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Heat and mass transfer phenomena occurring in a gypsum board exposed to fire conditions

D.A. Kontogeorgos[1], M.A. Founti

[1] National Technical University of Athens, School of Mechanical Engineering, Thermal Engineering Section, Laboratory of Heterogeneous Mixtures & Combustion Systems, Heroon Polytechniou 9, Zografou Campus, 15780 Polytechnioupoli-Zografou, Athens, Greece

ABSTRACT: In this paper, the simultaneous heat and mass transfer phenomena occurring in a gypsum board exposed to fire conditions are investigated. For this purpose, the in-house developed code named HETRAN, has been used in order to predict the heat and mass transfer characteristics within gypsum boards. The code solves numerically a set of mass and energy conservation equations appropriate for the heat and mass transfer through porous building materials, assuming homogeneity, local thermodynamic equilibrium and mass transfer due to diffusion and pressure gradients. Predictions of the temperature evolution within the gypsum sample, with and without mass transfer, are compared to experimental data, revealing the significant effect of vapor migration through the sample, in the board behavior under elevated temperatures. The water vapor released during the dehydration process, fills in the pores and induces concentration and pressure gradients, which force water vapor to move towards both directions, affecting the temperature field inside the gypsum board.

1 INTRODUCTION

Gypsum plasterboards are widely used in the building industry for a variety of applications as an aesthetically pleasing, easily worked but mechanically enduring facing material for walls and ceilings. Additionally, they are easy to apply and exhibit good mechanical and thermal properties. In the context of building fire safety, gypsum plasterboards are capable of slowing the penetration of fire through walls and floors, due to the endothermic gypsum dehydration process that takes place in high temperatures [Mehaffey et al. (1994), Sultan (1996), Manzello et al. (2007)a and b].

Several computational efforts have been made in the past to predict the thermal behavior of gypsum boards under fire conditions. Most of the researchers have performed only heat transfer calculations using an effective specific heat in order to incorporate the dehydration process into their model [Mehaffey et al. (1994), Sultan (1996), Takeda & Mehaffey (1998), Clancy (2001), Ghazi Wakili et al. (2007), Thomas (2002), Kontogeorgos et al. (2008), Wullschleger & Ghazi Wakili (2007)] or the concept of moving dehydration front from the heated to the unheated side [Axenenko & Thorpe (1996), McGraw & Mowrer (1999)]. However, simultaneous heat and mass transfer analysis in gypsum boards when subjected to fire conditions showed that vapor migration inside the gypsum porous structure could be an important issue and should be taken into account [Ang & Wang (2004), Ang & Wang (2009), Kontogeorgos & Founti (2010)].

In the current work, the simultaneous heat and mass transfer mechanisms occurring inside a gypsum board exposed to fire conditions are investigated. For this purpose, the in-house developed code HETRAN [Kontogeorgos et al. (2008), Kontogeorgos & Founti (2010)] is used and the predictions of the temperature evolution within the gypsum samples, with and without mass transfer, are compared with experimental data, revealing the importance of vapor migration in the gypsum board behavior under elevated temperatures. Finally, mass concentration and pressure distributions, inside the gypsum sample, depict that the vapor moves towards both directions.

1.1 Gypsum thermo-chemistry

Commercial gypsum boards consist mainly of the crystalline mineral calcium sulphate combined with ca. 21% by weight chemically bound water, known as calcium sulphate dehydrate ($CaSO_4 \cdot 2H_2O$). In many cases, gypsum boards usually contain an amount of absorbed free water (≤4%) [Mehaffey & Sultan (1992), Mehaffey et al. (1994), Gerlich et al. (1996), Axenenko & Thorpe (1996), Thomas (2002)], as well as calcium carbonate ($CaCO_3$) [Ghazi Wakili et al. (2007), Ghazi Wakili & Hugi (2009)], magnesium carbonate ($MgCO_3$) [Ghazi Wakili & Hugi (2009)] and/or other fire resistant materials.

When gypsum boards are heated to temperatures above 80^{o}C, the chemically bound water dissociates from the crystal lattice and, together with the free moisture, evaporates. This process, known as "dehydration" of gypsum, and takes place at temperatures between ~80^{o}C and ~250^{o}C, depending on the heating rate [McIntosh et al. (1990), Paulik et al. (1992), Mehaffey et al. (1994)]. During the dehydration, a large amount of heat is absorbed and the heat transfer through the gypsum board is practically delayed until the process is completed.

The dissociation of the chemical bound water takes place in two stages. In the first stage, the calcium sulphate dihydrate loses 75% of its water, thus forming calcium sulphate hemi-hydrate ($CaSO_4 \cdot 1/2H_2O$):

$$CaSO_4 \cdot 2H2O \leftrightarrow CaSO_4 \cdot \frac{1}{2}H_2O + \frac{3}{2}H_2O \uparrow \tag{1}$$

Upon further heating, a second reaction occurs, where the calcium sulphate hemi-hydrate loses the remaining water to form the calcium sulphate anhydrate ($CaSO_4$):

$$CaSO_4 \cdot \frac{1}{2}H_2O \leftrightarrow CaSO_4 + \frac{1}{2}H_2O \uparrow \tag{2}$$

When gypsum board is fully dehydrated, at temperatures near 400^{o}C, a third, slightly exothermic reaction occurs, in which the molecular structure of the soluble crystal (anhydrate III) irreversibly reorganizes itself into a lower insoluble energy state (anhydrate II) (hexagonal to orthorhombic) [King et al. (1971), Saloua Sebbahi et al. (1997), Cave & Holdich (2000), Manzello et al. (2007) a,b]:

$$CaSO_4(\mathrm{III}) \rightarrow CaSO_4(\mathrm{II}) \tag{3}$$

A reduction of gypsum mass may be observed at temperatures between 600-800^{o}C, which corresponds to the decomposition of magnesium carbonate [Ghazi Wakili & Hugi (2009)] and calcium carbonate [Ghazi Wakili et al. (2007), Ghazi Wakili & Hugi (2009)]:

$$MgCO_3 \rightarrow MgO + CO_2 \uparrow \tag{4}$$

$$CaCO_3 \rightarrow CaO + CO_2 \uparrow \tag{5}$$

At temperatures near 1200°C another endothermic reaction occurs, which corresponds to the transition of insoluble anhydrate II to anhydrate I [Saloua Sebbahi et al. (1997), Cave & Holdich (2000)]:

$$CaSO_4(\mathrm{II}) \rightarrow CaSO_4(\mathrm{I}) \tag{6}$$

Finally, at temperatures near 1250°C gypsum mass is further reduced due to the decomposition of calcium sulphate anhydrate [Saloua Sebbahi et al. (1997)]:

$$CaSO_4 \rightarrow CaO + SO_2 \uparrow + \frac{1}{2} O_2 \uparrow \tag{7}$$

2 MATHEMATICAL MODELING

In order to simulate the thermal behavior of the gypsum board when exposed at elevated temperatures the in-house developed code HETRAN [Kontogeorgos et al. (2008), Kontogeorgos & Founti (2010)] was used. The software solves numerically a set of mass and energy equations appropriate for the heat and mass transfer phenomena occurring in porous materials. The main assumptions of the code are the homogeneity of the porous material, the local thermodynamic equilibrium and that the mass transfer is owed to diffusion and pressure gradients.

The code solves generalized form of 1-D conservation equations:

$$A_f \frac{\partial f}{\partial t} = \nabla \bullet \left(B_f \nabla f\right) - \nabla \bullet \left(\mathbf{C_f} f\right) + Q_f \tag{8}$$

Table 1 tabulates the variables and coefficients used in each conservation equation.

Table 1 Variables and coefficients of the generalized conservation equation

f	A_f	B_f	$C_\mathbf{f}$	Q_f
$c_g^{(k)}$	ϕ	D_{eff}	$\mathbf{U}_g^D$	$\frac{\partial m_g'''^{(k)}}{\partial t}$
T	$(1-\phi)\rho_s C_s + \phi \sum_{k=1}^{N^g} c_g^{(k)} C_{p,g}^{(k)}$	k_{eff}	$\sum_{k=1}^{N^g} C_{p,g}^{(k)} \left(\mathbf{j}_{diff}^{(k)} + \mathbf{j}_{pres}^{(k)}\right)$	$\phi \frac{\partial P_g}{\partial t} + \frac{\partial Q'''}{\partial t}$

The mean filtration velocity field of the gas phase mixture is calculated from Darcy's law:

$$\mathbf{U}_g^D = -\frac{\mathbf{K}}{\mu_g} \nabla P_g \tag{9}$$

The gaseous phase consists of ideal gases and the gas phase mixture total pressure is the summation of each component's partial pressure. The mass fluxes due to diffusion and pressure gradients are calculated from Fick's and Darcy's law, respectively:

$$\mathbf{j}_{diff}^{(k)} = -D_{eff} \nabla c_g^{(k)} \tag{10}$$

$$\mathbf{j}_{pres}^{(k)} = c_g^{(k)} \mathbf{U}_g^D \tag{11}$$

Finite volume techniques [Patankar (1980)] are used in order to discretize the 1-D balance eq. (8) and after the discretization the set of equations is summarized into one ordinary differential system [Kontogeorgos & Founti (2010)]:

$$\frac{d\mathbf{f}}{dt} = \mathbf{F}(t, \mathbf{f}) \tag{12}$$

The above ordinary differential system is solved using the Gear's Backward Differentiation Formula (BDF) [Gear (1971)] method, with automatic control step size and order.

2.1 *Vapor production term*

As mentioned above, during the dehydration process water vapor is produced and migrates through the pores of the gypsum board. The vapor production term can be calculated from Thermogravimetric Analysis (TGA) measurements [Ghazi Wakili et al. (2007), Ghazi Wakili & Hugi (2009)], where the sample is very small and it is assumed that vapor leaves the sample immediately after its production. The vapor mass that is produced can be calculated from the initial mass of the gypsum sample, $m_{0,G}$, minus the mass of the gypsum samples at a specific temperature, m_G. Assuming that the volume of the sample remains constant, the vapor production rate can be calculated from:

$$\frac{\partial m'''_{vapor}}{\partial t} = -\frac{dm'''_G}{dT}\frac{\partial T}{\partial t} \tag{13}$$

The heat that is absorbed by the sample during dehydration is the summation of the energy needed for the dissociation of the chemically bound water from the crystal lattice of the gypsum, for the evaporation of this amount of water and for the free moisture. Thus, the source term of the energy equation can be calculated from:

$$\frac{\partial Q'''}{\partial t} = L_v \frac{\partial m'''_{f,vapor}}{\partial t} + \left(L_v + \frac{E_C}{0.21}\right)\frac{\partial m'''_{c,vapor}}{\partial t} \tag{14}$$

Where L_v is the latent heat of evaporation and E_C is the energy needed for the dissociation of the chemically bound water from the crystal lattice of the gypsum board, which can be taken equal to 87kJ/kg [Elbeyli & Piskin (2004)]. Assuming that the free moisture content is very small, eq. (14) becomes:

$$\frac{\partial Q'''}{\partial t} = \left(L_v + \frac{E_C}{0.21}\right)\frac{\partial m'''_{vapor}}{\partial t} = -\left(L_v + \frac{E_C}{0.21}\right)\frac{dm'''_G}{dT}\frac{\partial T}{\partial t} \tag{15}$$

3 TEST CASE

In order to validate the HETRAN code, predictions are compared with experimental data [Ghazi Wakili et al. (2007)], where a gypsum board plate of size 1.25m × 1.05m × 0.012m was subjected to the standard ISO 834 fire [ISO 834-1 (1999)].

3.1 *Boundary conditions*

A 12 mm thick solution domain, with heat and mass boundary conditions allocated to each boundary node, was simulated. The pressure along the boundaries is considered to be atmospheric and the mass flow at all boundaries is specified as diffusive-convective mass flow [Ahmed & Hurst (1997), Ang & Wang (2004), Ang & Wang (2009)].

In the ambient side, it is assumed that the air temperature is 20 ^{o}C and relative humidity 40%. In this case, the mass boundary condition for vapor is a convection boundary condition (eq. (16)), whereas the heat boundary condition is a convection and radiation boundary condition (eq. (17)).

$$\left.\left(\mathbf{j}_{diff}^{(vapor)}+\mathbf{j}_{pres}^{(vapor)}\right)\bullet\mathbf{n}\right|_{\mathbf{x}=\mathbf{X}_{BOUND}} = h_m\left(c_{g,amb}^{(vapor)}-c_{g,wall}^{(vapor)}\right) \tag{16}$$

$$\left.-k_{eff}\nabla T\bullet\mathbf{n}\right|_{\mathbf{x}=\mathbf{X}_{BOUND}} = h_c\left(T_{amb}-T_{wall}\right)+\varepsilon\sigma\left(T_{amb}^4-T_{wall}^4\right) \tag{17}$$

The mass concentration of air at the boundary is calculated via Dalton's law.

The heat transfer convection coefficient and the emissivity were set to be h_c=10 W m^{-2} K^{-1} and ε=0.9, respectively, while the mass transfer convection coefficient was chosen to be h_m=9.55×10^{-3} m s^{-1}, calculated from $h_m=1/(\rho_{air}C_{p,air})\times(\mathrm{Pr}/\mathrm{Sc})^{2/3}\times h_c$ [Ahmed & Hurst (1997)], with all the variables in this equation taken at ambient temperature.

For the "fire side", the measured temperature on the surface of the sample was used as wall temperature boundary condition, thus avoiding inaccuracies involved in the procedure of defining the convective and radiative heat transfer due to the experimental enclosure-furnace [Wickström (2004)]. Assuming that the fuel is methane, the vapor mass fraction inside the furnace was calculated, from the stoichiometric combustion of methane, to be Y_{vapor}=0.1239. The vapor mass concentration inside the furnace was calculated from:

$$c_{vapor}(t)=Y_{vapor}\rho_{mix}=Y_{vapor}\frac{P_{amb}MW_{mix}}{R_g T_{fire}(t)} \tag{18}$$

3.2 *Physical properties*

The physical properties of the simulated gypsum board were taken from the literature. The porosity, the permeability and the diffusion coefficients were chosen to be $\phi = 0.68$ [Craft et al. (2008)] and $K = 10^{-15}\,m^2$ [Bear (1972)] (similar to sandstone), $D_{eff} = \phi D_{AB}/\tau$ and $\tau = 1.869$ [Blondeau et al. (2003)]. The diffusion coefficient of water vapor in air was chosen to be D_{AB}=2.56×10^{-5} m^2 s^{-1} [Schwertz & Brow (1951)]. The rest of the physical properties, i.e. effective density, specific heat and thermal conductivity were taken from literature [Ghazi Wakili et al. (2007)].

4 RESULTS AND DISCUSSION

4.1 *Temperature evolution*

In Figure 1, HETRAN predictions, with and without mass transfer, of the temperature evolution inside the gypsum board are compared with experimental data [Ghazi Wakili et al. (2007)] (position x=0mm corresponds to the ambient side, whereas position x=12mm corresponds to the "fire side"). It is clearly shown that the introduction of vapor mass transfer in the model improves agreement with the experimental data, in comparison to the heat transfer calculations. The observed small over and under predictions of the calculated temperature field with the combined heat and mass transfer mechanisms can be associated to the constant mass transfer physical properties, i.e. porosity, permeability, diffusion coefficient, mass transfer coefficient etc, that are taken into account in this investigation. Numerical experiments indicated that the additional amount of energy offered to the dehydration process due to mass transfer amounts approximately to 191kJ/kg, which corresponds to ca. 42% increase in the dehydration energy of 450kJ/kg [Ghazi Wakili et al. (2007)], and it is very close to the ca. 45% estimated in the work of Ang & Wang [Ang & Wang (2009)].

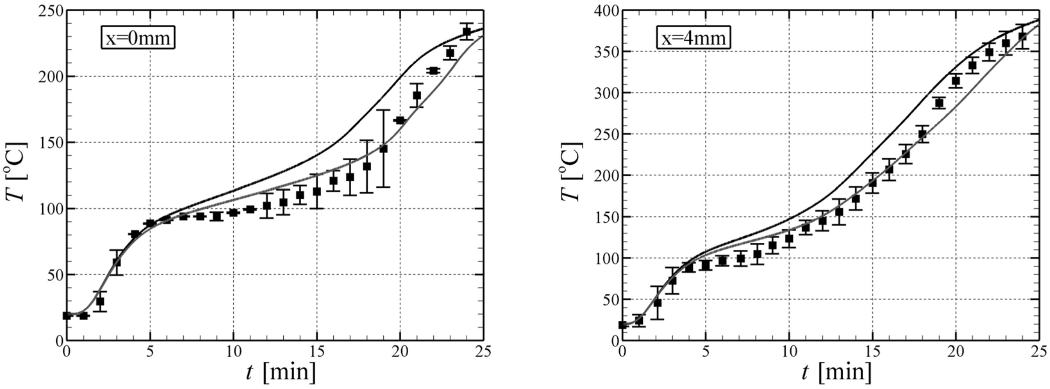

Figure 1. Comparison between HETRAN predictions, with (grey solid line) and without (black solid line) mass transfer, and experimental data (square symbols) [Ghazi Wakili et al. (2007)] of the temperature evolution inside the gypsum board.

4.2 *Mass concentration and pressure distributions*

Figure 2 illustrates the spatial distribution of the vapor (fig. 2a) and air (fig. 2b) mass concentration, as well as the gas phase mixture total pressure (fig. 2c) at different time steps. As gypsum is heated, the free moisture and the chemically bound water evaporate and water vapor is released inside the pores of the gypsum board increasing its mass concentration (fig. 2a). The increase of vapor mass concentration creates concentration gradients which make vapor to diffuse towards both directions (heated and unheated side). On the other hand, air is pushed out of the pores by the produced water vapor, decreasing its mass concentration (fig. 2b). At the fire side there is lack of air, due to the combustion taking place at the furnace, creating an air mass concentration gradient with the ambient side, forcing air to move to the fire side. Finally, vapor production increases pore pressure and pressure gradients are developed inside the gypsum sample (fig. 2c), forcing the gas phase mixture to move towards both directions.

4.3 *Conclusions*

This paper studies the simultaneous heat and mass transfer mechanisms occurring in a gypsum board when subjected to the ISO 834 fire curve. Predictions with the in-house developed code HETRAN, with and without mass transfer, of the temperature evolution inside the gypsum sample revealed the significant influence of vapor migration to the gypsum board behavior under fire conditions. Spatial distributions of vapor mass concentration and mixture total pressure indicated that vapor migrates toward both the heated and unheated side of the gypsum board.

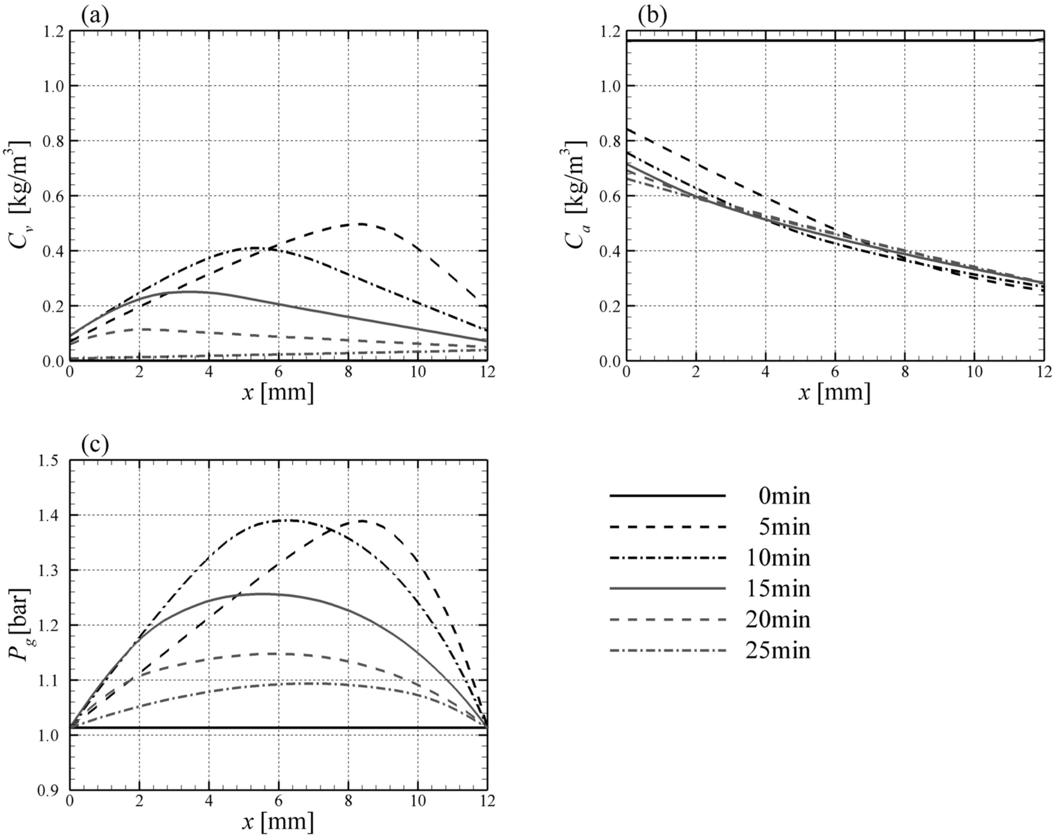

Figure 2. Spatial distribution of: a) vapor mass concentration, b) air mass concentration and c) mixture total pressure at different time steps.

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