Numerical Modelling of the Hydration of Cement in Concrete

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Abstract: The early age mechanical behaviour of concrete is characterised by the evolution of the hydration of cement with gains in strength and the onset of crack inducing residual strains. These effects justify special attention when high performance concrete is used, as due to their potential to mobilize substantially high levels of heat of hydration. This has led to the recent development of alternative thermo-chemical and thermo-chemo-mechanical models, with the objective of predicting the early age behaviour of concrete structural elements.

A hybrid-mixed finite element formulation is used to model the thermo-chemical process of hydration of cement in concrete. This formulation is based on the direct approximation of the temperature, hydration degree and heat flux fields using high-order approximation bases to enhance its implementation using coarse meshes of superelements. It can be implemented in out-of-the-shelf computers but its structure is suitable to parallelization for large-scale applications.

The basic equations of transient thermal problems are extended to include the heat generation caused by the cement hydration, the kinetics of which is assumed to be governed by the Arrhenius law. Particular attention is paid to the modelling the hydration laws that characterize different types of cement, and, also, to the modelling of the alternative initial and boundary conditions that may occur in practical applications and in the emulation of experimental testing conditions.

Thus, to model phased construction, the initial conditions can be stated in terms of known hydration degree fields and prescribed temperature or temperature rate fields. In what regards boundary conditions, and besides the standard conditions on prescribed heat flux and/or temperature, the formulation is written to model conduction, convection and radiation laws, under variable environmental conditions.

The resultant transient problem is non-linear. Consequent upon the approximation criteria that are used to set up the finite element formulation, the algebraic solving system is symmetric, highly sparse and well-suited to parallelization and adaptive refinement. These properties are exploited to minimize storage requirements and enhance speed in solution.

The performance of the formulation is illustrated with one-, two- and three-dimensional testing problems. They are taken from the literature and include the assessment of the results obtained in the emulation of experimental testing and monitoring. A set of tests designed to assess the robustness of the finite element formulation is also presented.

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