 070011
[13] Lukovic Mladen and Ye Guang 2016 Effect of Moisture Exchange on Interface Formation in the Repair System Studied by X-ray Absorption Materials 2 9(1)
[14] Ibragimov R A and Pimenov S I 2016 Influence of mechanochemical activation on the features in the of hydration of cement Magazine of Civil Engineering 2 3-12
[15] Ibragimov R A, Pimenov S I and Izotov S I 2015 Effect of mechanochemical activation of binder on properties of fine-grained concrete Magazine of Civil Engineering 2 63-69
[16] Chen X and Wu S 2013 Influence of water-to-cement ratio and curing period on pore structure of cement mortar Construction and Building Materials 38 804-812
[17] Fischer N, Haerdtl R and McDonald P J 2015 Observation of the redistribution of nanoscale water filled porosity in cement based materials during wetting Cement and Concrete Research 68 148-155
[18] Dvorkin L, Bezusyak A, Lushnikova N and Ribakov Y 2012 Using mathematical modeling for design of self compacting high strength concrete with metakaolin admixture Construction and Building Materials.37 851-864

[19] Ivanov A N and Trembitskiy M A 2011 Foam concrete of certain average density for thermal insulation of attics floors Magazine of Civil Engineering 8(26) 19-24

[20] Fedosov S V, Roumyantseva V E, Krasilnikov I V and Narmania B E 2017 Formulation of mathematical problem describing physical and chemical processes at concrete corrosion International journal for computational civil and structural engineering 13 2 45-49

[21] Fedosov S V, Roumyantseva V E, Krasilnikov I V and Konovalova V S 2018 Physical and mathematical modelling of the mass transfer process in heterogeneous systems under corrosion destruction of reinforced concrete structures IOP Conference Series: Materials Science and Engineering 456 012039

[22] Mizonov V, Yelin N, Kotkov A and Fedosov S 2017 Theoretical study of sheet construction materials drying with reversible supply of drying gas JP journal of heat and mass transfer 14 3 411-420

[23] Kosheleva M K, Novikova T A and Rudobashta S P 2016 Structural, adsorption, and mass-transfer properties of polycaproamide Fibre chemistry 47 5 372-376

[24] Rudobashta S P, Kosheleva M K and Kartashov E M 2015 Nonstationary mass transfer near the surface of a cylindrical body Journal of engineering physics and thermophysics 88 6 1320-1328

[25] Lykov A V and Mikhailov Yu A 1963 Theory of heat and mass transfer (Moscow-Leningrad: Gosudarstvennoe energeticheskoe izdatel'stvo) p 535

[26] Keltsev N V 1988 Principles of adsorption techniques (Moscow: Himiya) p 592

[27] Taburkin V I, Doronina M V, Udartseva O V, Solovev D B 2019 The Grounds of Subject Area of Technosphere Studies IOP Conference Series: Earth and Environmental Science 272 paper № 032022. [Online]. Available: https://doi.org/10.1088/1755-1315/272/3/032022