THCM model of concrete at early ages and its extension to tumor growth numerical analysis

Giuseppe Sciumè

Keywords: multi-physics, multiphase, hydration, shrinkage, creep, cell division, necrosis.

Prediction of concrete strain at early age may be a critical point on the design of some classes of civil engineering structures. Among these are massive structures like concrete dams, reactor's containments in nuclear power plants, tunnels, etc., in which hydration is accompanied by an important increase of temperature.

Cement hydration is a thermo-activated reaction and therefore the rise of temperature, not well dissipated in mass concrete, increases the rate of reaction which may become very important inducing a ΔT of the order of 40-60 °C. The positive thermal strain associated with heating is very often restrained by an existing substrate, or self-restrained due to the cast geometry, leading to compressive stress. Then, during the subsequent cooling phase the volume of concrete decreases progressively and also this compressive stress decreases; however, due to the greater stiffness of the material (Young's modulus changes a lot with hydration) the stress in certain parts of the structure becomes of traction and may induce diffuse cracking or traversing localized cracks. Furthermore, thermal strain is coupled with hygral strain (autogenous and drying shrinkage) and creep strain (basic and drying creep) and this makes modeling the mechanical behavior of concrete at early age a very demanding task.

To deal with such problems, a multiphysics model for concrete at early age is here presented [1]. Concrete is modeled as multiphase system consisting of three phases: a solid phase, *s*, a liquid phase, *l*, and a gaseous phase, *g*. The solid phase contains several species: anhydrous grains of cement, aggregates, and hydrates (CSH, etringite, etc.). The liquid phase is liquid water and the gaseous phase is modeled as an ideal binary gas mixture of dry air and water vapour.

The mathematical model shares the general conservation equations of mass, energy and linear momentum of Gawin *et al.* [2], whereas several originalities have been introduced at the constitutive level and these are listed below.

The equation used for the desorption isotherm has been properly modified to take into account its dependence on the hydration degree of concrete: this is a key point of the model because together with the adoption of a hydration dependent Biot's coefficient allows to compute with fine accuracy the hygral strain during hydration. Thanks to the adoption of a relevant porosity function which respects stoichiometry, the instantaneous and time dependent parts of autogenous shrinkage come out mechanically from the effective stress principle, without a dedicated constitutive equation. The mechanical damage is considered and coupled with creep to take into account that cracking may occur also at lower tensile stress than the tensile strength, due to strain excess.

The model has been implemented in Cast3M (FE code of the French Atomic Agency), in a partially uncoupled form: the THC solution impacts on the mechanical one, but not *viceversa*. This partial uncoupling is suitable when – such as in the considered case – cracks opening and strains are relatively small for having an influence on mass and heat transports.

The participation to the French international Benchmark ConCrack[1] has allowed to test the effectiveness of the developed model. A large massive beam with restrained longitudinal strain has been modeled and the agreement between the obtained numerical results and the experimental ones has been very satisfactory [3].

This model is also exploitable for repaired structures [1]. Two repaired beams analyzed experimentally in [4], have been modeled and their behavior compared with that of a reference beam (not repaired). The two beams have been repaired using two wholly different concretes: an ordinary concrete (w/b = 0.62) and an ultra-high performance fiber reinforced concrete (w/b = 0.22).

Going from the material scale (experimental tests used to identify the parameters of the model) to the structure one (modeling of the reference and repaired beams), an agreement between the numerical and experimental results has been achieved qualitatively and quantitatively. The analyzed cases have confirmed that the factors influencing mainly the behavior of repairs are: installation and environmental conditions, the repair's geometry and the materials' properties. Concerning the repair material, elastic modulus, tensile strength and creep potential impact critically on the success of a repair. Creep in particular has a chief role because it relaxes the tensile stress and moderates cracking.

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[1] This benchmark has been organized within the National French project CEOS ('Comportement et Evaluation des Ouvrages Spéciaux vis-à-vis de la fissuration et du retrait').

A specific procedure for the identification of the material parameters has been also defined. This procedure, based on four[2] experimental tests, allows to easily identify the input parameters, and despite the sophistication of the model makes it reasonably exploitable for industry and for many cases of practical interest.

An important part of the PhD thesis concerns tumor growth modeling: this work has been carried out within the context of a collaboration between my Italian PhD Director (B. Schrefler) and the Methodist Hospital of Houston.

The mathematical model developed for tumor growth is based on multiphase porous media mechanics and has relevant formal analogies with that of concrete at early age (phases' transport, intra-phase and inter-phase exchanges of mass, etc.).

Tumor is modeled as a four-phase system which consists of a solid phase, the extracellular matrix (ECM), and three immiscible fluid phases. The fluid phases are the interstitial fluid (IF), tumor cells (TC) and healthy cells (HC), with the latter two phases modeled as adhesive fluids. Being the tumor growth strongly influenced by nutrients availability, the diffusion of oxygen coming from the nearby existing vessels is also considered. Several cases of biological interest like tumor spheroids and tumor cords have been modeled, and numerical results, although not extensively validated, are qualitatively in agreement with experiments.

At the beginning a unique pressure was considered for both cell populations ($p^{TC} = p^{HC}$) [5]. Nowadays, appropriate constitutive relationships for the pressure difference among each pair of fluid phases have been introduced, allowing for different pressures in the three fluid phases [6]. These relationships respect the relative wettability of fluids and take into account explicitly fluid–fluid interfacial tensions, resulting in a more realistic modeling of cell adhesion and invasion.

High interfacial tension at the TC–HC interface support a rapid growth of the malignant mass, with a relevant amount of HC which cannot be pushed out by TC and remains in place; conversely, a lower TC–HC interfacial tension tends to originate a more compact and dense tumor mass with a slower growth rate of the overall size. This enhancement together with the recent relaxation of the assumption of a rigid ECM [7], generalize the model and allow to properly take into account the physical properties of the host tissue in which tumor grows and evolves.

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[2] (i) adiabatic calorimetry test; (ii) tests for measuring autogenous and drying shrinkage and loss of mass; (iii) measures of final Young's modulus and tensile strength (possibly also their evolution with time); (iv) basic and drying creep tests.

The next step of this very stimulating research in the introduction of tumor vascularization and the modeling of angiogenesis. The expected overall outcome is a tumor growth model which takes into account neovascularization and allows to model drugs delivery; this would make it useful in predicting tumor proliferation and its response to different therapeutic regimens.

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