DETERMINATION OF THERMAL PROPERTIES OF HARDENING CONCRETE CONTAINING HIGH CALCIUM FLY ASH

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ABSTRACT
A numerical and experimental investigation on thermal behavior of young concrete is presented. It has been performed to establish the range of possible applications of concrete containing non-standard addition of reactive high calcium fly ash. The proposed model of temperature distribution in hardening concrete is based on the non-linear IHTP (inverse heat transfer problem) solution. Changes in properties of concrete during setting and hardening are included in the model. The proposed approach consists of several stages. First the temperature measurements in a one-dimensional form are performed using real size concrete materials. Then the method of lines is used to solve the one dimensional heat equation. The results are treated as an input to IHTP for determination of thermal properties of concrete: specific heat capacity, thermal conductivity and heat of hardening. To solve IHTP the pattern search method is used, which does not require the calculation of the gradient of the objective function. In the third step the direct heat conduction problem is solved. Own, based on finite element method, software TMC (Thermal & Mechanical modeling of Concrete) is used to predict temperature field. The obtained numerical results have been compared with experimentally measured temperature in concrete and a fair agreement has been found.

INTRODUCTION
Hardening of concrete is a complicated physicochemical process which liberates a huge amount of heat. The temperature of hardening concrete in structure can exceed values which are safe for its durability. Therefore it is important to know the temperature field on planning stage because in that case we can avoid such type of dangerous situation (i.e. include cooling pipe network or change concrete mix composition). But to predict the transient temperature field it is necessary to know the equation which describes the process and boundary and initial conditions. Many authors report that heat transfer equation in form (1) describes the temporal evolution of temperature of a hardening concrete structure (Ballim 2004, Carslaw & Jaeger 1959):

$$c\rho\frac{\partial T}{\partial t}-\frac{\partial}{\partial x}\left(k_x\frac{\partial T}{\partial x}\right)-\frac{\partial}{\partial y}\left(k_y\frac{\partial T}{\partial y}\right)-\frac{\partial}{\partial z}\left(k_z\frac{\partial T}{\partial z}\right)=Q \qquad (1)$$

where: ρ – density, c – heat capacity, T – temperature, t – time, x, y, z spatial coordinates, k_x, k_y, k_z thermal conductivity in direction x, y, z respectively.

To solve equation (1) we have to know values of coefficients c, ρ, k_x, k_y, k_z and function Q which denotes the internal heat source. These values are time, spatial and temperature dependent (Bentz, 2008, Bentz et al, 2011). Nevertheless many authors use these properties as constant (i.e. Ballim 2004), often argue that it is hard to estimate exact values that change over time. The authors of this paper in their work use innovative cement binders with high calcium fly ash (Garbacik et al, 2010) which composition (and hence the thermal properties) also varies depending on the date of delivery (see Table 1). Thus, for accurate modeling it was necessary to develop a procedure which allows to test each type of binder before using it in structure. To determine the thermal properties of hardening concrete containing high calcium fly ash the authors use inverse heat transfer problem (IHTP) solution. The literature related to IHTP is vast, but only one article covers the topic of this work (Phillips et al, 2007). Phillips has applied the genetic algorithm to estimate thermal diffusivity, heat generation and convective coefficient, but he has used only the synthetic data. In this work real data collected from measurements were used. Figure 1 shows flow a chart of the used procedure. In this investigation the temperature field in a two dimensional object is estimated on the basis of point temperature measurements in the one dimensional mold and an inverse problem solution. To enable an easy use of numerical procedures a graphical user interface called TMC was built (Figure 2).

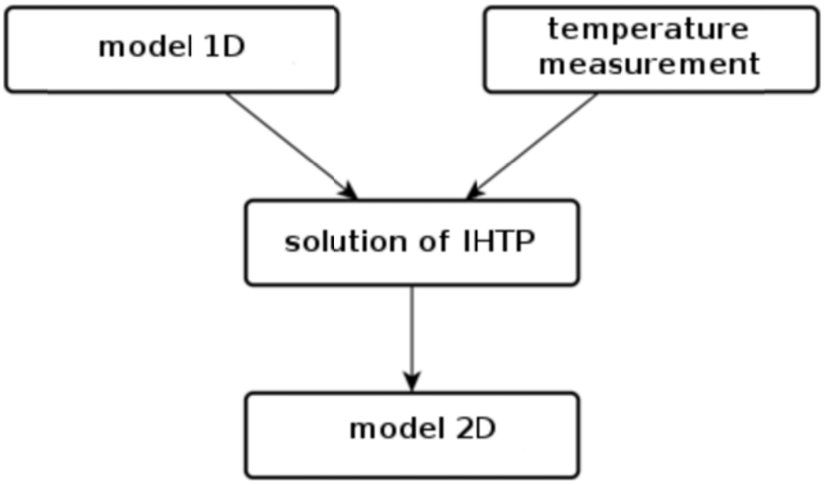

Figure 1: Flow chart of the test procedure

Table 1: The compositions of high calcium fly ash from Bełchatów Power Station from different supplies.

component	**Fly ash 1** 16.03.2010	**Fly ash 2** 19.05.2010	**Fly ash 3** 28.06.2010	**Fly ash 4** 10.11.2010	**Fly ash 5** 25.03.2011
SiO_2	33.62%	35.41%	40.17%	45.17%	40.88%
Al_2O_3	19.27%	21.86%	24.02%	20.79%	19.00%
Fe_2O_3	5.39%	6.11%	5.93%	4.58%	4.25%
CaO	31.32%	25.58%	22.37%	20.60%	25.97%
MgO	1.85%	1.49%	1.27%	1.49%	1.73%
SO_3	4.50%	4.22%	3.07%	2.96%	3.94%
K_2O	0.11%	0.13%	0.20%	0.19%	0.14%
Na_2O	0.31%	0.16%	0.15%	0.23%	0.13%
P_2O_5	0.17%	0.16%	0.33%	0.14%	0.10%
TiO_2	1.21%	1.22%	1.01%	1.37%	1.52%
Mn_2O_3	0.07%	0.06%	0.06%	0.06%	0.04%
SrO	0.20%	0.17%	0.16%	0.13%	0.17%
ZnO	0.02%	0.02%	0.02%	0.02%	0.01%
CaO_{free}	2.87%	1.24%	1.46%	1.18%	1.07%

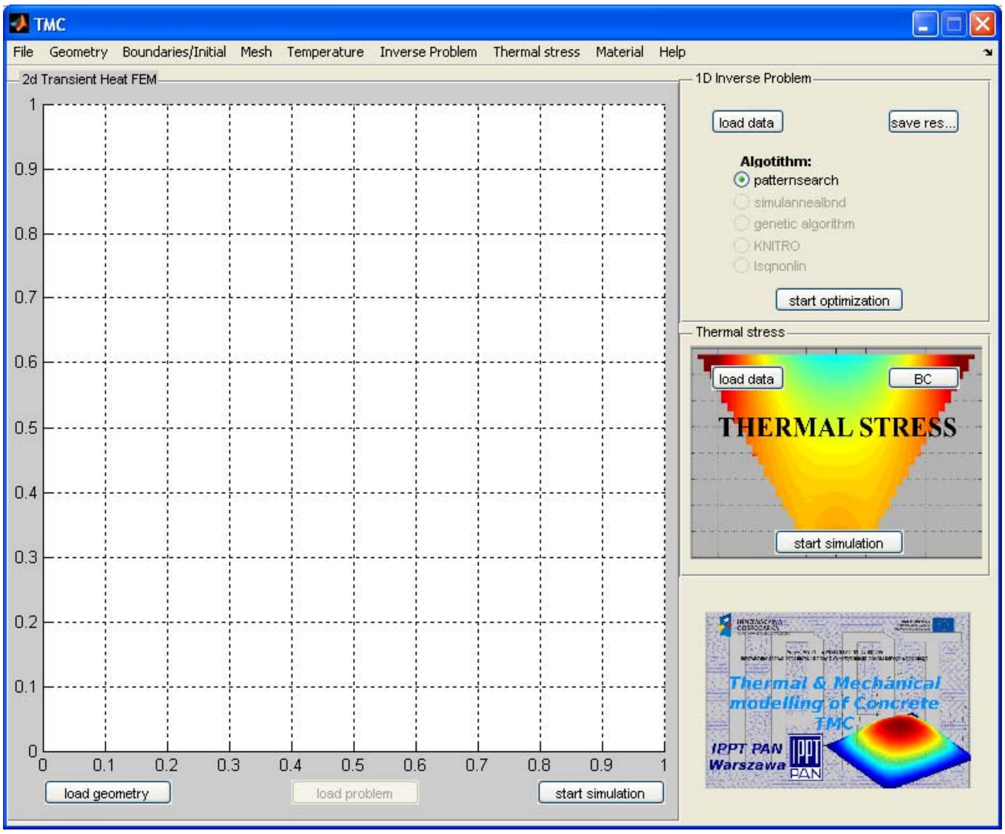

Figure 2: The developed graphical user interface of TMC in-house software.

MATHEMATICAL MODEL

Determination of temperature field by equation (1) is possible if the boundary and initial conditions are known. In this case the initial condition is written as:

$$T(t=0,x,y,z)=T_0(x,y,z) \tag{2}$$

where T_0 denotes the initial temperature field.

The boundary conditions in the general case can be written as a function φ depending on time, location, temperature and temperature gradient:

$$\varphi(x,y,z,t,T,\nabla T)=0 \tag{3}$$

In one dimensional case the Dirichlet boundary conditions are used.

The heat equation (1) is solved by in-house software called TMC, which also consists of IHTP module. IHTP is defined as an optimization problem and to solve it functions k, c and Q are parameterized in this way:

$$k_x=k_y=k_z=k(t_e)=\begin{cases} a_k t_e+b_k, & 0\le t_e<72h \\ 72a_k+b_k, & t_e\ge 72h \end{cases} \tag{4}$$

$$c=c(t_e)=\begin{cases} a_c t_e+b_c, & 0\le t_e<72h \\ 72a_c+b_c, & t_e\ge 72h \end{cases} \tag{5}$$

$$Q=Q(t,t_e)=\frac{t_e}{t}\sum_{i=1}^{n} q_i\,N_i(t_e) \tag{6}$$

The following notation is used:

- t_e is the equivalent time:

$$t_e = \int_0^t \beta(T)dt' = \int_o^t exp\left(\frac{E}{R}\left(\frac{1}{293} - \frac{1}{273+T}\right)\right)dt' \tag{7}$$

where E is the activation energy and R is the universal gas constant.

- N_i are linear shape functions for one-dimensional finite element,
- a_k, b_k, a_c, b_c, q_i are unknown coefficients which are determined by solving the IHTP.

Next equation (1) in 1D case is solved and results T^n are compared with the measured temperature T^e by the norm defined as (Özisik & Orlande, 2000):

$$E(\boldsymbol{a}) = (T^e - T^n)^T(T^e - T^n) + \gamma \sum_{p=1}^{P} a_p^2 \tag{8}$$

where γ is a regularization parameter, a_p unknown parameters (a_p={a_k, b_k, a_c, b_c, q_i}), P is a number of unknown parameters.

The value of the objective function E is minimized by non-gradient direct search algorithm (Audet & Dennis, 2003). It should be noted that the problem described by equations (1) and (9) is not well-posed in the sense of Hadamard, because its solution is not unique. To avoid this problem the IHTP is solved twice. For the first time with the heat equation in the following form:

$$\frac{\partial T}{\partial t} - \alpha\frac{\partial^2 T}{\partial x^2} = \tilde{Q} \tag{9}$$

where $\tilde{Q}$ is a heat source: $\tilde{Q} = \frac{Q}{\rho c}$, and α is a thermal diffusivity: $\alpha = \frac{k}{\rho c}$, which is parameterized in the same manner like c and k:

$$\alpha = \alpha(t_e) = \begin{cases} a_\alpha t_e + b_\alpha, & 0 \le t_e < 72h \\ 72a_\alpha + b_\alpha, & t_e \ge 72h \end{cases} \tag{10}$$

where, a_α and b_α are unknown coefficients.

Subsequently the IHTP is solved with equation (1) and additional constrains from the previous solution and information on the mold thermal insulation, which had been estimated on the basis of a cooling sand temperature measurement.

EXPERIMENT

The solution of IHTP requires point temperature measurements in the one dimensional mold. Figure 3 shows the geometry of this mold and the temperature sensors positions. Thermal isolation of the mold is made of polyethylene foam and polystyrene to minimize heat loss through the walls (Brandt et al, 2011). For experimental verification of the proposed method, a two dimensional trapezoidal mold (Figure 4) has been developed. In this case seven sensors were used to measure the temperature. Due to the symmetry of the problem the sensors were placed in the same part of the mold. The data acquisition system consists of a data logger and set of sensors, it records temperature data automatically with high time resolution (Brandt et al, 2011). In both cases the ambient temperature is also recorded.

The experiment has been carried out for the three concrete mixtures: PP50-0, P50-0, P50-60-Ws whose compositions are given in Table 3. In the mixture P50-60-Ws 60% of cement was replaced by high calcium fly ash in relation to the reference mixture P50-0. In the mixture PP-50-0 a double amount of cement was used in comparison to the reference mixture.

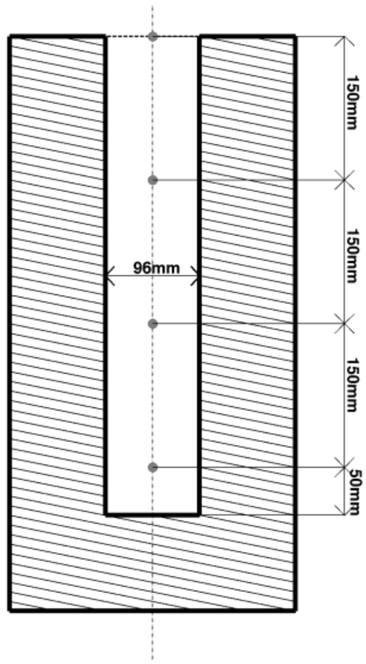

Figure 3: One-dimensional mold scheme with the temperature sensors positions.
Hatched area indicates the thermal insulation.

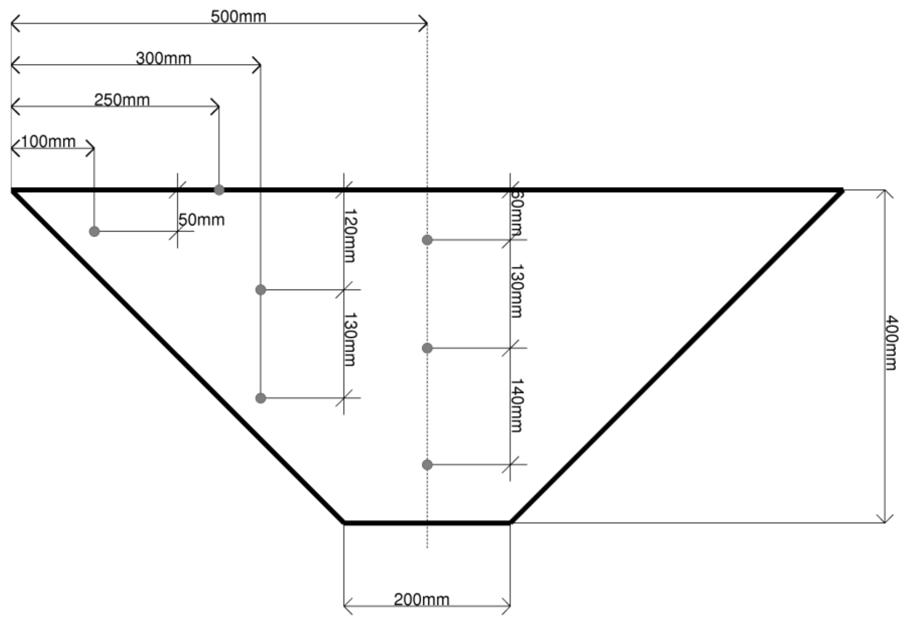

Figure 4: The two-dimensional mold and the temperature sensors positions.

Table 2: The composition of mixtures to study self-heating of concrete.

Component of concrete mix	The content of components in a mixture:		
	PP-50-0	P-50-0	P-50-60-Ws
Cement CEM I 42,5R	800	400	160
Sand 0-2mm	290	580	547
Coarse aggregate 2–8mm	305	625	625
Coarse aggregate 8-16mm	295	615	615
High calcium fly ash	0	0	120
Water	400	200	200

RESULTS AND DISCUSSION

Figure 3 shows the temperature evolution in one dimensional mold for P-50-0 mix, the data is used to solve the IHTP and determine thermal properties of particular mixture. As mentioned in the previous section, experimental tests have been conducted for three concrete mixes, and the result of IHTP for each mixture (coefficients *a* and *b* from equations 4 and 5) are presented in Tables 3 and 4. Based on these results it can be inferred that the specific heat increases with the age of concrete, while the thermal conductivity is a decreasing function of time in each case. Figure 5 shows a determined heat of hardening for mixture PP-50-0. Error bars result from the average of ten runs of IHTP algorithm. Their small values mean that the algorithm gives reproducible results. This information allows to estimate the temperature evolution in a two-dimensional object using in-house FEM software. Figures 7, 8 and 9 show a comparison between numerical model and experiments in 2D case. The best agreement between result of computation and experiment has been obtained for P-50-0 mixture (Figure 7). However for the other two cases the differences are acceptable. The sharp drop in temperature for the mixture PP-50-0 was caused by change of boundary conditions (for the first 20 hours the mold was covered with polystyrene foam), which was included in the model.

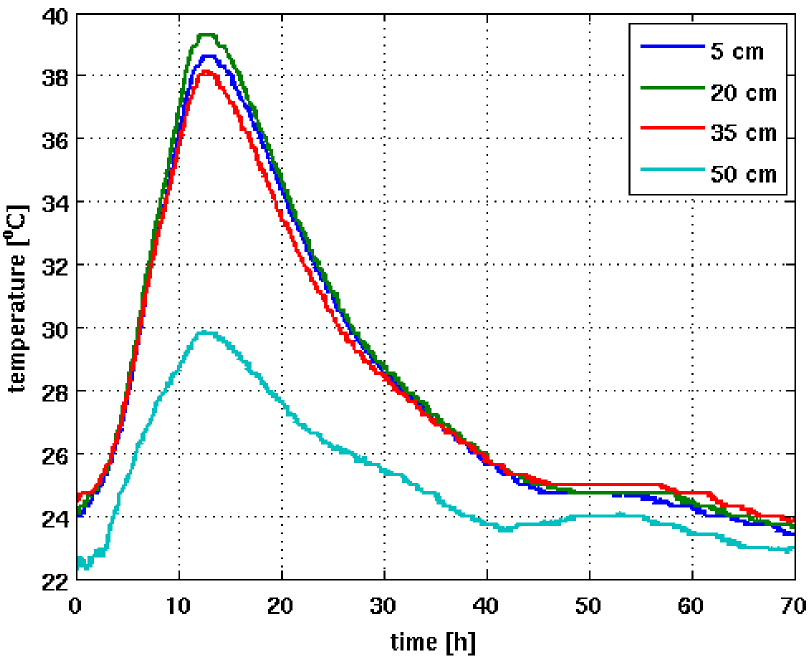

Figure 5: Temperature evolution in 1D mold - mixture P-50-0 (the numbers in the legend indicate the position of temperature sensors).

Table 3: Specific heat coefficients determined by IHTP.

a_c [J/kgKh]	b_c [J/kgK]	Mixture
0.0578	915.77	PP-50-0
0.1928	910.1	P-50-0
0.0729	912.1	P-50-60 WS

Table 4: Thermal conductivity coefficients determined by IHTP.

a_k [W/mKh]	b_k [W/mK]	Mixture
-0.0021	1.628	PP-50-0
-0.0037	1.592	P-50-0
-0.0018	1.398	P-50-60 WS

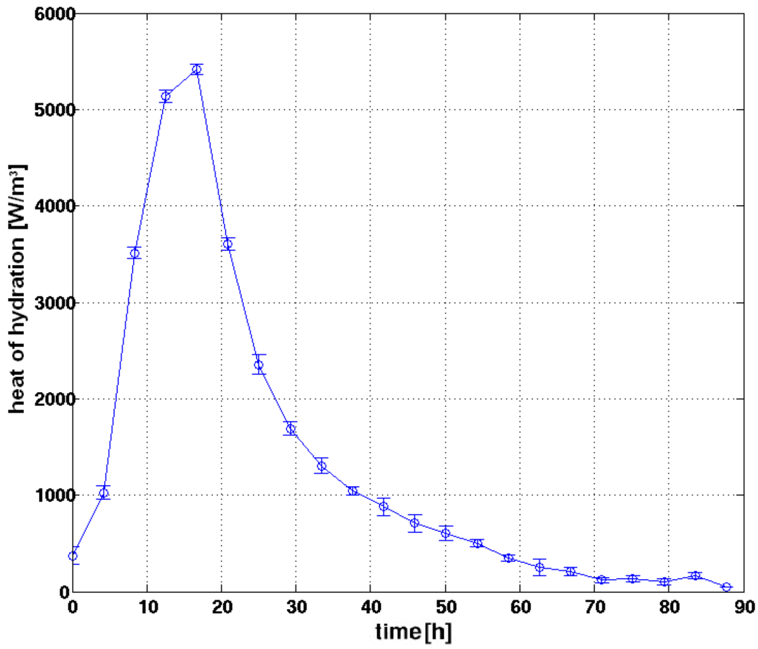

Figure 6: Mixture PP-50-0: heat of hardening detremined by IHTP.

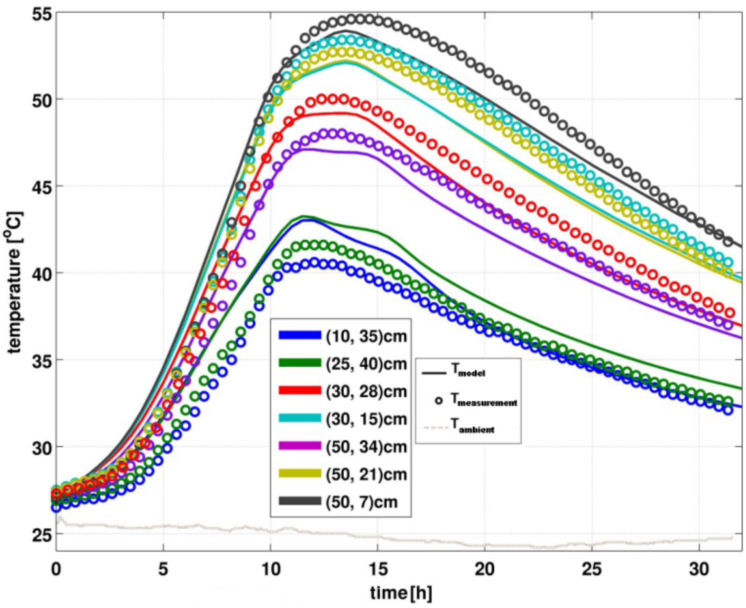

Figure 7: Temperature evolution in 2D mold - mixture P-50-0 (the numbers in the legend indicate the position of temperature sensors).

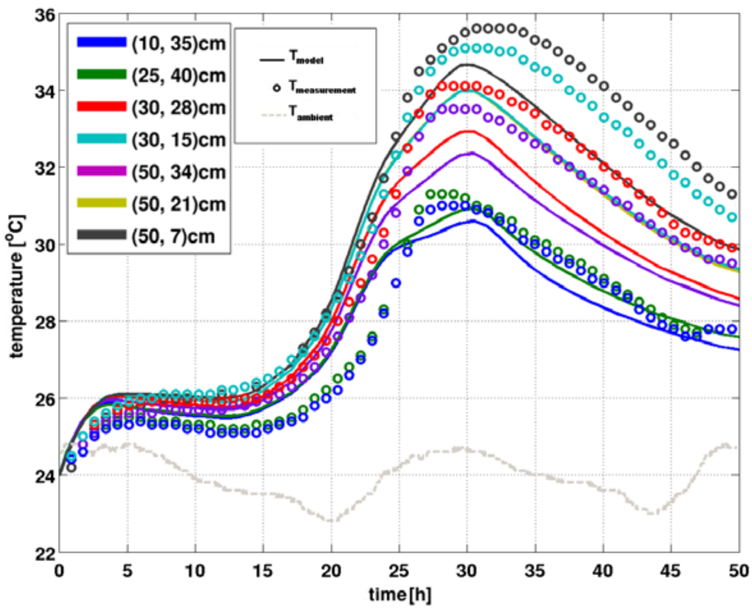

Figure 8: Temperature evolution in 2D mold - mixture P-50-60 Ws (the numbers in the legend indicate the position of temperature sensors).

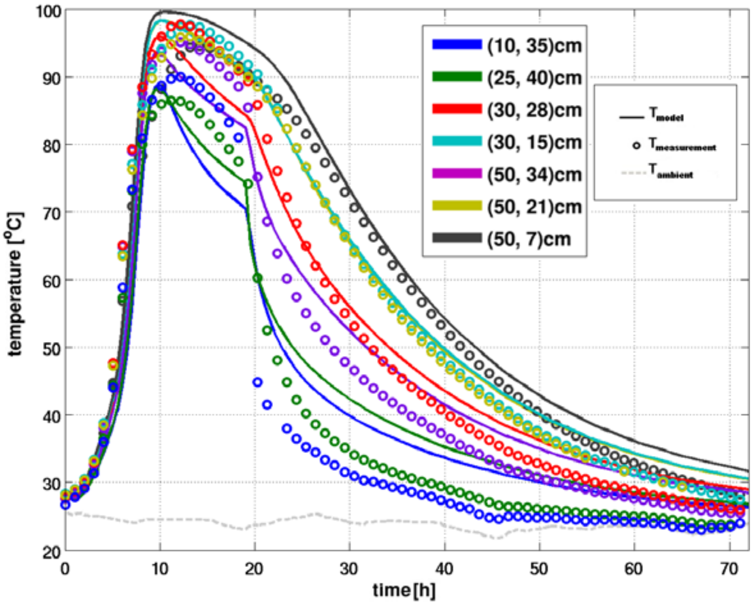

Figure 9: Temperature evolution in 2D mold - mixture PP-50-0 (the numbers in the legend indicate the position of temperature sensors).

CONCLUSIONS

The presented method of determination of thermophysical parameters of concrete at early ages was based on the solution of the inverse heat transfer problem (IHTP). For this purpose a proprietary algorithm for solving the task of heat conduction based on the finite element method and algorithm for solving the inverse problem has been developed. The obtained results of the simulations are consistent with experimental data, which indicates that this procedure can be adequate in real size structure. The advantage of the developed method is a possibility of determination the heat of hardening for any concrete mixture without knowledge about its composition. Furthermore, after analyzing a larger set of measurements it will be possible to assess the impact of individual components of the concrete mixture on the thermophysical parameters.

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