MODELING OF HEAT AND MASS TRANSFER INDUCED BY HIGH TEMPERATURE IN CONCRETE

M. RODRÍGUEZ[*] C.M. LÓPEZ[*] AND I. CAROL[*]

[*] Department of Geotechnical Engineering and Geo-Sciences
Universidad Politécnica de Cataluña
Jordi Girona 1, Edif. D2, E-08034 Barcelona, Spain
e-mail: mariana.rodriguez@upc.edu,carlos.maria.lopez@upc.edu,ignacio.carol@upc.edu

Key words: Heat and mass transfer in concrete, High temperature.

Abstract. In the context of a long term development of a general meso-mechanical model for concrete under mechanical and environmental actions, this paper describes the on-going work to represent the heat and moisture transfer in concrete subject at high temperatures, which causes water movement and pore pressure build up. Temperature distributions are obtained from separate thermal diffusion analysis (uncoupled), and only one pressure variable is considered to describe the water transfer process where the water dehydration is included. The formulation is largely based on Bazant & Thonguthai's model [1], which made no distinction between liquid and vapor water. However, in its original form that model predicted pressures far too great at high temperatures when all water was in vapor form, which motivates some modifications along the line proposed by Tenchev et. al.[2], which make the model comply also with the perfect gas law in the limit case at the critical temperature of 374,15ºC. A simple academic example for temperatures between 27 and 600ºC is presented to show the behaviour of the model.

1 INTRODUCTION

Concrete subject to high temperatures undergoes two main degradation mechanisms. The first one is related to the incompatibility of thermal deformations between aggregates and cement paste. The second one corresponds to the heat and mass transfer taking place in the concrete microstructure as the result of high temperatures, which causes water evaporation and pore pressure build up.

Thermal and moisture diffusion models are usually based on the heat and mass water conservation equations and the well-known *Fick's Law* of diffusion and *Fourier's Law* for the heat flow. These two diffusion processes may be considered coupled, or temperatures may be obtained from a separate thermal analysis and then applied as an input data on the water transfer process. The moisture diffusion analysis in turn may be represented with two independent variables (typically the two pressures of gas and water vapor or capillary pressure) [2,3], or be simplified to only one unknown variable [1]. For temperature below the critical point of water (374.15ºC), one must also distinguish between saturated and non-saturated (partially saturated) concrete; and in this case a constitutive equation for the pore state saturation it needed. For higher temperature above the critical point, liquid water phase

does not exist, and the equations of an ideal gas may be considered.

In the case of partial saturation, additional equations are needed to relate the water content of the pore system, to the partial pressure of the water vapor P_v and the capillary pressure P_c. These relations are a function of temperature T, and typically involve the degree of saturation S and the pore radius r distribution. In the literature, these relations may take different forms; in Geotechnical literature the *water retention curves* relate the degree of saturation to the temperature and capillary pressure $S=S(P_c,T)$; in materials science *sorption-desorption isotherms* relate water content to vapor pressure or relative humidity and temperature $w=w(H,T)$, where $H= P_v/P_{sat}$ and the saturation pressure being a function of temperature $P_{sat} = P_{sat}(T)$.

One of the best known models is that of Bazant & Thonguthai's [1], which is based on a single primary unknown variable P_v, and proposes a set of *isothermal desorption curves* that are shown in Figure 1(left). These *curves* have been used by many other authors, and in particular Tenchev [2] has modified the curves and extended the formulation to consider separate liquid water and water vapor (Figure 1 right).
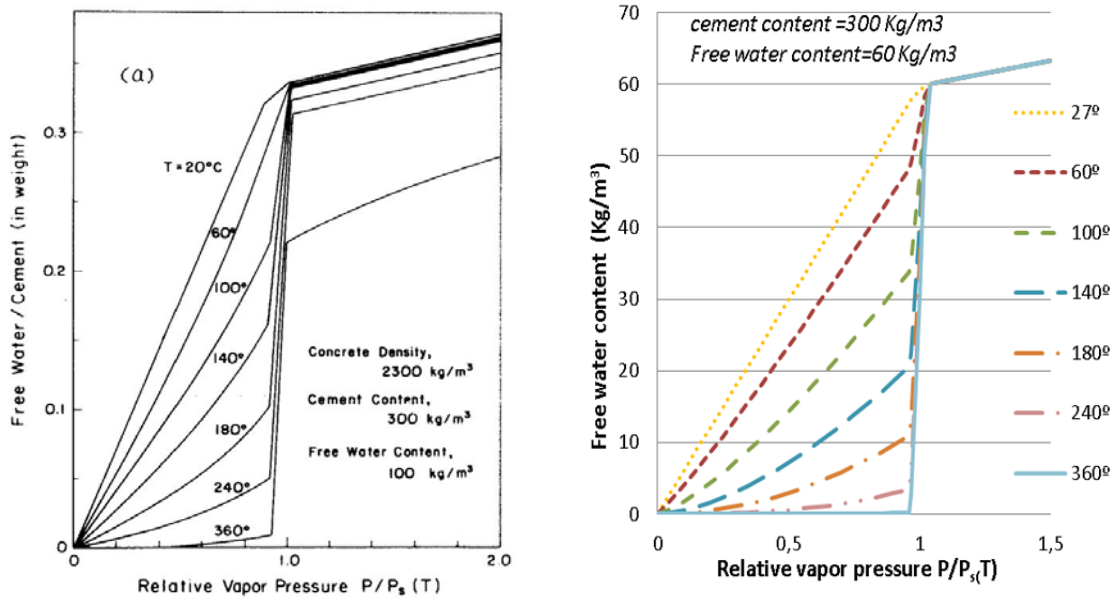

Figure 1: Isothermal desorption curves by Bazant & Thonguthai 1978 [1] and Isothermal desorption curves used in Tenchev *et. al.*2001 [2].

Gawin & Schrefler 1996 [3], consider liquid water and water vapor separately in the mass transfer formulation, which are related through the saturation of liquid water, which are defined as a function of capillary pressure, $S=S(P_c)$, for a given temperature.

In the literature one can find different expressions for the degree of saturation of liquid water as a function of the capillary pressure [4-8]. Normally the empirical equations $S=S(P_c)$ proposed are inaccurate when the saturation is close to zero since, in this field not much care is paid to the behavior at low water content [9]. Moreover, most empirical equations become singular when *residual water content* is reached (Figure 2 left), so this type of expressions may seem not optimal for numerical modeling. A relationship of the type $S=S(r)$, with r=pore radius, seem to be more suitable (Figure 2 right). The pore radius and capillary pressure are

related through the *Laplace Equation*, *P$_c$=2σ/r*, where *σ* is the surface tension, *σ= σ(T)*.
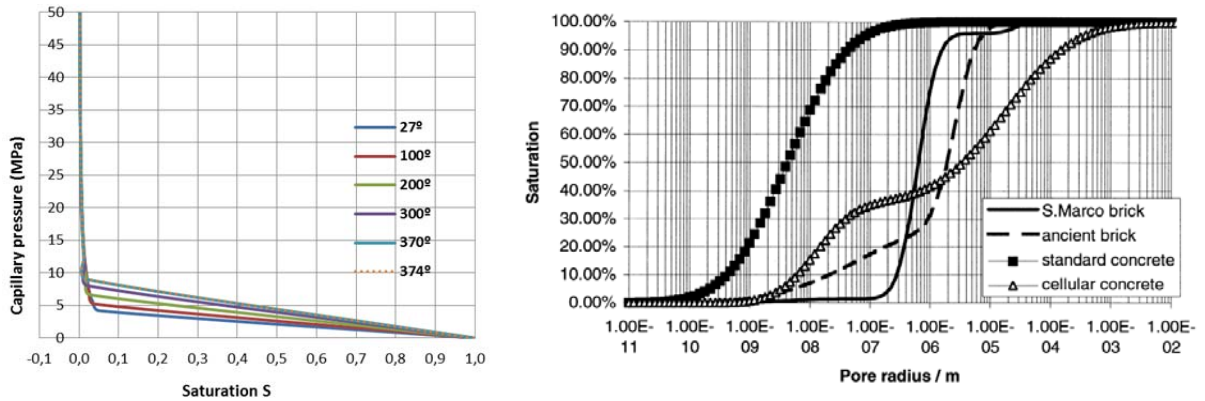

Figure 2: Left: *S-P$_c$* curves used in Gawin & Schrefler 1996 [3]. Right: Typical *S-r* curve extracted from Baggio *et. al.* 1997 [9] (right).

Previous work of the author´s group was focused on the study of the mechanical effects of the thermal deformations due to the incompatibility between aggregates and cement paste [10, 11], via meso-structural FE model with fracture-based zero-thickness interface elements [12, 13]. The present paper describes the state of on-going work to represent the thermal and moisture diffusion in cement paste by means of a numerical FE formulation, which will be then coupled the existing meso-mechanical model to analyze the influence on the concrete damage.

2 THERMAL AND MOISTURE DIFFUSION MODEL

As already indicated, in the present study the moisture diffusion model has to be finally inserted as part of a general meso-mechanical model in which cracks are represented in a discrete manner via zero-thickness interface elements, the opening of which will influence strongly the diffusion properties and provide H-M coupling. As usual in the development of complex systems, initially each part is taken in its simplest version, and only after the overall behavior has been verified, the individual components can be replaced with more elaborate versions.

In this context, the moisture and thermal diffusion FE model considered in this study is deliberately simple. Besides temperature *T*, it considers a single pore pressure variable *P*, that in most situations may be interpreted as the partial pressure of the water vapor in the pores *P$_v$*.

In this context, the heat and water mass conservation equations may be expressed as:

$$\rho C \frac{\partial T}{\partial t} = -div(k_T grad T) \tag{1}$$

$$\frac{\partial w}{\partial t} = -div(k_w grad\ P) + \frac{\partial w_d}{\partial t} \tag{2}$$

in which *ρ* and *C* are the mass density and heat capacity of concrete, *k$_T$* is the heat conductivity, *w* is the total mass of free water per m³ of concrete; *w$_d$* is the mass of chemically bound water that is released to the pore as a result of the dehydration process (dehydration of the solids in cement paste as a result of heating); and *k$_w$* is the moisture flow permeability

given as a function of temperature and pressure, $k_w = k_w(T,P)$ taken from Bazant & Thonguthai's model [1] with slight modifications.

The third ingredient required in the model is the relation between water content w and vapor pressure P_v and temperature T, and for that one needs to distinguish two cases:

1) If temperature is above the critical point $T > 374.15°C$, all water is in vapor form, and the equation of perfect gases is assumed:

$$w = \phi \rho_v, \qquad \rho_v = \frac{P}{R_v T_a} \tag{3}$$

where ρ_v is the water vapor density, R_v is the universal gas constant of the vapor phase and T_a is the absolute temperature.

2) If temperature is below the critical point $T < 374.15°C$, the total free water content w, is again taken as a simplified version of the isothermal desorption curves of Bazant & Thongutai's [1] (Figure 1 left), as follows:

(a) for the un-saturated zone:

$$w = c \left(\frac{w_1 \left(\frac{P}{P_s} \right)}{c} \right)^{\frac{1}{m(T)}} \quad for\ H \le 0.96; \quad H = \left(\frac{P}{P_s} \right) \tag{4}$$

$$with \quad m(T) = 1.04 - \left[\frac{z}{22.34 + z} \right]; z = \frac{T + 10}{T_0 + 10}^2$$

b) for the saturated zone

$$w = \frac{\phi}{v_l} * \left(1 + 0.12 \left(\left(\frac{P}{P_s} \right) - 1.04 \right) \right) \quad for\ H \ge 1.04 \tag{5}$$

$$with \quad \phi = \left[\phi_0 + \frac{w_d(T) - w_{d0}}{\rho_0} \right]$$

c) for the transition zone, $0.96 < P/P_s < 1.04$:

$$w = A * \left(\frac{P}{P_s} \right)^3 + B * \left(\frac{P}{P_s} \right)^2 + C * \left(\frac{P}{P_s} \right)^1 + D ; \ si\ 0.96 < H < 1.04 \tag{6}$$

In previous equations w_l is the saturation water content at 25°C; c is the mass of cement content per unit volume of concrete; P_s is the vapor saturation pressure; v_l is the specific volume of liquid water, ϕ is the porosity; ϕ_0 is the initial porosity at T_0; $(w_d - w_{d0})$ is the decrease of weight (per unit volume) of chemically bound water from T_0 to T; and ρ_0 is the density of liquid water at T_0. In equation (6), A, B, C and D are parameters which may be temperature-dependent.

However, the original version of the above formulas, led to excessive pore pressures when all water is in vapor form, as seen in Figure 3, where the predictions of that model are plotted on the classical P-v diagram (for constant T) of the water. Also, those formulas would not provide a smooth transition at the critical point of 374.15°C. To remedy all that, the following changes are introduced: water content is decomposed into liquid and vapor contibutions via the saturation degree S, as:

$$w = w_l + w_v \tag{7}$$

$$w_l = S \, \phi \, \rho_l \tag{8}$$

$$w_v = (1 - S) \, \phi \, \rho_v \tag{9}$$

with the liquid density $\rho_l = \rho_l(T)$, and the vapor density ρ_v given by the ideal gas equation (3b). Now, following Tenchev [2], it is assumed that the prediction from formulas (4)-(6) yield not total water content but only liquid phase w_l, and then from (8) one can obtain the degree of saturation S, and then use (9) and (3b) to calculate the total water content. This procedure leads to much more reasonable P-v diagrams on the gas-only region on the right-hand side of the dome, as shown in Figure 3.
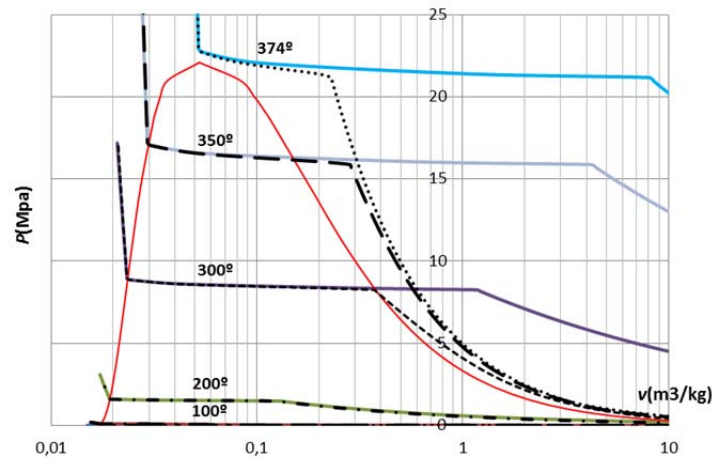

Figure 3: *P-v* curves (at constant *T*), for the porous medium according the original (solid lines) and modified Bazant model (dashed lines). Note that the original model would predict specific volumes much larger than the ones actually possible when all the water is in gas form, and that this does not happen with the modified model.

Finally, the dehydration process is assumed to start at about 105ºC, and the expression used is similar to that of Bazant and Thonguthai´s [1]:

$$w_d(T) = w_h^{105} * f(T) \tag{10}$$

in which $w_h{}^{105}$ is the hydrated water content at 105ºC and *f(T)* is a function which represents the amount of water that is dehydrated when reaching higher temperature. Function *f(T)* is obtained by fitting experimental data of the weight loss measurements on heated concrete specimens, which can be obtained from the literature [14-16]. The expression used for *f(T)* is shown in equation (11).

$$f(T) = w_f * \left[1 - \exp^{\left(-k*\left(\frac{T}{T0}\right)^P \right)} \right] + m*(T - 105), \tag{11}$$

where w_f, *k, m, T_0* and *p,* are constants fitting parameters which varies for different concretes and T represent the temperature.

3   RESULTS

The preliminary example of application presented in this section is a simplified version the one used in Tenchev *et. al.* 2001[2] and Davie *et. al.* 2006 [17]. It consists of solving the 1D pressure distribution and water content in the direction perpendicular to the exposed surface, of a thick cement wall. The numerical analysis is made on a long and narrow 2D FE domain of 20×0.2cm (horizontal×vertical), which is discretized with a single row of 200 linear rectangular elements and the left vertical end corresponds to the exposed surface.

Previous to the moisture calculation, temperature distributions are obtained from a separate thermal diffusion analysis, where the (left vertical) exposed edge is subject to temperature increments from 27 to 600ºC according to the ISO 834 curve [18], condition which is applied *via* mixed Newman-Dirichlet boundary condition (heat flow proportional to the difference of the resulting surface temperature with the desired prescribed value, proportionality constant h). Thermal flow is assumed null on the other three faces of the FE domain, and the initial temperature value is 27ºC for all nodes of the mesh. The resulting temperature distribution is then applied as an input for the moisture diffusion analysis, with a constant vapor pressure value assumed prescribed on the (left vertical) exposed edge of the domain, while moisture flow is assumed null on the other three faces. The initial vapor pressure value was $3,567e^{-3}$ MPa for all nodes of the mesh, which corresponds to a saturated state at $T_0=27$ºC. For simplicity, in this first example no dehydration has been considered.

Thermal parameters used are: $\rho= 2300$ Kg/m^3; $C=1171$ J/KgºC; $k_{T=}$ 66 J/min m ºC and the convective heat transfer coefficient, $h=$ 6500 J/min m^2 ºC. For moisture diffusion analysis parameters used are: $k_{w=}$ $6e^{-10}$ m/min ($1e^{-11}$ m/s) constant value in whole process; $c=300$ Kg/m^3; $w_l=$ 60 Kg/m^3; $T_0=27$ºC; $n_0=0.06$; $R_v=46.15$ m/ºC; $\rho_l = \rho_l$ (T) obtained from thermodynamic tables of water [19].
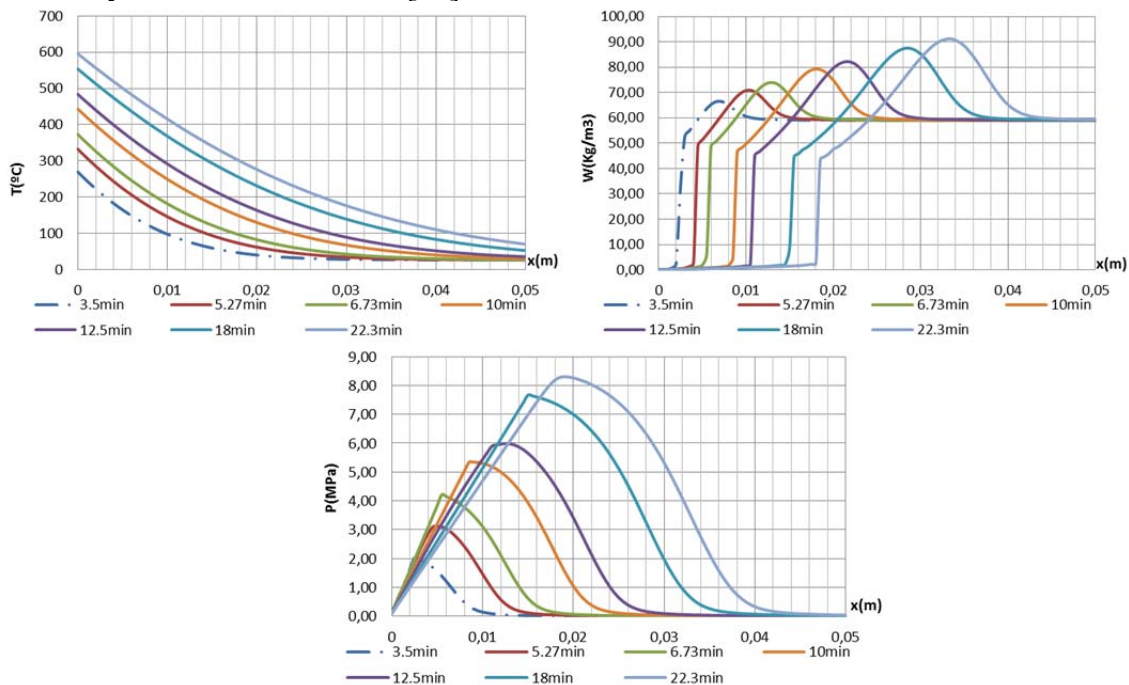

Figure 4: Distribution of temperature prescribed (upper left); free water content (upper right) and pressure (down) as a function of the distance from the fire exposed edge for 3.5, 5.27, 6.73, 10, 12.5, 18 and 22.3 minutes.

Figure 4 shows the curves of temperature prescribed *T*, and resulting water content *w* and vapor pressure *p*, as functions of *x* (depth in the cement wall), for seven different heating times of 3.5, 5.27, 6.73, 10, 12.5, 18 and 22.3 minutes. Only the part of the mesh affected by the process is represented (from *x*=0 to 0.05m), the rest remains in initial conditions. The results turn out qualitatively similar to those obtained in the literature, in which as the high temperatures penetrate the material, a front of low water content and high vapor pressure also moves into the material at around the location of the 200-250ºC front.

In the curves for water content *w*, from left to right, it possible to distinguish a dry zone (near the exposed edge), a sudden moisture front (jump on the curves) and a high zone where water content increases reaching values up to 50% higher than the initial state (w_l=60 Kg/m3). This is the result of moisture migration from the zone with highest vapor pressures near the exposed surface, towards the inner part of the wall, while from the pressure peak to the left moisture would escape to the wall surface. For each time, the location of the maximum vapor pressure *p* marks pretty well the limit of the dry zone in corresponding *w* curve.

4   CONCLUDING REMARKS

The model described for moisture diffusion in cement at high temperatures constitutes a first attempt of a formulation to be implemented in the more general context of a meso-level mechanical model of concrete already developed and verified in a large variety of situations. At this stage of development, the model is based on existing formulations [1,2] conveniently modified so that some unrealistic pressures at high temperatures are not predicted. The results obtained seem to represent realistically some aspects of the phenomenon, although also exhibit some concepts that may be clearly improved.

A new version of the model based on the pore distribution curve *S(r)* and Kelvin equation, is currently under development. In this case the transition from non-saturated to saturated concrete are implicitly given from the *S(r)* curve. With it, it is expected to improve some aspect of the model, while still using a single pressure field variable at the nodes.

ACKNOWLEDGMENTS

REFERENCES

[1] Bazant, Z.P. and Thonguthai, W. Pore pressure and drying of concrete at high temperature. *Nuclear Engineering Mechanics Division*, 104, pag. 1059-79 (1978).

[2] Tenchev, R.T., Li, L.Y. and Purkiss, J.A. Finite element analysis of coupled heat and moisture transfer in concrete subjected to fire. *Numerical Heat Transfer, Part A,* 39:685-710, (2001).

[3] Gawin, D. and Schrefler, B.A. Thermo-hygro-mechanicla analysis of partially saturated porous materials. *Engineering Computations,* vol. 13, nº 7, pp:113-143,(1996).

[4] Baroghel-Bouny, V., Mainguy, M., Lassabatere T. and Coussy O. Characterization and identification of equilibrium and transfer moisture properties for ordinary and high-performance cementitious materials. *Cem Con Res*, 29, pp.1225-1238, (1999).

[5] Meschke, G., M.ASCE, and Granberger, S. Numerical modelling of coupled hygromechanical degradation of cementitious materials. *Journal of engineering mechanics* (2003).

[6] Li, X., Li, R., and Schrefler, B.A. A coupled chemo-thermo-hygro-mechanical model of concrete at high temperature and failure analysis. *International Journal for Numerical and Analytical Methods in Geomechanics,* 30, 635-681, (2006).

[7] Gawin, D., Majorana, C.E., and Schrefler, B.A. Numerical analysis of hygro-thermal behavior and damage of concrete at high temperature. *Mechanics of Cohesive-Frictional Materials*, 4, 37-74, (1999).

[8] Gawin, D., Pasavento, F., and Schrefler, B.A. Modelling of hygro-thermal behavior and damage of concrete at high temperature above the critical point of water. *International Journal for Numerical and Analytical Methods in Geomechanics,* 26, 537-562, (2002).

[9] Baggio, P., Bonacina, C., and Schrefler, B.A. Some considerations of modelling heat and mass transfer in porous media. *Transport in Porous Media,* 28, 233-251, (1997).

[10] Rodríguez, M., López, C.M. and Carol, I. High temperature effect in mortar and concrete specimens using a meso-mechanical model with fracture based zero-thickness interface elements. *XI COMPLAS*, CD-ROOM, (2011).

[11] Peréz, A., Rodríguez, M., López, C.M. and Carol, I. 3D-Mesomechanical analysis of cracking and spalling of concrete subjected to high temperature. *XII COMPLAS*, CD-ROOM, (2013).

[12] Carol, I., Prat, P. C., López, C.M. A normal/shear cracking model. Application to discrete crack analysis. *Engng. Mech. ASCE*, 123, pp. 765-773 (1997).

[13] Carol, I., López, C.M. and Roa, O. Micromechanical analysis of quasi-brittle materials using fracture-based interface elements. *Int. J. Num. Meth. Engng.,* Vol 52, pp. 193-215 (2001).

[14] Alonso, C., and Fernandez, L. Dehydration and rehydration processes of cement paste exposed to high temperature environments. *Journal of Materials Sciences* 39, 3015-3024, 2004.

[15] Alarcon-Ruiz, L., Platret, G., Massieu, E., and Ehrlacher, A. The use of thermal analysis in assessing the effect of temperature on cement paste. *Cement and Concrete Research* 35, 609-613, 2005.

[16] Harmathy, T.Z., and Allen, L.W. Thermal properties of selected masonry unit concretes. *Journal of the American Concrete Institute* 70, 132-142, 1973.

[17] Davie, C.T., Pearce, C.J. and Bicanic, N. Coupled heat and mass moisture transport in concrete at elevated temperatures- Effects of capillary pressure and adsorbed water. *Numerical Heat Transfer, Part A*, 49: 733-763, 2006.

[18] ISO834-1. Fire Resistance Test – *Element of Building constuctions*- Part 1: General Requirement, (1999).

[19] Cengel, Y.A., and Turner, R.H. Fundamentals of thermal-fluid sciences- Second edition. McGraw-Hill.