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Proficiency analysis of VCCTL results for heat of hydration and mortar cube strength

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HIGHLIGHTS

- A virtual cement testing model is evaluated using traditional laboratory metrics.
- Cement heat of hydration and compressive strength predictions are compared.
- Twenty type I, II, and III reference cements are simulated.
- Virtual laboratory performance is better than many physical laboratories.
- Proscribed model input characterization methods are not required in this context.

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ABSTRACT

This paper establishes proof of concept that computational modeling can emulate the performance of physical testing laboratories for heat of hydration and compressive strength testing of type I, II and III portland cements. Simulation of 20 reference cements in a modified Virtual Cement and Concrete Testing Laboratory produced compressive strength and heat of hydration results with mean absolute differences of 5.0% and 6.5% compared to experimental data obtained from the same cements through the proficiency sample program of the Cement and Concrete Reference Laboratory. The findings suggest computational modeling can be a practical, reliable and economical alternative to physical testing for portland cements.

1. Introduction

The Virtual Cement and Concrete Testing Laboratory (VCCTL) is a three dimensional, micro scale, cellular automata [1,2] model for the microstructural hydration and mechanical properties of portland cement based materials, and is the product of three decades of research and development [3–8]. Virtual materials are created by the user based on careful characterization of raw material properties, and used to construct a digital image approximation of an unhydrated cement paste microstructure. Hydration of the digital microstructure produces results that emulate physical testing, without the associated time or labor requirements.

Validations of the VCCTL and its predecessor, Cemhyd3D, have examined the sensitivity of the model to variation in inputs as well as errors associated with the digital image approximation method [9], and compared simulated results to plastic and hardened properties of Cement and Concrete Reference Laboratory (CCRL) reference cements [10,11]. Each of these studies focused on detailed characterization of two cements, but performed limited numbers of simulations. The results for each cement were calibrated by modifying a time-per-cycle constant, to produce the best agreement with experimental data. Robust model validations require reference cements with well characterized raw and hardened properties. CCRL maintains a proficiency sample program (PSP), in which homogenized cement samples are distributed to 1100 laboratories. Laboratories test for X-ray fluorescence (XRF) mineral oxide composition [12], phase composition per the Bogue equations, specific surface area according to Blaine air-permeability method [13], and compressive strength of mortar cubes. CCRL distributes samples in pairs to identify laboratory bias [14], and reports the results from all laboratories for each pair, including calculations of the precision of the different test methods [15].

The VCCTL is computationally expensive; a 28 day simulation requires two hours nominally on conventional computing

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hardware. We ported the code to the University of Florida's HiperGator supercomputing cluster and developed custom input generation and output parsing routines, enabling parallel execution of hundreds of thousands of simulations for the research project supporting this paper. This study simulated each reported laboratory measurement of cement composition and fineness for 20 CCRL cements to produce 10,000 virtual heat of hydration and mortar compressive strength tests in less than 48 h of real time. CCRL measurements of heat and compressive strength from the same cements provided validation references for virtual test results. The flow of inputs and outputs for a single simulation included several discrete operations, summarized in Fig. 1.

2. VCCTL inputs and function

The phase composition and particle size distribution (PSD) of cement are primary inputs for VCCTL simulations. Volume fractions, surface area fractions and two dimensional spatial distribution data for the four primary cement phases (C_3S, C_2S, C_3A, and C_4AF) are obtained via scanning electron microscopy (SEM) combined with energy dispersive X-ray spectroscopy (EDS). Phase

Table 1
Summary of measured particle size distributions, with 10th, 50th and 90th percentile particle diameters in microns.

CCRL ID	d10	d50	d90
176	2.2	10.4	22.6
177	2.1	11.1	31.5
178	2.1	11.0	27.1
179	2.3	10.6	23.3
180	1.9	11.1	30.3
181	2.0	11.1	32.3
182	2.7	12.0	29.3
183	2.2	11.0	25.4
184	2.3	11.8	29.8
185	2.8	11.7	29.8
186	2.4	11.2	26.8
187	2.2	11.5	26.8
188	2.4	12.1	32.3
189	2.4	11.0	23.4
190	2.7	11.2	24.4
192	1.8	11.8	33.2
194	3.1	11.4	25.9
195	1.8	11.4	34.7
196	1.6	10.2	25.7
198	2.1	11.3	33.3

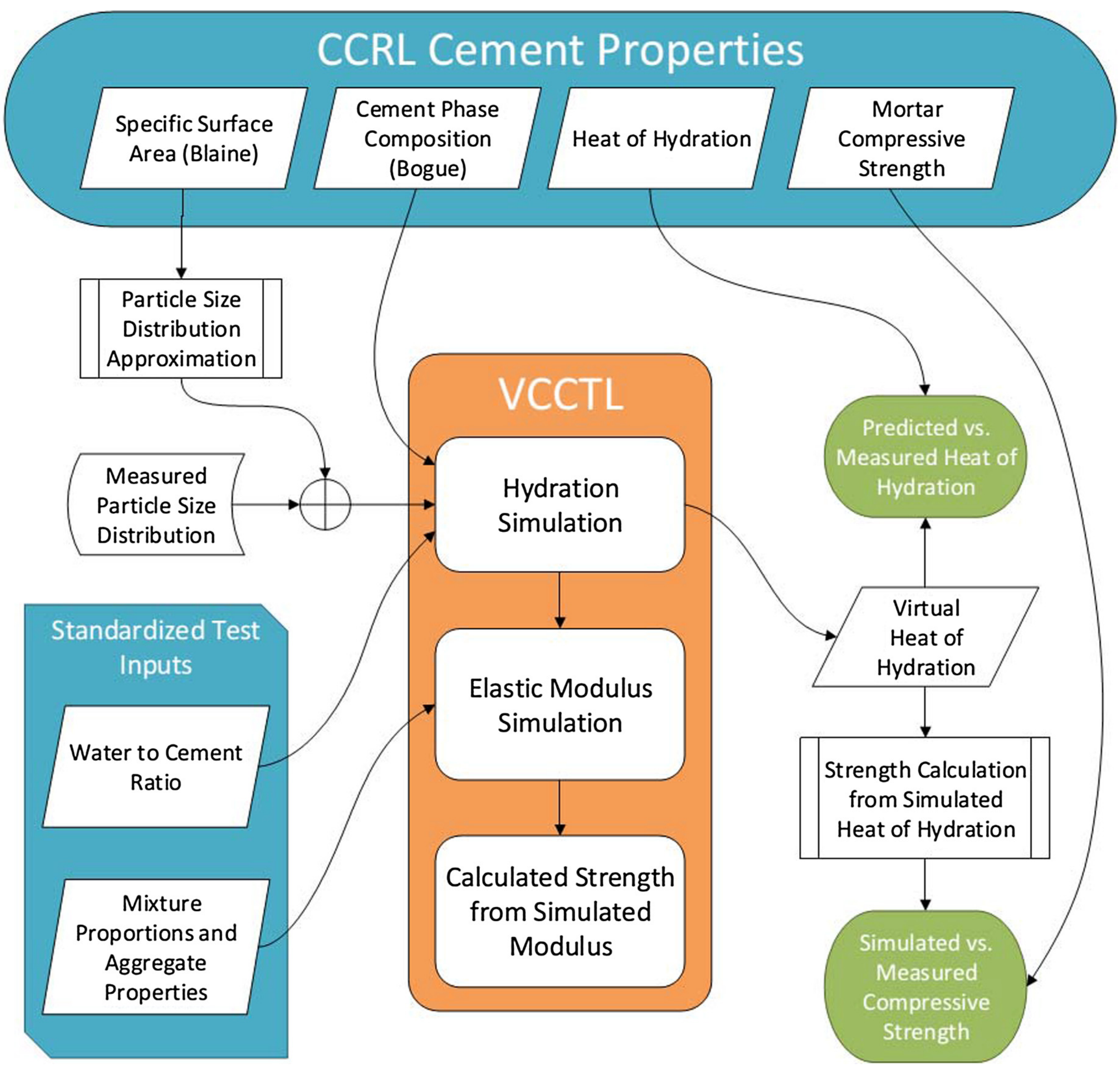

Fig. 1. Data flow for a single simulation performed in this study.