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Simulation of the hydration kinetics and elastic moduli of cement mortars by microstructural modelling

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ABSTRACT

The ability of the VCCTL microstructural model to predict the hydration kinetics and elastic moduli of cement materials was tested by coupling a series of computer simulations and laboratory experiments, using different cements. The novel aspects of this study included the fact that the simulated hydration kinetics were benchmarked using real-time measurements of the early-age phase composition during hydration by in situ X-ray diffraction. Elastic moduli are measured both by strain gauges (static approach) and by P-wave propagation (dynamic approach). Compressive strengths were measured by loading mortar prisms until rupture. Virtual samples were generated by VCCTL, using particle size distribution and phase composition as input. The hydration kinetics and elastic moduli were simulated and the numerical results were compared with the experimental observations. The compressive strength of the virtual mortars were obtained from the elastic moduli, using a power-law relation. Experimentally measured and simulated time-dependence of the major cement clinker phases and hydration product phases typically agreed to within 5%. Also, refinement of the input values of the intrinsic elastic moduli of the various phases enabled predictions of effective moduli, at different ages and different water-to-cement mass ratios, that are within the 10% uncertainty in the measured values. These results suggest that the VCCTL model can be successfully used as a predictive tool, which can reproduce the early age hydration kinetics, elastic moduli and mechanical strength of cement-based materials, using different mix designs.
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1. Introduction

In recent years, ever-improving computational resources have facilitated the study of the 3D microstructure of cementitious materials and its relationship with the physical properties, based on computer models that generate virtual materials and accurately simulate the mechanisms of microstructural development. An integrated approach that encompasses both measurement and modeling is fundamental to understanding experimental observations and to developing an advanced design of cement-based materials.

In this study, we test the capabilities of the Virtual Cement and Concrete Testing Laboratory (VCCTL) models [1–3] developed at the National Institute of Standards and Technology (NIST) to predict the hydration kinetics, elastic properties, and compressive strength of concrete binder materials. Similar validation studies have been published previously, but they have mostly focused on theoretical aspects of modelling the development of cement paste physical properties [4–7] and used indirect measurements of the hydration kinetics, based on the measurement of the degree of hydration [5,6], or empirical relations [4,8] rather than the measured variation of the phases present in the system, to calibrate the numerical results. In this work, we attempt to test the potential of VCCTL on mortar samples, as a predictive tool that can integrate experimental determinations for practical applications. For practical purposes, the comparison of simulated with measured variations of physical properties must be based on physical time rather than on the degree of hydration, which would require addi-

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Table 1
Oxide chemical composition measured by XRF for the cements and silica fume studied. The uncertainty associated with the measurements is less than 1%.

Cement	SiO_2	Al_2O_3	Fe_2O_3	MgO	CaO	Na_2O	K_2O	SO_3	Sum
C1	19.4	5.5	1.8	3.1	60.8	1.2	0.4	3.2	95.3
C2	20.6	4.6	2.5	1.7	65.5	–	0.7	2.5	98.1
C3	21.5	4.6	2.2	2.7	65.1	0.1	0.7	2.0	97.0
Silica fume	94.7	0.5	1.7	0.7	0.3	0.5	0.7	–	99.1

Table 2
Mineral phase proportions measured by XRD for the cements studied. Numbers in parentheses are estimated uncertainty expressed as percent by mass, based on the results of [11].

Phase	C1 (mass%)	C2 (mass%)	C3 (mass%)
Alite	60 (5)	58 (5)	58 (5)
Belite	19 (5)	13 (3)	17 (4)
Aluminate	8 (3)	8 (3)	9 (3)
Ferrite	4 (1)	7 (2)	3 (1)
Gypsum	2	1	1
Bassanite	3	1	4
Arcanite	1	–	–
Calcite	–	12	–
Periclase	2	–	2

tional measurements and additional sources of error. To achieve these aims, we focussed on the following aspects:

1. The accuracy of the simulated kinetics is benchmarked using in situ X-ray diffraction experiments coupled with Rietveld refinement, which returns the actual time-dependent phase composition of the hydrating cement paste. Both simulation and experiments were performed on three different cements, prepared at a different water-to-cement mass ratios (w/c) and cured at different temperatures.
2. A detailed evaluation of the intrinsic elastic properties relative to the individual phases is performed, based on a review of recent literature data. Particular focus is given to the elastic moduli of the C–S–H phase, whose values are extrapolated by a quantitative method.
3. Both static and dynamic elastic moduli, in addition to compressive strength, are measured for mortars with different composition and w/c, to establish the most appropriate method of measurement to be used for comparing actual and predicted properties.
4. A general working relationship between elastic moduli and strength is defined, based on different cements and w/c.

2. Materials and experimental methods

The starting materials used in this work were an ordinary CEM I 52.5R Portland cement and a limestone CEM II/A-LL 42.5R Portland cement[1] (hereafter C1 and C2). A third mix was obtained from a CEM I 52.5R cement blended with 5% and 10% by mass of silica fume (hereafter C3), and used to validate the relationship between elastic moduli and compressive strength. The solid oxide composition and mineralogical phase composition, as measured by X-ray fluorescence and X-ray diffraction, respectively, are shown in Tables 1 and 2. The particle size distributions, measured by laser scattering, are displayed in Fig. 1. The aggregate used for the mortar samples is a CEN normalized siliceous sand, having a mean solid density of 2620 kg/m^3, a bulk modulus of 33.2 GPa and a shear modulus of 24.5 GPa.

Mortar samples were used as reference test materials to study the accuracy of the computer model in predicting compressive strength and elastic moduli. The mortars were prepared by mixing 0.9 kg of cement with 2.7 kg of sand. The adopted mixing procedure and curing conditions were based on the EN 196-1 standard [10]. Three different w/c ratios were selected for C2 (0.5, 0.55 and 0.6), two for C1 (0.5 and 0.6) and one for C3 (0.5).

2.1. Compressive strength and elastic moduli measurements

Measurements of the mechanical and elastic properties were performed on mortar prisms with standard dimensions 40 mm × 40 mm × 160 mm. Compressive strength and elastic moduli measurements were performed at 1 d, 7 d, and 28 d of hydration for C1 and C2. For C3, compressive strengths were measured at 28 d 60 d of hydration, for additions of 5% and 10% by mass of silica fume.

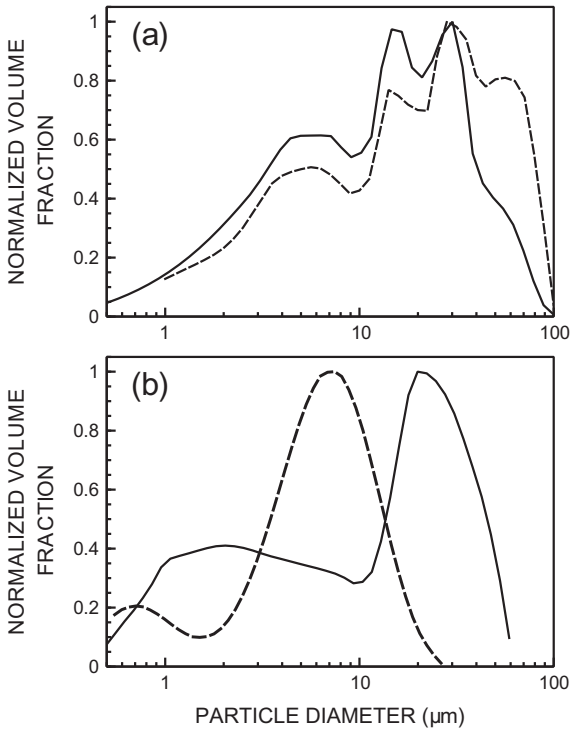

Fig. 1. Particle size distributions for the starting materials used in the study, displayed as probability density functions. (a) C1 (solid line) and C2 (dashed line) and (b) C3 (solid line) and silica fume (dashed line) Each curve is the average of three measurements, with the variability about the same as the thickness of the line.

The axial compressive strengths were measured by loading the mortar prisms between plates with dimensions 40 mm × 40 mm until rupture, as prescribed by the EN 196-1 standard [10].

The Young's modulus of each mortar prism was measured both by a dynamic and a static method. The dynamic measurements were made by a non-invasive method using the propagation of compressional waves (P-waves) through the sample. The dynamic Young's modulus E_d is calculated from the measured P-wave velocity according to

$$E_d = \frac{(1+\nu)(1-2\nu)}{1-\nu}\rho V_P^2 \quad (1)$$

where ν and ρ are the measured Poisson's ratio and density of the material, respectively. The Poisson's ratio of each mortar prism was measured by equipping the prisms with three strain gauges. Two gauges were placed on opposite faces in order to measure

[1] Cement types are defined based on the EN 197-1 standard [9].

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