Chemistry and Materials Research, Vol.4 2013
Special Issue for International Congress on Materials & Structural Stability, Rabat, Morocco, 27-30 November 2013

Virtual materials for the prediction of concrete mechanical properties

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Abstract. Physical properties such as compressive strength and elastic moduli are of the utmost importance for the structural stability and design of cement-based materials. These properties are strictly related to the microstructure of the binder paste, which in turn varies in time, as a function of the hydration kinetics. Therefore, the development of the elastic properties and mechanical strength can in principle be controlled by affecting the microstructure and hydration kinetics. This can be achieved through an appropriate mix-design, which encompasses a careful selection of phase proportions, grain-size distribution, amount of water and aggregates, and use of additives. Changing such variables by a trial-and-error process can be extremely time consuming and has a significant impact in terms of resources employed. Moreover, a fully quantitative approach to the study of the cement microstructure and hydration kinetics requires significant efforts in terms of experimental testing, often encompassing analytical techniques such as X-ray diffraction, scanning electron microscopy and isothermal calorimetry, among others. In this contribution, an alternative quantitative characterization of the cement paste in time is illustrated, based on the numerical modeling of cement-based systems. Virtual cement pastes and mortars are generated using the software VCCTL (http://www.nist.gov/el/building_materials/inorganic/vcctl.cfm), using as input parameters the clinker phase composition, the water/cement ratio, and the size and shape distribution of the particles. The elastic moduli and compressive strength of such virtual samples is then computed from the developed microstructure by a finite element method. Extensive calibration and testing has been performed against experimental data, and the good agreement between the calculated and measured elastic and mechanical properties shows that VCCTL can be used as a truly predictive tool. Although experimental testing remains a fundamental aspect of concrete science, the coupling of experiments with computational methods provides a viable tool towards a knowledge-based mix design, with a potential reduction of costs and environmental impact.

1 Introduction

The current worldwide production of cementitious binders amounts to about three billion tonnes per year [1]. The production of structural elements represents the most important application for concrete and other cement-based binders, although these materials are fruitfully used in other fields, such as the restoration of historical buildings and the treatment and environmental remediation of contaminated soils, e.g. by stabilization/solidification techniques.

Regardless of the specific application, the fundamental properties of any cementitious material are those related to its mechanical properties, durability and workability. All these properties are strictly related to the thermodynamics, hydration kinetics and microstrctural configuration of the specific system.

The control of these properties by a modern, knowledge-based, rather than purely empirical approach, requires a fully quantitative investigation of the physical variables involved in the hydration and microstructural development of these materials, which can in turn result in significant efforts in terms of experimental time, overall cost, and use of raw materials.

In this contribution, an alternative characterization of the processes related to the microstructural development of cementitious binders, based on numerical simulations, is illustrated.

In particular, virtual cement pastes and mortars are generated by the VCCTL (Virtual Cement and Concrete Testing Laboratory) microstructural model, developed at the National Institute of Standards and Technology (NIST) to predict the hydration kinetics, elastic properties, and compressive strength of concrete binder materials.

The ability of VCCTL to predict selected mechanical properties of cementitious materials is tested by coupling a series of computer simulations and laboratory experiments, performed on industrial samples.

2 Materials and experimental methods

An ordinary Portland cement and a limestone Portland cement were used as test materials for this study. Cement pastes were obtained by mixing these cements with deionised water with different w/c values, and used to monitor the hydration kinetics by means of in-situ X-ray diffraction. In particular, the first 24 hours of hydration were investigated by this method, which allows the determination of the time-dependent phase composition of the hydrating cement paste.

Moreover, a series of mortar samples were obtained by the addition of a normalized siliceous sand. The elastic moduli and compressive strength of the mortars were experimentally determined at 1, 7 and 28 days of hydration. In particular, dynamic elastic moduli were obtained by recording the velocity of P-waves propagated through the samples.

The axial compressive strengths were measured by loading the mortars between parallel plates, having dimensions of 40 mm x 40 mm, until rupture.

3 Numerical model

The computational model VCCTL simulates the hydration kinetics and microstructural development of cement pastes, under a variety of curing conditions, based on the implementation of probabilistic rules to mimic the dissolution, diffusion, and precipitation of the phases present in the system [2]. The phase composition, w/c ratio and particle size distribution of the cement, as well as the amount, grading and physical properties of the aggregate (i.e. density, bulk and shear moduli) are supplied as input by the user. The output, at each simulated hydration time, is represented by a three-dimensional digital microstructure, in which each voxel is assigned a unique index, representative of a given cement phase (Figure 1).

The simulated microstructure is used as input for the calculation of the elastic moduli and compressive strength of the material, by a combination of finite element and effective medium theory calculations [3].

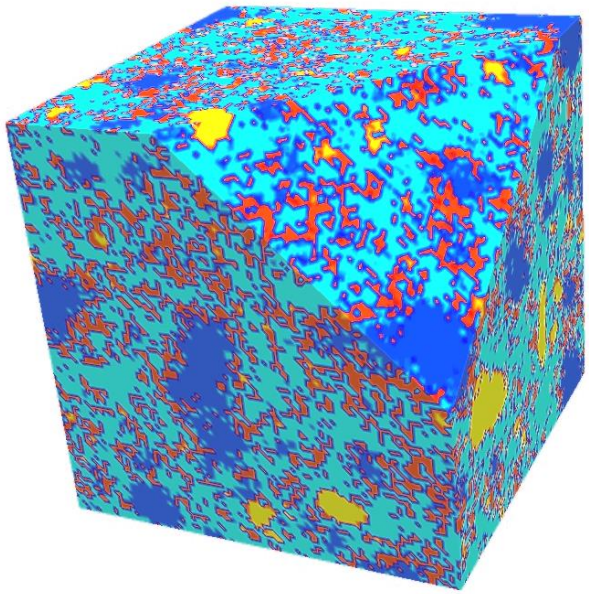

Figure 1. Example of virtual cement paste generated by VCCTL.

4 Results

VCCTL was used to simulate: a) the early age hydration kinetics of virtual cement pastes analogous to those investigated experimentally by in-situ X-ray diffraction; b) the development of mechanical properties of virtual mortar samples analogous to those used for the experimental testing.

The simulated rates of reaction of the phases present in the cement pastes are in good agreement with those measured experimentally. In particular, Figure 2 displays the good performance of VCCTL in reproducing the volume variation of both C-S-H and capillary porosity, which are crucial to the mechanical properties of the hardened paste.

The calculated compressive strength at 1, 7 and 28 days are displayed in Figure 3. The comparison with the measured values shows a very good agreement between predicted and actual compressive strengths, at any hydration time.

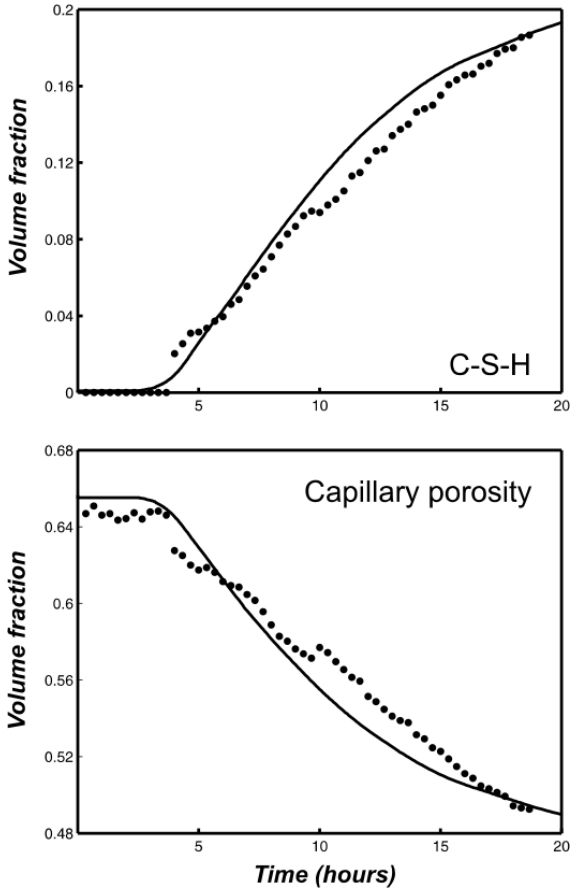

Figure 2. Comparison between the experimental (dots) and simulated (solid line) evolution of the volume fraction of C-S-H and capillary porosity for an ordinary Portland cement paste.

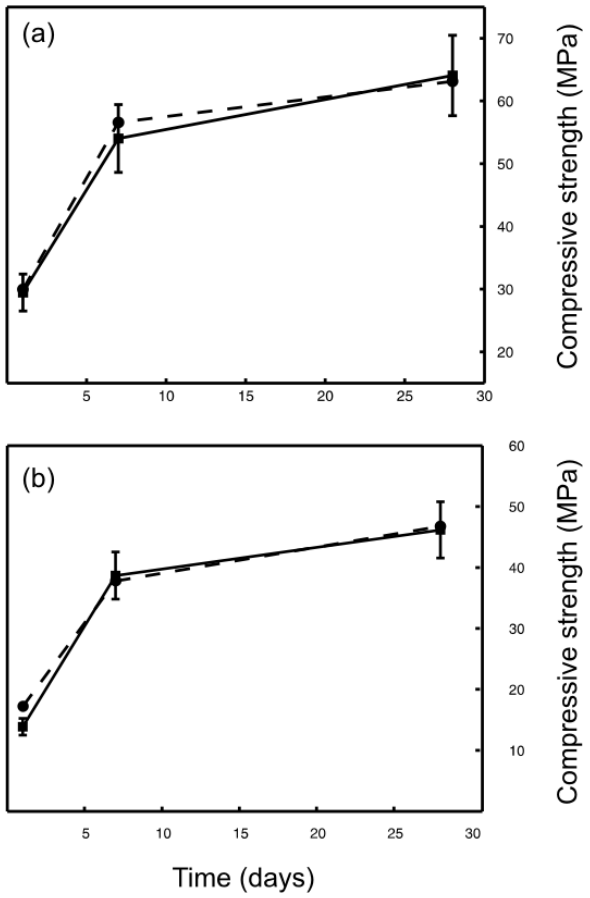

Figure 3. Comparison between the experimental (squares and solid lines) and simulated (circles and dashed lines) for an ordinary Portland cement mortar (a) and a limestone Portland cement mortar (b). Both simulations and experimental measurements were performed at 1, 7 and 28 days of hydration, and the lines included in the graphs only represent a visual aid. The vertical lines represent the range of uncertainty of the experimental measurements.

5 Summary and conclusions

In this study, the potential of the numerical model VCCTL to predict the hydration kinetics and mechanical properties of cement-based materials was tested. In particular, the properties of virtual materials generated by VCCTL were compared with those of real cement pastes and mortars.

The results have shown that the predicted hydration kinetics and mechanical properties of materials based on an ordinary Portland cement and a limestone Portland cement are in good agreement with the experimental determinations.

These results show that numerical models for predicting mechanical properties of mortar and concrete are a potentially powerful tool for a knowledge-based design of cementitious materials.

References

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