

A HYGRO THERMO MECHANICAL MODEL FOR CONCRETE

A JEFFERSON*, A CHITTEZ*, R TENCHEV[†], G COLE[†], P LYONS[†], J OU*

* Cardiff University
The Parade, Cardiff, UK, CF24 3AA
e-mail: JeffersonAD@cf.ac.uk, www.cardiff.ac.uk

[†] LUSAS
Forge House, High Street, Kingston Upon Thames, Surrey UK,
e-mail: Paul.Lyons@lusas.com, www.lusas.com

Key words: Concrete, plasticity, damage, hydration, shrinkage, creep, porosity

Abstract: The paper presents an overview of a finite element approach for the analysis of the Concrack benchmark RL1. The approach adopted includes a thermo-hygro component which is coupled to a mechanical model which includes non-linear mechanical, aging, shrinkage and long term creep behaviour. The thermo-hygro model solves the mass balance equations for water vapour and liquid water as well as the enthalpy balance equation. A particular focus of the paper is on the model used to describe the development porosity with hydration. It is concluded that a correct treatment of porosity development over time is essential for the proper simulation of the Concrack material data and benchmarks.

1 INTRODUCTION

The paper considers the analysis of one of the benchmark problems from the CEOS.fr project [1] using a hygro-thermo-mechanical model implemented in the finite element program LUSAS.

An overview of the modelling approach is provided but particular attention is paid to the simulation of early age porosity and its importance in the analysis. The reason for concentrating on this aspect is that in an earlier presentation by the authors at a benchmarking workshop, entitled Concrack2 [1], the authors' results for early age shrinkage were inaccurate and one of the reasons identified for this was an inconsistency between the liquid mass-balance and the porosity development model being used.

The evolution of shrinkage and porosity are closely linked phenomena. The hydration of cement and external drying remove water from the cement matrix and this gradually empties the space or pores of liquid and results in

menisci at liquid-gas interface where capillary pressures manifest [2]. The capillary tensions cause stresses in the skeleton and lead to macroscopic shrinkage. Thus, porosity development has a significant influence on the estimation of shrinkage.

The overall approach to simulating hygro-thermal behaviour is similar to that of Gawin et al [3] with the exception that only one fluid phase is considered rather than two. This is possible due to the assumption that the gas pressure is maintained at atmospheric.

A staggered approach is taken to simulating the hygro-thermal (H-T) and mechanical components of the analysis in which a hygro thermal step is followed by a mechanical step.

2 GOVERNING H-T EQUATIONS

The averaged macroscopic mass balance equations for liquid (capillary and absorbed water) and vapour phases are as follows;

$$\dot{\bar{\rho}}_w + \text{div}(J_w) = -\dot{m}_v - \dot{m}_h \quad (1)$$

$$\dot{\bar{\rho}}_v + \text{div}(J_v) = \dot{m}_v \quad (2)$$

where \dot{m}_v is the rate of mass transfer during evaporation of liquid water, \dot{m}_h is the rate of liquid water mass used in hydration which represents the sink/source term, $\bar{\rho}_\pi = \eta S_\pi \rho^\pi$ is the averaged density of phase ($\pi = w$ or v), η is the porosity of the medium, S_π is the degree of saturation of phase π , ρ^π is the bulk density of phase, the superior dot denotes the time derivative with respect to solid skeleton and J_π denotes the mass flux of phase π .

The macroscopic enthalpy balance equation for the multi-phase medium, assuming that all the phases are in thermal equilibrium, is as follows:

$$\overline{\rho C_p} \dot{T} + \text{div}(-k_T \text{grad}(T)) = -\dot{m}_v H_v + \dot{Q}_h \quad (3)$$

Where, T is the temperature of the medium, $\overline{\rho C_p} = \sum_\pi (\bar{\rho}_\pi C_p^\pi)$ is the thermal capacity, k_T is the effective thermal conductivity of cement paste, H_v is the specific enthalpy of evaporation and \dot{Q}_h is the rate of heat generation of hydration. In the current model there is no constitutive law for \dot{m}_v , but this problem is solved by combining equations (1) and (2) into a single expression.

3 CONSTITUTIVE LAWS AND HYDRATION MODEL

Liquid phase advection/permeation is assumed to obey Darcy's law and diffusion of the vapour phase to follow Fick's law:

$$J_w = -\frac{k^i k^{rw}}{\mu^w} \text{grad}(p^w - \rho^w \mathbf{g}) \quad (5)$$

$$J_v = -\frac{M^w}{RT} D^v \text{grad}(p^v) \quad (6)$$

where k^i is the intrinsic permeability coefficient dependent on the degree of hydration, k^{rw} , μ^w , p^w and M^w are the relative permeability coefficient, the dynamic viscosity, pressure and molar mass of phase w , \mathbf{g} is the gravity vector, R is the ideal gas constant, D^v represents the effective diffusivity of vapour in the air while p^v is the water

vapour pressure. The capillary curve defined in eq. (7) provides the relationship between capillary pressure p^c and S_w . The expression adopted is a version of van Genuchten's equation [4] used by Baroghel-Bouny et al. [5].

$$S_w = \left[1 + \left(\frac{p^c \xi_0}{a_c p_{atm} \xi} \right)^{\frac{b}{b-1}} \right]^{-\frac{1}{b}} \quad (7)$$

where a_c and b are material parameters, p_{atm} is the atmospheric pressure and ξ_0 is the surface energy at reference temperature. Clapeyron's state equation correlates pressure to mass concentration, Kelvin's equation delineates internal relative humidity, h_r , whilst Laplace equation defines p^c as a function of surface tension, σ and pore radius, r :

$$\rho^\pi = \frac{p^\pi M^\pi}{RT} \quad (8)$$

$$h_r = \exp\left(\frac{-p^c M^w}{\rho^w RT}\right) \quad (9)$$

$$p^c = \frac{2\sigma}{r} \quad (10)$$

The curing of the cementitious material is described by Schindler and Folliard's hydration model [6]:

$$\Gamma(t_e) = \Gamma_\infty \exp\left[-\left(\frac{\tau_{sf}}{t_e}\right)^{\beta_{sf}}\right] \quad (12)$$

where Γ is the degree of hydration at equivalent time t_e , Γ_∞ is the ultimate degree of hydration at complete theoretical hydration whereas τ_{sf} and β_{sf} are the hydration time and shape parameters. t_e takes into account the coupled effect of time and temperature on different thermal curing methods on the basis of Arrhenius rate theory for chemical reactions.

4 AGING PROPERTIES, CREEP & SHRINKAGE

Elastic properties and strengths are assumed to depend directly upon the degree of hydration. For example, the elastic modulus is

given by

$$E(\Gamma) = E_f \Gamma_r^{c_E} \quad (13)$$

where c_E is a constant, and $\Gamma_r = \Gamma / \Gamma_\infty$

Creep is simulated with a modified form of Bazant's solidification theory [7], in which -at each time interval during curing- there is an addition of a stress free rheological unit which comprises different proportions of a long-term and a short-term Maxwell unit. The idea is illustrated below:

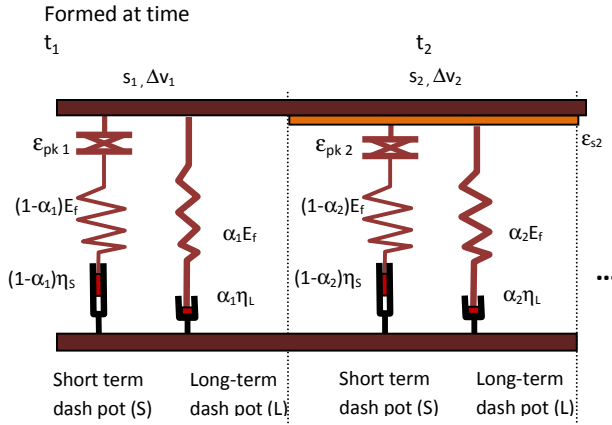


Figure 1: Solidification creep model.

Autogenous and drying shrinkage are computed from changes in the degree of saturation and degree of hydration. Here we have not used p^c to compute shrinkage but rather chosen nonlinear functions of S_w and Γ . It is noted that once hydration is complete, experimental data shows that there is a remarkably linear relationship between weight loss and drying shrinkage for a normal environmental range of humidity [8], i.e.

$$\dot{\epsilon}_{ds} = \beta_{ds} \dot{S}_w$$

5 MECHANICAL MODEL

The constitutive model for concrete is based on a modified version of the model described in [9]. Two major modifications have been made for the work on simulating early age behaviour. The first involve a modification of the plastic and damage evolution functions such that they depend upon the degree of hydration. Results from an example analysis using the data from Yi et al [10] is shown in

Figure 2.

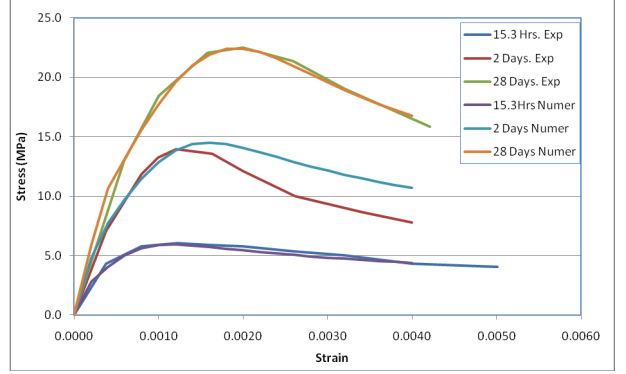


Figure 2: Compressive response for different times.

The second major change involves using an entirely smooth relationship for rough crack contact as well as an approach to the solution of the nonlinear equations which does not involve using a negative tangent modulus. These changes have greatly improved the stability of the solution process. Details are to be given in a forthcoming publication.

6 DEVELOPMENT OF POROSITY WITH HYDRATION

As mentioned in the Introduction, the primary focus of the paper is on the development of porosity over time and the need for an approach which is consistent with the moisture mass balance equation.

A few hours after mixing, the cement paste is plastic and all the pores are filled with pore solution. During this period all the chemical shrinkage manifest itself into an external volume change and the water degree of saturation remains constant and close to 1. Later, when a percolation threshold hydration degree is exceeded, the paste starts to gain stiffness and, due to shrinkage, voids are formed within the mix. In the second stage of hydration the small voids nucleate into larger pores leading to a stabilised capillary network. Two types of pores can be identified inside the hydrated paste according to their size: capillary pores $\geq 12\text{nm}$ and gel pores $\leq 12\text{nm}$ [11]. In the early stages, capillary pores are predominant, but, as the hydration process proceeds, the proportion of gel pores gradually increases with respect to the capillary ones. A

shift of the pore size distribution to smaller pores with time is measured. Experimental evidence suggests an essentially linear relationship between porosity and degree of hydration [12]. In this paper, porosity is estimated from the quantity of cement paste constituents at the end of the chemical reactions and by assuming that the reaction products advance proportionally with the overall hydration degree of the paste. Powers' model [13] for cement hydration provides a general expression of porosity which for concrete has the form:

$$\eta(\Gamma) = \frac{\frac{w_0}{c_0} + \frac{V_{ea}\rho^w}{c_0} - \left[\Gamma \cdot C_\eta \frac{\rho^w}{c_0} + V_s(\Gamma) \frac{\rho^w}{c_0} \right]}{\frac{\rho^w}{\rho_c} + \frac{w_0}{c_0} + \frac{V_{ea}\rho^w}{c_0} + \frac{\sum V_{agg} \rho^w}{c_0}} \quad (13)$$

where η is porosity, $\frac{w_0}{c_0}$ is the water cement ratio, C_η material coefficient, V_{ea} is the volume of entrapped air, ρ_c is the density of cement, $V_s(\Gamma)$ is the volumetric strain do to autogenous shrinkage, and $\sum V_{agg}$ is the volume of aggregates. C_η differentiates capillary from total porosity and is obtained by evaluating the quantities of water forms using stoichiometry of the four main clinker minerals. The chemical reactions considered for these components essentially follow those given in references [11] and [14].

An example simulation is presented using an experiment undertaken by Baroghel-Bouny [5], in which autogenous drying takes place. The relative humidity referred to on the graph is internal relative humidity calculated from equation 9.

7 CONCRACK BENCHMARK

Full details of the Concrack benchmark (RL1) and associated material data are given on the project web site [1].

As mentioned earlier, one of the concerns regarding the authors' earlier simulations was an inability to correctly predict the material test data for autogenous drying.

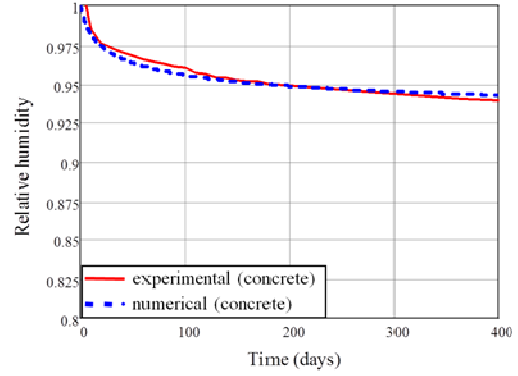


Figure 3: Autogenous drying of concrete.

Using the refined porosity and shrinkage models, this situation has improved and an illustrative graph showing the prediction of the autogenous response from the Concrack material data is given in Figure 4.

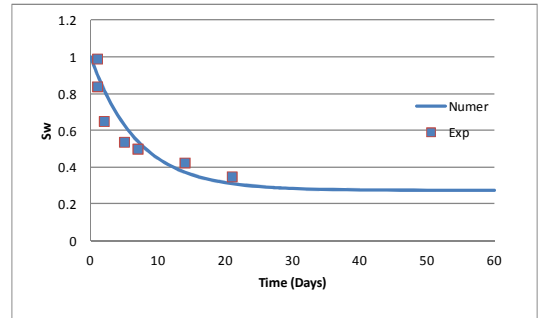


Figure 4: Autogenous drying for Concrack material.

Direct moisture content values were not available for the RL1 benchmark but temperatures, strains and displacements were available. The predictions regarding temperature and overall deformation are given in Figures 5 & 6.

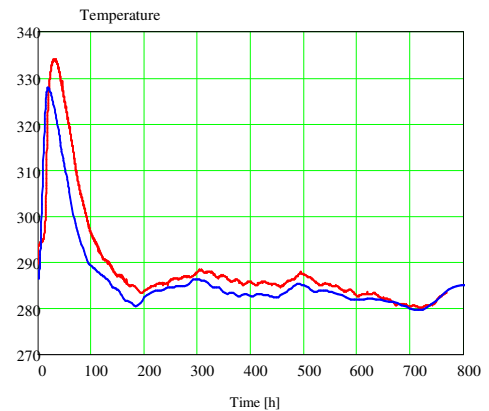


Figure 5: Temperature variation for Concrack test RL1

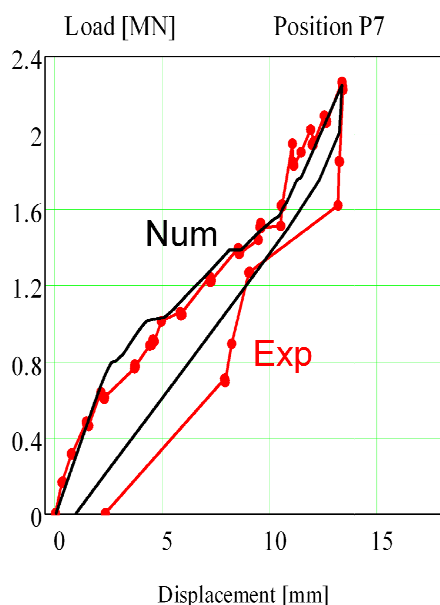


Figure 6: Overall response for Concrack test RL1

8 CONCLUDING REMARKS

The paper has presented an overview of an approach to the analysis of the time dependent behaviour of concrete along with some illustrative results for the Concrack benchmark RL1.

In addition, more detailed information is provided on one aspect of the approach, namely the porosity development model. A correct treatment of porosity development over time was found to be an essential for the proper simulation of the Concrack material data and as well as for the full scale tests themselves.

REFERENCES

[1] <http://www.concrack.org/>
 [2] Coussy, O. *Poromechanics*, Wiley (2004)
 [3] Gawin D., Pesavento F., Schrefler B. A. 2006. Hygro-thermo-chemo-mechanical Modelling of Concrete at Early Ages and Beyond. Part I: Hydration and Hygro-thermal Phenomena, *Int. J. Numer. Meth. Engng*, 67, 299-331
 [4] van Genuchten M. T., 1980. A Closed-form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils, *SoilSci. Soc. Am. J.*, 44, 892-898

[5] Baroghel-Bouny V., Mainguy M., Lassabatere T., Coussy O., 1999. Characterization and Identification of Equilibrium and Transfer Moisture Properties for Ordinary and High-Performance Cementitious Materials, *Cement and Concrete Research*, 29, 1225-1238
 [6] Schindler A.K. and Folliard K.J., 2005. Heat of Hydration Models for Cementitious Materials, *ACI Journal*, 24-33
 [7] Bazant, Z.P., Cusatis, G. and Cedolin, L., 2004. Temperature Effect on Concrete Modelled by Microprestress-Solidification Theory. *Journal Engineering Mechanics, ASCE*, pp691-699
 [8] Barr B, Hoseinian S.B, Beygi M.A., 2003. Shrinkage of concrete stored in natural environments. *Cement and Concrete Composites*, 25(1), 19-29
 [9] Jefferson A. D ., 2003. Craft - a plastic-damage-contact model for concrete. I. Model theory and thermodynamic considerations, *International Journal of Solids and Structures* , 40(22) 5973-5999
 [10] Yi, S-T, Kim, J-K and Oh, T K., 2003. Effect of strength and age on the stress-strain curves of concrete specimens. *Cement and Concrete Research* 33, 1235-1244
 [11] Jennings H. M., 2008. Refinements to colloid model of C-S-H in cement: CM-II, *Cement and Concrete Research*, 38, pp. 275-289
 [12] Cook R.A., Hover K.C., 1999. Mercury Porosimetry of Hardened Cement Pastes, *Cement and Concrete Research*, 29, 933-943
 [13] Powers T. C., Brownyard T. L., 1947. Studies of the Physical Properties of Hardened Portland Cement Paste, *Journal of the American Concrete Institute*, 43.
 [14] Feldman R.F., 1973. Helium Flow Characteristics of Rewetted Specimens of Dried Portland Cement Paste, *Cement and Concrete Research*, vol. 3, nr. 6, 777-790.