Modeling Heat and Moisture Transport During Hydration of Cement-Based Materials in Semi-Adiabatic Conditions

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Abstract

Introduction

The process of accelerated curing of pre-cast concrete consists of increasing the temperature within a saturated water vapor atmosphere during several hours; therefore, it consumes a considerable amount of energy. A typical steam-curing cycle is shown in Figure 1. In this process, the cement hydration has a significant importance in the thermal behavior of concrete, since it has an effect on both the material properties and performance. Therefore, it is essential to understand the chemical reaction-heat and mass transport process condition interaction, in order to optimize the curing process.

The aim of the present work is to simultaneously model cement hydration and heat and moisture transport in cement-based materials using a continuum approach to simulate semi-adiabatic curing conditions.

Use of COMSOL Multiphysics® software

A multiphysics model that describes hydration and heat and mass transport in cement-based materials was developed. The model utilizes two variables to describe the chemical kinetics; equivalent time and degree of hydration in the form of Domain Ordinary Differential Equations. The hydration reactions are described by a maturity function that uses this equivalent time, thereby describing the change in the degree of hydration based on the time-temperature history.

These equations are coupled to a heat balance, using the COMSOL® Heat Transfer Module, and moisture content (two phases: liquid and vapor) using the Partial differential equations module in its general form.

The 2D axisymmetric model-geometry implemented represents a simple semi-adiabatic laboratory calorimeter. It consists of four subdomains; the cylinder of cement-based material; the

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surrounding plastic container; the insulation wall, and the air between the top specimen surface and the container lid.

The parameters of the maturity function and the activation energy were obtained by experimental isothermal calorimetry studies conducted at different temperatures on pastes and mortars with various water-to-cement ratios (w/c) by mass. The requisite thermal properties of thermal conductivity and specific heat were measured using a Hot-Disk Thermal Constants Analyzer.

Results

The simulated temperature distribution achieved when the maximum temperature is reached for the model-geometry is shown in Figure 2, using the axisymmetric model.

Figure 3 presents the measured and predicted temperature in cement-paste specimens at two different w/c, during both heating and cooling periods. The cooling stage occurring after approximately two days fits well in the case of w/c=0.30, but shows an overprediction in the case of w/c=0.45. In this latter case, some heat could have been dissipated due to water evaporation, which was not taken into account in the current model.

The model is also able to compute the degree of hydration (Figure 4) and moisture loss by the consumption of water by the chemical reactions.

Conclusions

A Multiphysics model that describes temperature evolution, degree of hydration and moisture content was developed and the results show good agreement with experimental results. The model was used to simulate the temperature evolution in the semi-adiabatic calorimetric test, and simulation predictions compared favorably with the measured experimental data. In the future, the model will be extended to consider geometries and boundary conditions typically encountered in a pre-cast plant.

Reference

Bentz, D.P., Transient plane source measurements of the thermal properties of hydrating cement pastes. Materials and Structures, 40, pp.1073–1080 (2007).

Chini, A. R., Effect of elevated curing temperatures on the strength and durability of concrete. Materials and Structures, 38(281), pp.673–679 (2005).

Freiesleben Hansen, P Pedersen, J., Maturity Computer for Controlled Curing and Hardening of Concrete. Nordisk Betong, pp.19–34 (1977).

Hua, C., Acker, P. and Ehrlacher, A, Analyses and model of the autogenous shrinkage of hardening cement paste. I. Modeling at macroscopic scale. Cement and Concrete Research, 25(7), pp.1457–1468 (1995).

Mark, J.E., Physical Properties of Polymers Handbook, Springer Science Business Media (1990).

Pang, X. et al, A comparison study of Portland cement hydration kinetics as measured by chemical shrinkage and isothermal calorimetry. Cement and Concrete Composites, 39, pp.23–32 (2013).

Smilauer, V. and Krejci, T, Multiscale model for temperature distribution in hydrating concrete. International Journal for Multiscale Computational Engineering, 7(2) (2009).

Villmann, B. et al, Time-dependent Moisture Distribution in Drying Cement Mortars. Results of Neutron Radiography and Inverse Analysis of Drying Tests Determination of Moisture Transport Parameters and Moisture Profiles by Inverse Analysis., 20(1), pp.49–62 (2014).

Xu, Q. et al, Modeling hydration properties and temperature developments of early-age concrete pavement using calorimetry tests. Thermochimica Acta, 512(1-2), pp.76–85 (2011).

Figures used in the abstract

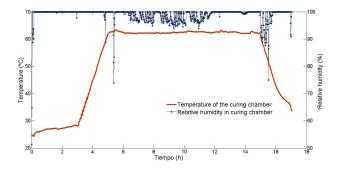


Figure 1: Typical steam curing conditions.

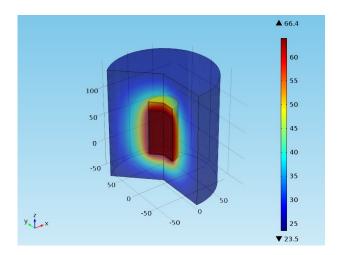


Figure 2: Temperature distributions in the simulated semi-adiabatic calorimetric test at a degree of hydration of 0.35 at 12 h in cement paste with w/c=0.3.

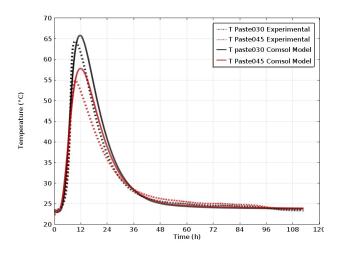


Figure 3: Comparison of evolution of measured temperature in the semi-adiabatic calorimetric test with the simulation in cement pastes with w/c=0.3 and 0.45.

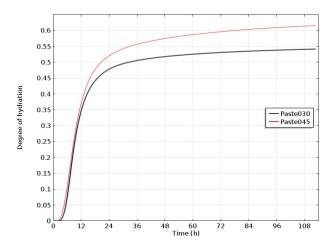


Figure 4: Simulated average degree of hydration in cement pastes with w/c=0.3 and 0.45.