Diffusion mechanisms and drying of concrete at elevated temperatures

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1 INTRODUCTION

Concrete properties depend strongly on temperature and moisture content. In addition, gradients of temperature and moisture content provoke internal stresses and microcracks in the material which also influence its mechanical behaviour. The prediction of the coupled transfer of heat, moisture and, eventually, air is therefore becoming more and more important in the design of PCRV's [Weber 1987]. In spite of many excellent contributions which have appeared on this subject a great number of questions remains, as yet, unanswered. At elevated temperatures this situation is even more complex because of the thermal instability of HCP. As a consequence both proper interpretation of results of usually quite expensive experiments and development of sound theoretical models are very intricate.

The present contribution is an attempt to construct a theory for the simultaneous flow of heat, water, and air at elevated temperatures. In an accompanying paper [Kamp 1987a] we presented a model which permits the prediction of the transport parameters of HCP and concrete on the basis of the elementary transport processes in individual pores of the material, as a function of temperature, moisture content, and pore size distribution.

The macroscopic theory discussed here is a logical extension of this model. A computer program, COUPFLO/1, was developed to simulate the flow phenomena in concrete slabs. In its present version, the program assumes the porous structure to be unaffected by temperature changes; i.e. only thermodynamic effects are taken into account. A second version which is currently being implemented, will use temperature dependent pore size distributions, such as determined, e.g., by Schneider [1985].

2 THEORY

Starting point for the development of the theory is the statement of conservation of mass and energy.

The following equations are then easily derived :

(1) $$\frac{\partial u}{\partial t} + \nabla \cdot J^u = Q^u \qquad \text{(conservation of water)}$$

$$\frac{\partial g}{\partial t} + \nabla J^g = Q^g \qquad \text{(conservation of gas) and} \tag{2}$$

$$\frac{\partial (\rho c^* T)}{\partial t} + \nabla \cdot J^h = Q^h \qquad \text{(conservation of energy)} \tag{3}$$

where u = water content, J^u = water flux, Q^u = water source (or water sink), g = gas content, J^g = gas flux, Q^g = gas source, ρc^* = heat capacity of the (moist) material, J^h = heat flux and Q^h = heat source.

For a thermally inert material, the water source and gas source terms are zero, and heat production or heat consumption are caused only bny condensation of water vapour or evaporation respectively. In the general case, however, these source terms must account for the hydration or thermal decomposition of HCP, and, eventually, the decomposition of some types of aggregates, e.g. limestone.

Summarizing, the following source terms are actually implemented :

$$\begin{aligned} Q^u &= 0 \\ Q^g &= 0 \\ Q^h &= \frac{L}{M} J^L \end{aligned} \tag{4}$$

where L = latent heat, M = molar mass, and J^L = production of liquid water in a point. The only gas considered in this case is, of course, air.

Latent heat of pore water is a function of relative humidity and temperature :

$$L(H,T) = L^B(T) - RT\ln H \tag{5}$$

where $L^B(T)$ = latent heat of bulk water, approximately given by :

$$L^B(T) \simeq 56500 - 42T \quad [\text{J/mole}] \tag{6}$$

For the calculation of J^L one must, in principle, consider liquid water and water vapour separately. The structure of HCP is supposed to be composed by microporous clusters of hydration products separated by macropores. Under usual condition micropores are filled with liquid water (capillary condensation) and the bigger pores contain water vapour only. Based on this model we assume that the transport through such a material can be looked upon to be a two-step process in series, i.e. liquid water transport within the clusters and vapour transport in the intercluster space. Thus it is supposed that water has to evaporate to cross the intercluster space. Macroscopically then the production of liquid is given by :

$$J^L = \frac{\partial}{\partial t}(u - u^v) \simeq \frac{\partial u}{\partial t} \tag{7}$$

where u = total water content, u^v = vapour content per unit volume of porous material.

Turning next our attention to the flow of water vapour and air, we remark that, at least for the limited temperature range for which the present implementation of the model is valid, both components flow independently of each other through molecular streaming (so called Knudsen flow).

The following expression can be derived for the flux of air :

$$(8) \qquad J^a = -\frac{32}{27\pi}\frac{e}{\bar{c}^a}\frac{\langle (r-t)^3\rangle_e}{\langle r^2\rangle}\left[\nabla p^a - \frac{p^a}{2T}\nabla T\right]$$

where e = porosity, $\bar{c}^a$ = thermal velocity of air molecules, p^a = air pressure, t = thickness of the adsorbed layer, and $\langle\rangle_e$ denotes an average taken over the "empty" pore space.

A similar formula can be derived for the flux of water <u>vapour</u> :

$$(9) \qquad J^v = -\frac{32}{27\pi}\frac{e}{\bar{c}^v}\cdot p^s\frac{\langle r-t\rangle^3 e}{\langle r^2\rangle}\left[\nabla H + \frac{H}{T}\left[\frac{L}{RT} - \frac{1}{2}\right]\nabla T\right]$$

where $\bar{c}^v$ = thermal velocity of water vapour molecules, and p^s = saturated vapour pressure.

For transport in series of water vapour and liquid water, the total water flux J^u is simply given formally by the following expression :

$$(10) \qquad J^u = a(u)J^v$$

where a(u) is an amplification factor which depends solely on (liquid) water content, and approaches unity for low water contents.

The heat flux is composed of three contributions : heat conduction in the humid solid, convection of air and convection of water :

$$(11) \qquad J^h = -\lambda\nabla T + c^a{}_T J^a + c^v{}_T J^u$$

where λ = thermal conductivity, c^a = heat capacity of air, and c^v = heat capacity of water vapour.

Thermal conductivity is approximately a linear function of water content :

$$(12) \qquad \lambda = \lambda^d + \frac{u}{u_{max}}(\lambda^w - \lambda^d)$$

where λ^d = conductivity of the dry solid, λ^w = conductivity of the wet solid, and u_{max} = maximum water content of the solid.

If we consider the time-derivatives given in equ. (1)-(3), we observe that the water content at equilibrium as a function of H and T is given by :

$$(13) \qquad U(H,T) = f(H^{T/T_o}, T_o)$$

where $f(H,T_o)$ = sorption isotherm at reference temperature.

Air content can be expressed easily in terms of air pressure, temperature, and water content :

$$(14) \qquad g = \frac{p^a M^a}{RT} \left(e - \frac{u}{\rho}\right)$$

Finally, heat capacity is roughly a linear function of moisture content :

$$(15) \qquad (\rho c)^* = u c^u + \rho^s c^s$$

where c^u = heat capacity of (liquid) water, and $p^s c^s$ = heat capacity of the (dry) solid.

3 NUMERICAL ANALYSIS

Equations (1)-(15) form a closed systen with three unknowns : H, p^a and T, which can be solved by standard finite element analysis. A 1D computer program to solve this problem has been described by Kamp [1987b].

The program uses the Crank-Nicholsen time marching scheme. The resulting non-symmetric system of equations is solved by means of Gauss-Seidel iteration. In order to speed up (vektor) calculations, the transport coefficients were calculated for a large number of temperatures and humidities and stored on file by means of a preprocessor.

As an example, we calculated the transport phenomena in a 50 cm thick concrete slab, which is supposed to be heated at one side from 20^0C to 150^0C in five hours, after which the temperature is kept constant. Initially, the slab is assumed to be in equilibrium at 80 % RH. The transport coefficients were calculated as described elsewhere [Kamp & al. 1987a]. Atmospheric conditions (T = 20^0C, p^a = 1 atm, H = 50 %) are assumed to be at the side which was not heated, whereas a "leaky" oven (no hermetic liner) was simulated at the heated side (total pressure 1 atmosphere, relative humidity corresponding to 50 % RH at 20^0C).

Figures 1-4 show the evolution of relative humidity, air pressure, temperature and moisture content as a function of time. As can be inferred from Fig. 4 a water "front" is predicted, which proceeds to the cold side of the slab. This is caused by condensation of water vapour in colder regions, an effect which may even cause the concrete to become supersaturated with liquid water. Figs. 5 and 6 show the water flux at the heated side and the weight loss curve respectively. The water flux curve shows a sharp peak which drops rapidly once the maximum temperature at the edge has been attained. Several mechanisms are responsible for this :

a) drying out of the material near the edge is almost stopped, and

b) moisture flow from the inner regions towards the (dry) edge is hampered by the temperature gradient.

Generally speaking, reasonable qualitative agreement with experimental results reported by Schneider und Herbst [1986] can be observed. The maximum increase of the total pressure observed by Schneider and Herbst was about 1.7 Bar after 35 hours. Results shown in Figs. 1 and 2 lead to a corresponding pressure of 2.0 Bar after 24 hours.

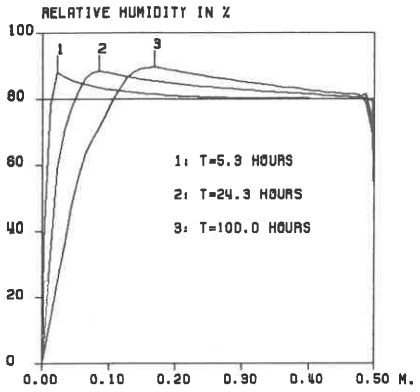

Figure 1 Relative humidities.

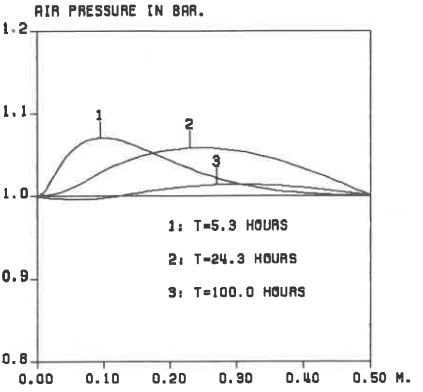

Figure 2 Air pressures.

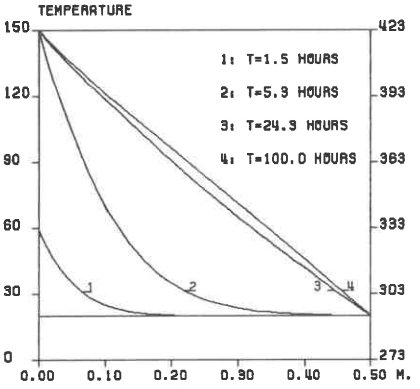

Figure 3 Temperatures.

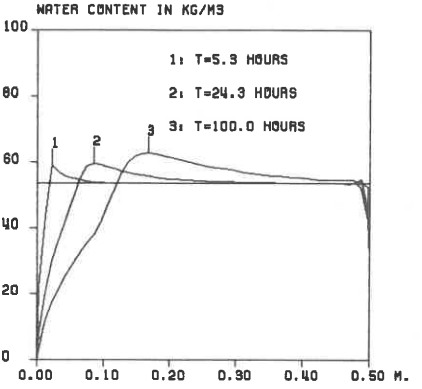

Figure 4 Water contents.

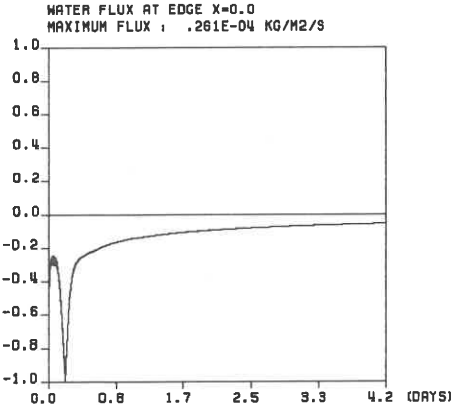

Figure 5 Water flux at heated edge.

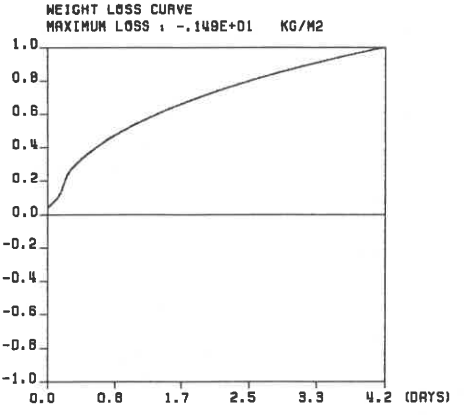

Figure 6 Weight loss.

The temperature gradient shown in Fig. 3 agrees reasonably well with experimental results given in the same report. Finally the weight loss shown in Fig. 6 compares reasonably well within the accuracy of the experiments and the numerical predictions (measured : about 2 kg, calculated : 1 kg after 35 hours).

4 CONCLUSIONS

A mathematical model for the analysis of the simultaneous flow of heat, moisture and air is presented. In its present form, the model predicts reasonably well the heat and mass transfer in concrete at moderately high temperatures (elevated temperatures) and not too high moisture contents.

In order to describe the characteristic flow phenomena at higher temperatures the model must be extended on the following points :

1) Hydration and thermal decomposition of HCP must be incorporated in the analysis.

2) Flow of water vapour and air must be described by the complete set of "Dusty-Gas" equations [Cunningham 1980].

3) The influence of temperature on the pore size distribution (coarsening of the microstructure and crack formation) must be taken into account.

4) Relative humidity must be replaced by another "moisture potential" (see for example [Kiessl 1983]) which permits a "smoother" description at high moisture contents.

Implementation of these extensions is under way.

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