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

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Introduction: The process of accelerated curing of pre-cast concrete process 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 reactions coupled to the heat and mass transport process, in order to optimize the curing process.

Use of COMSOL Multiphysics: The model utilizes two variables to describe the chemical kinetics; the equivalent time and the degree of hydration in the form of Domain Ordinary Differential Equations.

$$\frac{dt_e}{dt} = \exp\left[\frac{E}{R}\left(\frac{1}{T_r}-\frac{1}{T}\right)\right] \qquad t=0 \;\; then \;\; t_e=0$$

$$\frac{d\alpha}{dt} = \exp\left[\frac{E}{R}\left(\frac{1}{T_r}-\frac{1}{T}\right)\right]\cdot\frac{\alpha_u\beta}{t_e}\left(\frac{\tau}{t_e}\right)^{\beta}\exp\left[-\left(\frac{\tau}{t_e}\right)^{\beta}\right] \qquad t=0 \;\; then \;\; \alpha=0$$

These equations are coupled to a heat balance, using the COMSOL Heat Transfer module. Liquid (w) and vapor (h) phases were considered in the moisture content transport.

$$\rho_i Cp_i \frac{\partial T}{\partial t} = \nabla\cdot\left(k_i\nabla T\right)+Q_i$$

$$\rho_s\frac{\partial w}{\partial t} = \frac{\partial h}{\partial x}\left[\rho_s\cdot D_l(h)\frac{\partial w}{\partial x}+D_v(h)\frac{\partial h}{\partial x}\right]+S$$

The inner boundaries are continuous, in the exterior are a convective boundaries.

$$\mathbf{n}\cdot\left[(k\nabla T)_{\Omega 1}-(k\nabla T)_{\Omega 2}\right]=0 \qquad -\mathbf{n}\cdot(-k\nabla T)=q_0=h\cdot(T_{ext}-T)$$

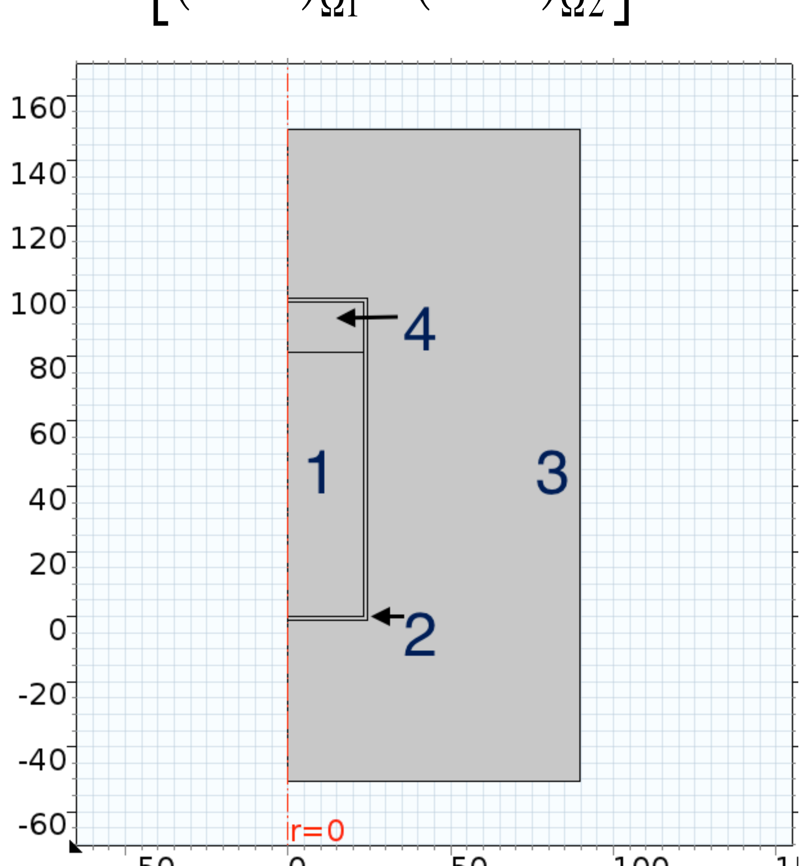

Figure 1. Geometry

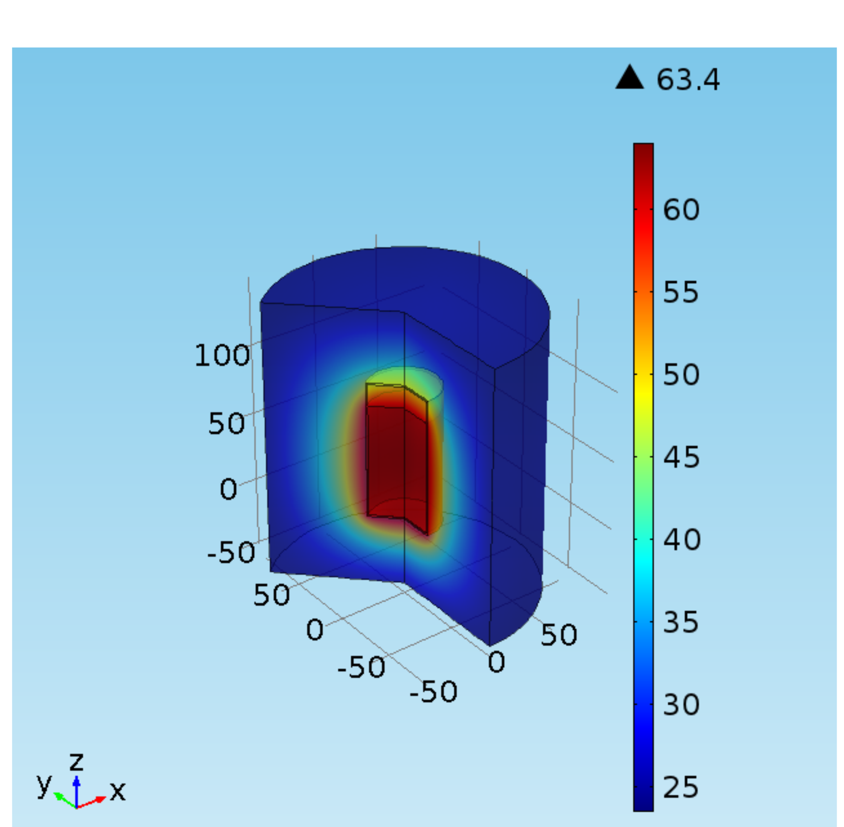

Figure 2. Axisymmetric temperature profile

Results: The simulations show a good agreement. The evolution of temperature shows two stages (Figure 4), heating (solid line) and cooling (dotted line). The model is also able to compute the degree of hydration and moisture content.

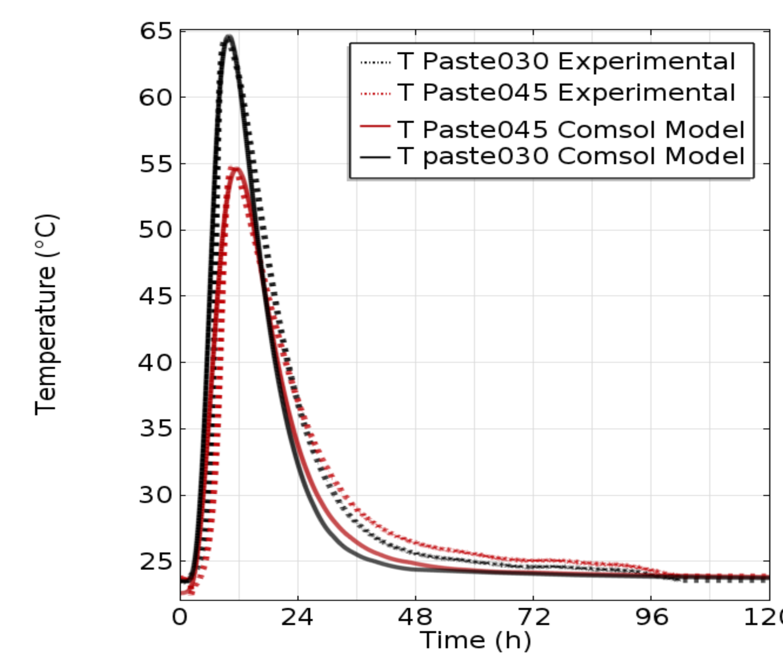

Figure 3. Experimental vs simulated

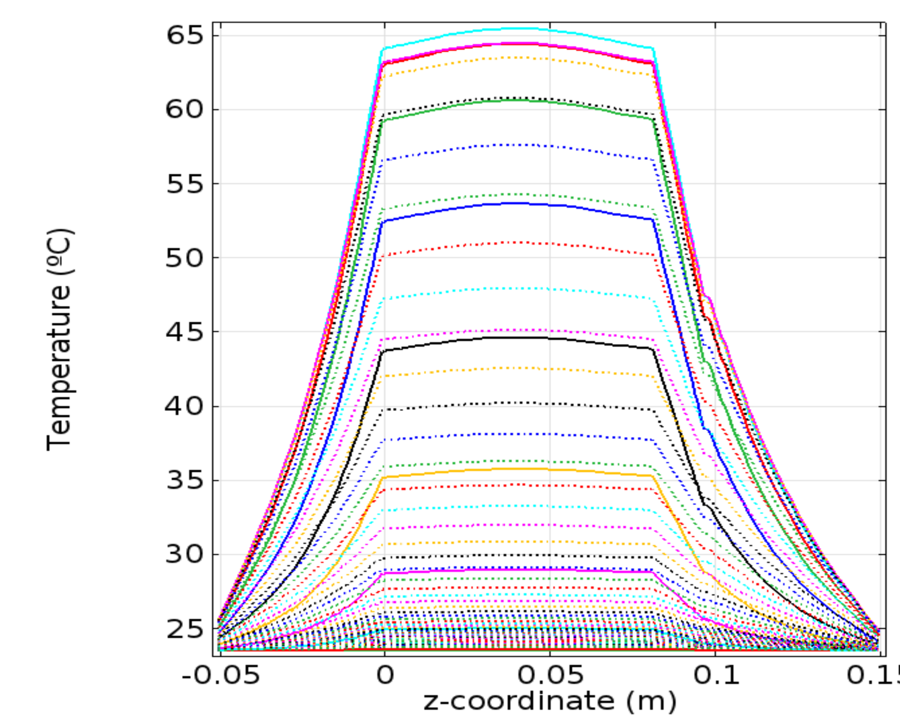

Figure 4. Temperature along z axis

The thermal properties, C_p and k, were experimentally determined

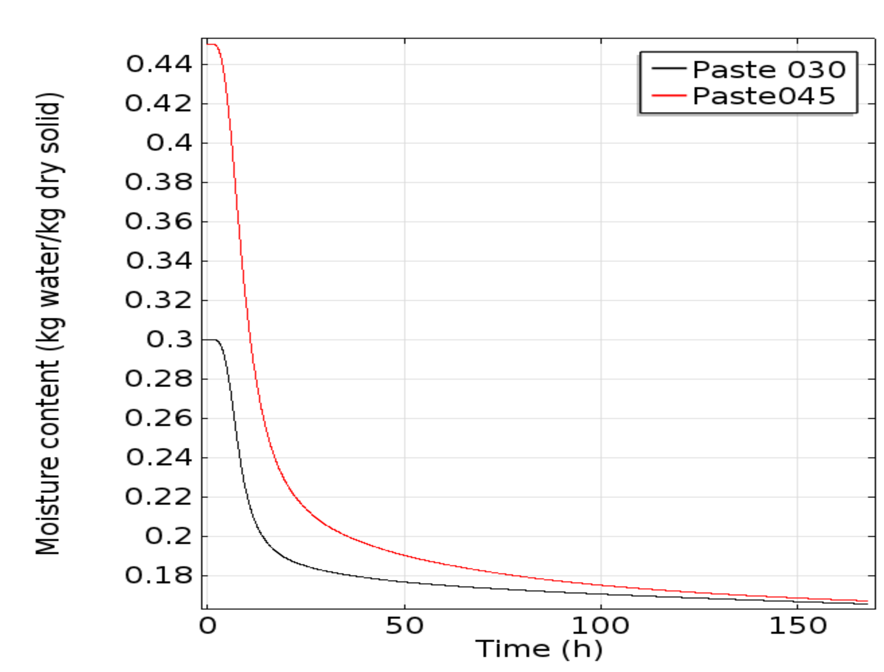

Figure 5. Moisture content

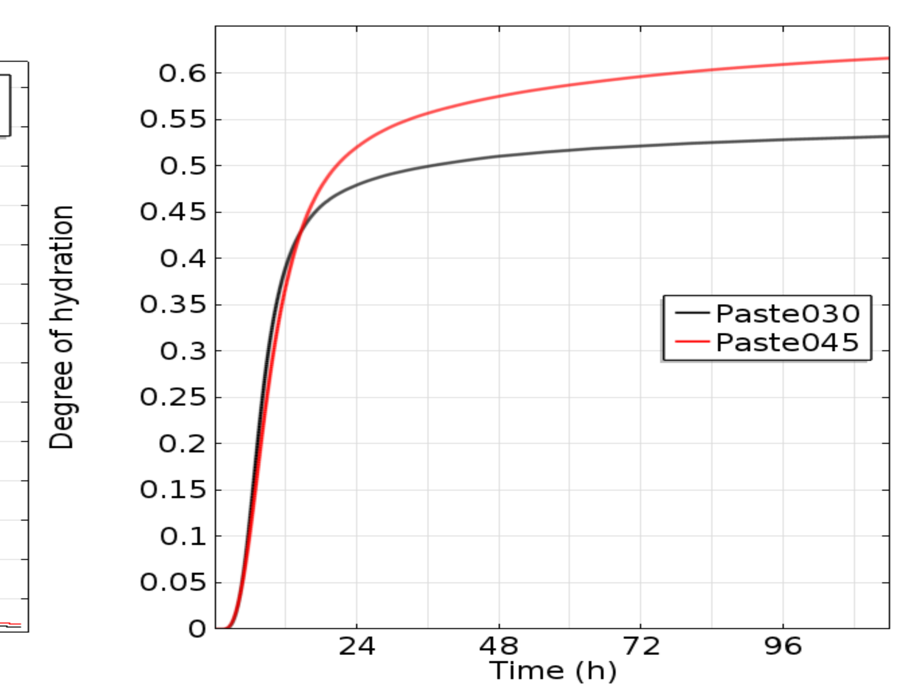

Figure 6. Degree of hydration

Conclusions: A Multiphysics model that describes heat conduction, degree of hydration and moisture content was developed. The model was used to simulate the temperature evolution in a semi-adiabatic calorimetric condition. The temperature evolution simulated using this model showed a good agreement with experimental data. The next step of the work will be to extend the simulations to the semi-adiabatic conditions used for curing mortars.

References:

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