THE INFLUENCE OF THERMODIFFUSION CROSS EFFECT ON THE TEMPERATURE AND MOISTURE DISTRIBUTION IN EARLY AGE MASS CONCRETE

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Abstract

The issues related to the determination of the thermal and moisture fields in the early age massive concrete are discussed in the paper. The coupled equations, which govern the heat and mass transfer in early age mass concrete as well as the initial and boundary conditions are presented. Next, the discretization in the space was made with the use of the finite element method and the finite difference method was introduced for the discretization in time. As the result the matrix form of the heat and moisture transfer equations was obtained. To recognize the real influence of the thermodiffusion cross effect on the distribution of the temperature and moisture over the curing process, a few comparative analyses were done. The object of the conducted analyses was the massive foundation slabs.

Streszczenie

Zagadnienia prezentowane w artykule są związane z wyznaczaniem pól termiczno-wilgotnościowych w początkowym okresie twardnienia betonowych elementów masywnych. Przedstawiono sformułowanie wariacyjne zagadnienia początkowo-brzegowego, które opisuje zjawiska termiczno-wilgotnościowe w konstrukcji masywnej. Wykorzystując metodę elementów skończonych, dokonano dyskretyzacji zagadnienia w przestrzeni, natomiast dyskretyzacji w czasie dokonano za pomocą metody różnic skończonych. W rezultacie otrzymano macierzową postać równań termodyfuzji w twardniejącym betonie. Celem zaprezentowanych analiz numerycznych masywnych płyt fundamentowych było zbadanie wpływu krzyżowego efektu termodyfuzji na rozkład pól termicznych i wilgotnościowych w czasie procesu twardnienia betonu.

Keywords: **Thermal Fields; Moisture Fields; Early Age Concrete; Mass Concrete; FEM Modelling.**

1. INTRODUCTION

The setting and hardening of concrete is accompanied by nonlinear temperature and moisture distribution. The rise of the concrete temperature during curing is the result of exothermic nature of the chemical reaction between cement and water. The total heat of hydration of cement is influenced by number of factors, such as type of cement, cement content or initial temperature. In massive concrete structures hydration heat as well as relatively low thermal conductivity of concrete can cause considerable temperature differences between the centre and the external layers of the structure. Furthermore, hydration process is accompanied by moisture migration due to the hydration process and moisture transfer to the environment. The early age deformation according to the arising nonlinear temperature and moisture fields may result in cracking of young concrete. Cracking at this moment has major consequences for the long term structural performance of concrete structure and on its durability and serviceability. Though the stress state resulting from the thermal-moisture deformations of early age concrete are the main considerations of engineers, but it must be supported by proper prediction of thermal and moisture fields. Mathematical description of the discussed fields in early age concrete is particularly complicated. It should be remembered that we consider a porous body consisting of three phases: liquid, gaseous phases and the solid matrix. Additionally, the process of coupled heat and moisture transfer in curing concrete is accompanied by chemical and structural changes. High level of the problem complexity and almost impossible creation of the model with taking into account full details of the problem lead to the simplified descriptions. This way the models are developed as a compromise between the physical necessities and possibility of practical applications. Among others the models for the porous material are proposed by Harmathy [1], De Vries [2], Bażant [3], Gawin [4].

The simplest models in this field are created without taking into account chemical and phase change process. Usually the concrete is considered as a mixture consisting of two components, namely porous matrix and water (Nowacki [5,6], Černy [7]). To formulate the equations of coupled heat and moisture transfer in early age concrete the application of laws of irreversible thermodynamics is used (Nowacki [5,6], Wyrwał [8], Gumiński [9]).

2. EQUATIONS OF HEAT AND MOISTURE TRANSFER IN MASS CONCRETE

There is no doubt that the heat and moisture transfer in early age concrete is the coupled process. So, the flux of heat is consisting of the flux due to the gradient of temperature as well of the gradient of moisture. Similarly, considering the flux of moisture, both gradient of moisture concentration and the gradient of temperature should be taken into account. Additionally, in inquired fields in mass concrete the heat production rate as well as the reduction of the moisture content due to the hydration process cannot be omitted. Accordingly, the coupled temperature and moisture fields in early age mass concrete can be described by the following equations (Klemczak [10]):

$$\dot{T} = div\left(\alpha_{TT}\ grad\,T + \alpha_{TW}\ grad\,c\right) + \frac{1}{c_b \rho} q_v \tag{1}$$

$$\dot{c} = div\left(\alpha_{WW}\ grad\,c + \alpha_{WT}\ grad\,T\right) - K\,q_v \tag{2}$$

where:

T – temperature, K,

c – moisture concentration, kg/kg,

α_{TT} – coefficient of thermal diffusion, m^2/s,

$\dot{T} = \frac{\partial T}{\partial t}$, $\dot{c} = \frac{\partial c}{\partial t}$ - time derivatives of temperature, moisture concentration,

α_{TW} – coefficient representing the influence of the moisture concentration on the heat transfer, $(m^2K)/s$,

α_{WW} – coefficient of moisture diffusion, m^2/s,

α_{WT} – thermal coefficient of moisture diffusion, $m^2/(sK)$,

c_b – specific heat, kJ/kgK,

ρ – density of concrete, kg/m^3,

K – coefficient of the water-cement proportionality, which described amount of water bounded by cement during the hydration process with the rate of heat generated per unit volume of concrete, m^3/J,

q_v – rate of heat generated per unit volume of concrete, W/m^3.

Initial and boundary conditions may be expressed as follows:

$$T(x_i, t=0) = T_p(x_i, 0) \tag{3}$$

$$c(x_i, t=0) = c_p(x_i, 0) \tag{4}$$

$$\mathbf{n}^T\left(\alpha_{TT}\,grad\,T + \alpha_{TW}\,grad\,c\right) + \tilde{q} = 0 \tag{5}$$

$$\mathbf{n}^T\left(\alpha_{WW}\,grad\,c + \alpha_{WT}\,grad\,T\right) + \tilde{\eta} = 0 \tag{6}$$

where $x_i \in (V \cup \partial V)$, $i = x,y,z$, T_p, c_p are the initial distribution of temperature and the initial concentration of moisture respectively, $\mathbf{n} = \left[n_x\, n_y\, n_z\right]^T$ is the vector normal to the boundary surface ∂V.

The heat flux $\tilde{q}$ depends on the temperature of the boundary surface $\hat{T}(x_i, t)$ and the outer temperature. Similarly, the moisture flux $\tilde{\eta}$ depends on the moisture content at the boundary surface $\hat{c}(x_i, t)$ as well as on the moisture content in surrounding air. Therefore, it can be written:

$$\tilde{q} = \frac{\alpha_p}{c_b \rho}\left[\hat{T}(x_i, t) - T_z(t)\right] \tag{7}$$

$$\tilde{\eta} = \beta_p\left[\hat{c}(x_i, t) - c_z(t)\right] \tag{8}$$

where α_p denotes the thermal transfer coefficient, $W/(m^2K)$, β_p is the moisture transfer coefficient, m/s.

At this point it is important to mention, that the coupled equations (1) and (2), which govern the heat and mass transfer in early age mass concrete are applied comparatively rare. In such models proposed for the description of thermal and moisture fields, the equations are formulated independently, with neglecting their coupling (Andreasik [11], Kiernożycki [12], SzarlińskI [13], Ślusarek [14], Jonasson [15]). The linear diffusion equation is based on the Fick's law:

$$\dot{c} = div(\alpha_{WW} \; grad \; c) - K \, q_v \tag{9}$$

Similarly, the heat transfer equation is formulated on the ground of the Fourier law:

$$\dot{T} = div(\alpha_{TT} \; grad \, T) + \frac{1}{c_b \rho} q_v \tag{10}$$

3. NUMERICAL IMPLEMENTATION

Equations (1) and (2) can be rewritten in the form suitable for the finite element method, which seems to be very efficient and widespread method for solving this type of problem. To formulate the finite element scheme the Galerkin procedure as a special case of the weighted residual method, can be used. Introducing the gradient operator:

$$\nabla = \left\{ \frac{\partial}{\partial x}, \quad \frac{\partial}{\partial y}, \quad \frac{\partial}{\partial z} \right\}^T \tag{11}$$

and respecting the boundary conditions we can write for Eq. (1):

$$\int_V W_i \left(\frac{\partial T}{\partial t} - \nabla^T (\alpha_{TT} \nabla T) - \nabla^T (\alpha_{TW} \nabla c) - \frac{1}{c_b \rho} q_V \right) dV + \\ + \int_{\partial V} W_i \left(\mathbf{n}^T (\alpha_{TT} \nabla T + \alpha_{TW} \nabla c) + \tilde{q} \right) dA = 0 \tag{12}$$

and for Eq. (2) :

$$\int_V W_i \left(\frac{\partial c}{\partial t} - \nabla^T (\alpha_{WW} \nabla c) - \nabla^T (\alpha_{WT} \nabla T) + K \, q_V \right) dV + \\ + \int_{\partial V} W_i \left(\mathbf{n}^T (\alpha_{WW} \nabla c + \alpha_{WT} \nabla T) + \tilde{\eta} \right) dA = 0 \tag{13}$$

where W_i is the weighting function.

Applying the first Green statement to reduce the order of derivative and following the Galerkin procedure, where the shape functions are used as weighting as well as assuming that the unknown functions are approximated by a linear combination of the shape functions:

$$T = \mathbf{N}\,\mathbf{T} \tag{14}$$

$$c = \mathbf{NC} \tag{15}$$

we can write the matrix form of Eq. (1) and Eq. (2) respectively:

$$\mathbf{K}_{TT}\mathbf{T} + \mathbf{K}_{TW}\mathbf{C} + \mathbf{P}\dot{\mathbf{T}} = \mathbf{F}_T \tag{16}$$

$$\mathbf{K}_{WT}\mathbf{T} + \mathbf{K}_{WW}\mathbf{C} + \mathbf{P}\dot{\mathbf{C}} = \mathbf{F}_W \tag{17}$$

where:

$$\mathbf{K}_{TT} = \sum_{e=1}^{n} \int_{V^e} (\nabla \mathbf{N})^T (\alpha_{TT} \nabla \mathbf{N}) dV \tag{18}$$

$$\mathbf{K}_{TW} = \sum_{e=1}^{n} \int_{V^e} (\nabla \mathbf{N})^T (\alpha_{TW} \nabla \mathbf{N}) dV \tag{19}$$

$$\mathbf{K}_{WW} = \sum_{e=1}^{n} \int_{V^e} (\nabla \mathbf{N})^T (\alpha_{WW} \nabla \mathbf{N}) dV \tag{20}$$

$$\mathbf{K}_{WT} = \sum_{e=1}^{n} \int_{V^e} (\nabla \mathbf{N})^T (\alpha_{WT} \nabla \mathbf{N}) dV \tag{21}$$

$$\mathbf{P} = \sum_{e=1}^{n} \int_{V^e} \mathbf{N}^T \mathbf{N} dV \tag{22}$$

$$\mathbf{F}_T = \sum_{e=1}^{n} \int_{V^e} \mathbf{N}^T \frac{1}{c_b \rho} q_v \, dV - \sum_{e=1}^{n} \int_{\partial V^e} \mathbf{N}^T \tilde{q} \, dA = 0 \tag{23}$$

$$\mathbf{F}_W = -\sum_{e=1}^{n} \int_{V^e} \mathbf{N}^T K \, q_v dV - \sum_{e=1}^{n} \int_{\partial V^e} \mathbf{N}^T \tilde{\eta} \, dA = 0 \tag{24}$$

and **T**, **C** are the matrixes of nodes values of temperature and moisture respectively, N = $\left[N_i \, N_j \, N_k \ldots \right]$ is the matrix of shape functions.

The time derivatives in Eq. (16) and Eq. (17) can be replaced by difference approximations:

$$\dot{\mathbf{T}} = \frac{\mathbf{T}^{t+1} - \mathbf{T}^t}{\Delta t} \tag{25}$$

$$\dot{\mathbf{C}} = \frac{\mathbf{C}^{t+1} - \mathbf{C}^{t}}{\Delta t} \tag{26}$$

and the equations (16) and (17) can be written in the form:

$$(1-p)\mathbf{K}_{TT}^{t+1}\mathbf{T}^{t+1} + p\mathbf{K}_{TT}^{t}\mathbf{T}^{t} + (1-p)\mathbf{K}_{TW}^{t+1}\mathbf{C}^{t+1} + p\mathbf{K}_{TW}^{t}\mathbf{C}^{t} + \mathbf{P}\frac{\mathbf{T}^{t+1}-\mathbf{T}^{t}}{\Delta t} = = p\mathbf{F}_T^{t} + (1-p)\mathbf{F}_T^{t+1} \tag{27}$$

$$(1-p)\mathbf{K}_{WT}^{t+1}\mathbf{T}^{t+1} + p\mathbf{K}_{WT}^{t}\mathbf{T}^{t} + (1-p)\mathbf{K}_{WW}^{t+1}\mathbf{C}^{t+1} + p\mathbf{K}_{WW}^{t}\mathbf{C}^{t} + \mathbf{P}\frac{\mathbf{C}^{t+1}-\mathbf{C}^{t}}{\Delta t} = = p\mathbf{F}_W^{t} + (1-p)\mathbf{F}_W^{t+1} \tag{28}$$

Assuming coefficients p as equals 0 we can write the above as:

$$\mathbf{K}_{TT}^{t+1}\mathbf{T}^{t+1} + \mathbf{K}_{TW}^{t+1}\mathbf{C}^{t+1} + \mathbf{P}\frac{\mathbf{T}^{t+1}-\mathbf{T}^{t}}{\Delta t} = \mathbf{F}_T^{t+1} \tag{29}$$

$$\mathbf{K}_{WT}^{t+1}\mathbf{T}^{t+1} + \mathbf{K}_{WW}^{t+1}\mathbf{C}^{t+1} + \mathbf{P}\frac{\mathbf{C}^{t+1}-\mathbf{C}^{t}}{\Delta t} = \mathbf{F}_W^{t+1} \tag{30}$$

The final set of governing equations is obtained under condition that coefficients α_{TT}, α_{TW}, α_{WW}, α_{WT} do not depend on time:

$$\mathbf{A}_T\mathbf{T}^{t+1} = \mathbf{B}_T \tag{31}$$

$$\mathbf{A}_W\mathbf{C}^{t+1} = \mathbf{B}_W \tag{32}$$

with:

$$\mathbf{A}_T = \mathbf{K}_{TT} + \frac{1}{\Delta t}\mathbf{P} \qquad \mathbf{B}_T = \frac{1}{\Delta t}\mathbf{P}\mathbf{T}^{t} + \mathbf{F}_T^{t+1} - \mathbf{K}_{TW}\mathbf{C}^{t+1} \tag{33}$$

$$\mathbf{A}_W = \mathbf{K}_{WW} + \frac{1}{\Delta t}\mathbf{P} \qquad \mathbf{B}_W = \frac{1}{\Delta t}\mathbf{P}\mathbf{C}^{t} + \mathbf{F}_W^{t+1} - \mathbf{K}_{WT}\mathbf{T}^{t+1} \tag{34}$$

Solving the set of equations (31) and (32) we obtain the temperature and the moisture concentration in time step (t+1), which are simultaneously the initial values $\mathbf{T}^t$, $\mathbf{C}^t$ for the next step of calculations. In the first step of calculations the values $\mathbf{T}^t$ and $\mathbf{C}^t$ are equivalent to the initial temperature and moisture concentration of concrete. Nonlinearity of the problem is hidden in the dependence of matrixes $\mathbf{B}_T$ and $\mathbf{B}_W$ upon unknowns $\mathbf{T}^{t+1}$ and $\mathbf{C}^{t+1}$. Therefore, the iteration at each time step is requisite. Description of the iterative procedure as well as the original computer program TEMWIL that was developed on the basis of Eq. (31) and Eq. (32) was given by Klemczak [10].

4. THE ANALYSES OF THE MASS CONCRETE SLABS

As it has been mentioned in chapter 2 usually the equations describing thermal and moisture fields are formulated independently, with neglecting their coupling. Therefore, the crucial question is how strongly the gradient of moisture influences the heat flux and consistently how the temperature gradient affects the moisture flux. Succeeding question is if the cross termodiffusion effect should be taken into account in estimation of thermal and moisture fields in early age concrete or it can be omitted without significant detriment. An attempt to answer these questions requires carrying out some comparative numerical analyses. Presented calculations were made for massive concrete slabs of base dimensions 10 m × 10 m and thickness 3 m or 1.5 m. It was assumed that the analyzed slabs were made of the following concrete mix: cement CEMII/BS 32.5R 350 kg/m^3, water 175 l/m^3, aggregate 1814 kg/m^3. The finite element mesh of analyzed slabs was showed in Fig. 1. Because of symmetry only the quarter of the slab is modeled. Essential elements of the slab that were used in presentation of calculation results were filled with black colour in Fig. 1. Table 1 presents symbol assigned to the analyzed slabs and some details connected with initial and boundary conditions for slabs such as type of formwork, time of formwork stripping, temperature of air and initial temperature of concrete.

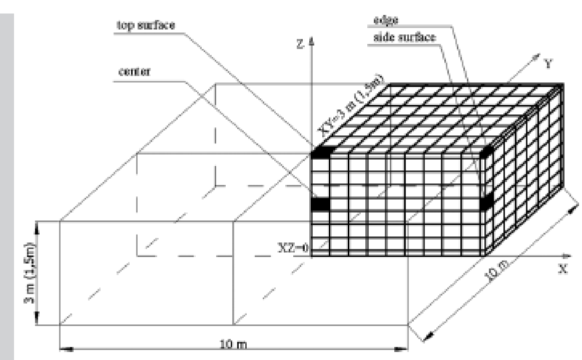

Figure 1.
Finite element mesh of the slab

Table 1.
Symbols of analyzed slabs

Symbol of the analyzed slab	The dimensions of the slabs, m	The outer temperature, °C	The initial temperature, °C	The time of shuttering removing, days	Protection of the top surface of the slab	Protection of the side and bottom surfaces of the slab
s_3m	10x10x3	20	20	>20	without protection	plywood 1.8 cm
s_1,5m	10x10x1.5	20	20	>20		
s_3m_r_5	10x10x3	20	20	5		
s_1,5m_r_5	10x10x1.5	20	20	5		

Table 2.
Thermal and moisture coefficients

Thermal fields		Moisture fields	
λ, $W / (mK)$	1.75	q_v, W/m^3	according to Fig. 2
c_b, $kJ / (kgK)$	1.0		
ρ, kg/ m^3	2340	K, m^3/J	$0.3\cdot10^{-9}$
α_{TT}, m^2/s	$7.47\cdot10^{-7}$	α_{WW}, m^2/s	$0.6\ 10^{-9}$
α_{TW}, $m^2\ K/s$	0 $9.375\cdot10^{-5}$	α_{WT}, $m^2/(sK)$	0 or $2\ 10^{-11}$ or $7\cdot10^{-11}$
α_p, $W/(m^2K)$	6.00 (without protection) 3.58 (plywood) 0.81 (plywood+soil)	β_p, m/s	2.78 (without protection) 0.18 (plywood) 0.12 (plywood+soil)
α_T, 1/°C	0.00001	α_W	0.001

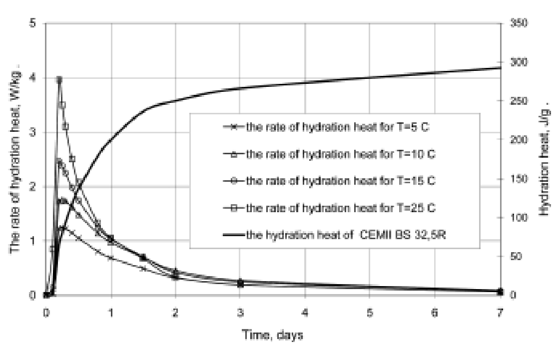

Figure 2.
The heat of hydration of CEM II BS 32.5R

Thermal and moisture coefficients necessary for calculation were set in Table 2. The values of coefficients were assumed according to literature suggestion (Černy [7], Andreasik [11], Kiernożycki [12], Szarliński [13], Witakowski [16]). The following values of coefficients related to the cross thermodiffusion effect were taken into account:

- $\alpha_{TW} = 0$, $\alpha_{WT} = 0$ – without thermodiffusion effect,
- $\alpha_{WT} = 9.375\cdot10^{-5}\ m^2K/s$, $\alpha_{WT} = 2\cdot10^{-11}\ m^2/(sK)$ – the lower value of the thermal coefficient of moisture diffusion,
- $\alpha_{TW} = 9.375\cdot10^{-5}$, $\alpha_{WT} = 7\cdot10^{-11}\ m^2/(sK)$ – the higher value of the thermal coefficient of moisture diffusion.

The analyses were made with the use of the original computer program TEMWIL (Klemczak [10]). For each considered slab (according to the symbol given in Table 1) temperature and moisture distribution were determined over 20 days of concrete curing. The results of the conducted numerical calculations are shown in Fig. 3÷6 (temperature distribution) and in Fig.7÷10 (moisture distribution).

Results for moisture distribution were presented with the use of the volumetric moisture content W (m^3/m^3), which is introduced in place of the mass concentration c (kg/kg). There is the following relation between mass concentration and volumetric moisture:

$$\rho c = \rho_w^{'} W \tag{35}$$

with

$$\rho_w^{'} = \frac{m_w}{V_w} \tag{36}$$

where

m_w – mass of water in comcrete, *kg*,

V_w – volume of water In concrete, m^3.

The results shown in already quoted figures can be summarized as follows:

- the temperature distribution over the investigated period of concrete curing is nearly identical for all analyzed slabs, despite the values of assumed coefficients. It means that the moisture gradient does not influence the flux of heat significantly and the thermodiffusion effect could be neglected in analyses of mass concrete elements. Such result is in the agreement with the suggestions given in the literature (Kiernożycki [12], Szarliński [13], Witakowski [16]),
- the moisture distribution over the investigated period, determined with taking into account the thermodiffusion cross effect or without this effect, is similar for all analyzed slabs but only for lower value of the thermal coefficient of moisture diffusion ($\alpha_{WT} = 2\cdot10^{-11}\, m^2/(sK)$). The lower loss of moisture was obtained in simulation with using coupled equation of heat and mass transfer,
- in case of higher value of the thermal coefficient of moisture diffusion the moisture distribution obtained with the use of coupled and independent equations differs. Visible differences in this case are obtained on side surfaces of slabs – on these surfaces (with shuttering) the accumulation of moisture is observed in the period when the temperature decreased.

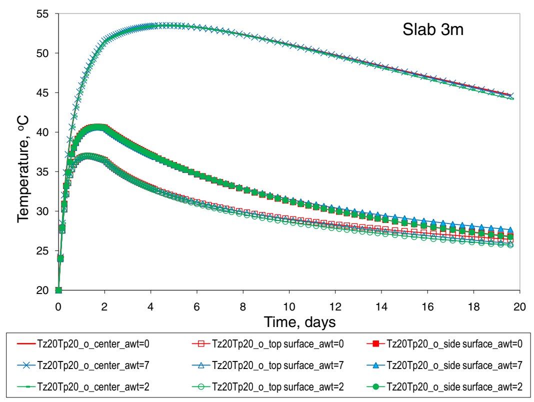

Figure 3.
Temperature distribution in the slab s_3m over the curing period for different value of coefficient α_{WT} (awt denotes α_{WT} x 10^{-11})

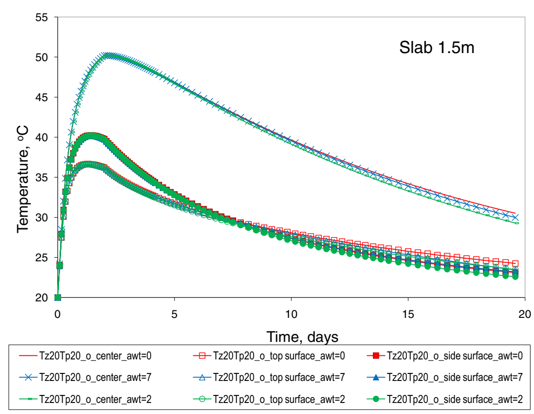

Figure 4.
Temperature distribution in the slab s_1.5m over the curing period for different value of coefficient α_{WT} (awt denotes α_{WT} x 10^{-11})

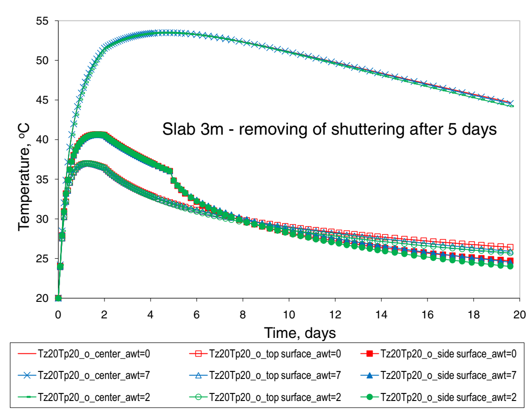

Figure 5.
Temperature distribution in the slab s_3m_r_5 over the curing period for different value of coefficient α_{WT} (awt denotes α_{WT} x 10^{-11})

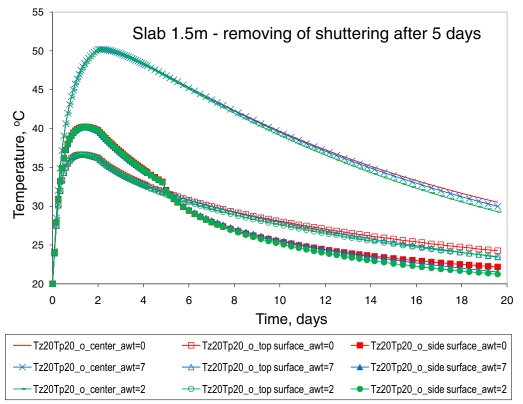

Figure 6.
Temperature distribution in the slab s_1.5m_r_5 over the curing period for different value of coefficient α_{WT} (awt denotes α_{WT} x 10^{-11})

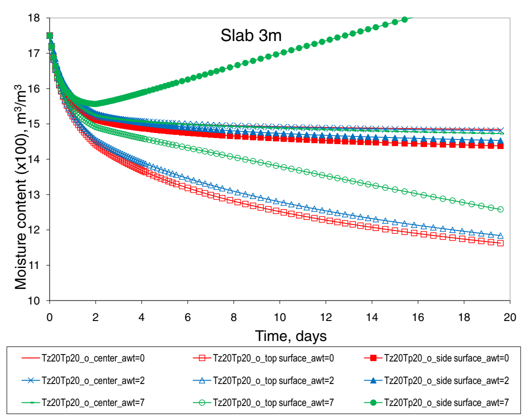

Figure 7.
Moisture distribution in the slab s_3m over the curing period for different value of coefficient α_{WT} (awt denotes α_{WT} x 10^{-11})

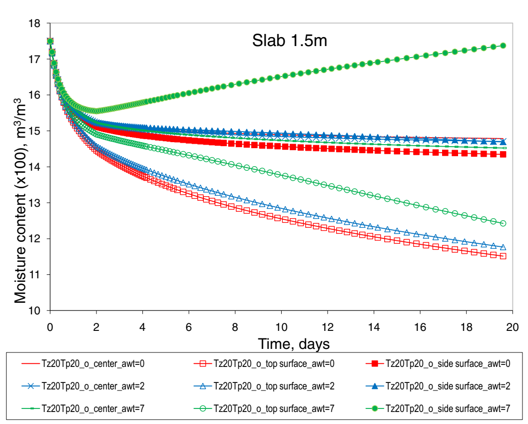

Figure 8.
Moisture distribution in the slab s_1.5m over the curing period for different value of coefficient α_{WT} (awt denotes α_{WT} x 10-$^{-11}$)

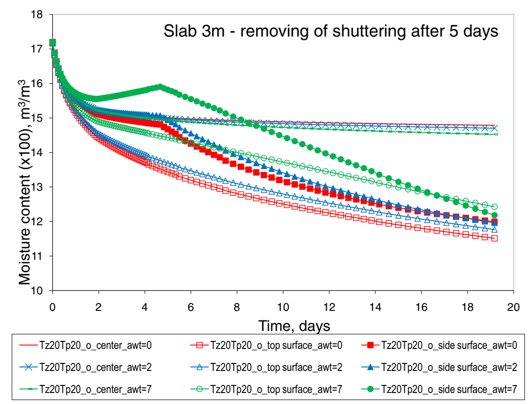

Figure 9.
Moisture distribution in the slab s_3m_r_5 over the curing period for different value of coefficient α_{WT} (awt denotes α_{WT} x 10^{-11})

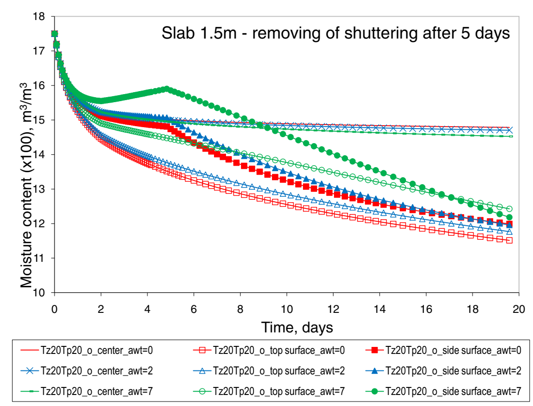

Figure 10.
Moisture distribution in the slab s_1.5m_r_5 over the curing period for different value of coefficient α_{WT} (awt denotes α_{WT} x 10^{-11})

5. CONCLUSIONS

Massive concrete elements are prone to early age cracking due to thermal and moisture effects associated with the hydration and curing process. Therefore, it is extremely important to predict the temperature and moisture distribution over the curing period properly. The most commonly used and practically accepted in this field are the equations, which neglect existing thermodiffusion cross effects. Coupled equations of thermodiffusion derived on the basis of irreversible thermodynamics laws are available in the literature, however, they are applied in the analyses comparatively rare for two major reasons. One of them is persuasion that thermodiffusion cross effect influenced the thermal and moisture fields in early age mass concrete inconsiderably. The second one is mainly connected with the technical difficulty with application of the coupled equations of thermodiffusion to the real engineering tasks. However, now this reason seems out of date due to the present-day development of numerical method dedicated to the solution of even more complicated mathematical equations.

The coupled equations of thermodiffusion, which govern the heat and mass transfer in early age mass concrete as well as the initial and boundary conditions are presented in the paper. The matrix form of the considered equations was the base for developing the original program TEMWIL, which enables the simulations of space concrete elements. To recognize the real influence of the thermodiffusion cross effect on the distribution of temperature and moisture over the curing process, a few comparative analyses were done. The object of the conducted analyses were the massive foundation slabs. The temperature distribution determined with taking into account thermodiffusion cross effect or without this effect in all analyzed slabs is almost identical. Such results suggest that the gradient of moisture does not influence the flux of heat significantly and in case of mass concrete elements the governing equations can be formulated independently, without the thermodiffusion cross effect.

The differences were obtained in moisture distribution determined with or without thermodiffusion cross effect. In this case the influence of temperature gradient on the flux of moisture is perceptible, but the weight of significance depends on the value of the thermal coefficient of moisture diffusion.

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