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ORIGINAL ARTICLE

Modeling the influence of limestone addition on cement hydration

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Abstract This paper addresses the influence of using Portland limestone cement "PLC" on cement hydration by characterization of its microstructure development. The European Standard **EN 197-1:2011** and Egyptian specification **ESS 4756-1/2009** permit the cement to contain up to 20% ground limestone. The computational tools assist in better understanding the influence of limestone additions on cement hydration and microstructure development to facilitate the acceptance of these more economical and ecological materials. μic model has been developed to enable the modeling of microstructural evolution of cementitious materials. In this research μic model is used to simulate both the influence of limestone as fine filler, providing additional surfaces for the nucleation and growth of hydration products. Limestone powder also reacts relatively slow with hydrating cement to form monocarboaluminate (AFmc) phase, similar to the mono-sulfoaluminate (AFm) phase formed in ordinary Portland cement. The model results reveal that limestone cement has accelerated cement hydration rate, previous experimental results and computer model "cemhyd3d" are used to validate this model.

1. Introduction

The use of blended cements, especially those containing limestone, seems to have many technical and economic benefits [1–3]. The beneficial effect of limestone cement is questionable, pervious researches reveal that limestone cement has several impacts on the mechanism and kinetics of cement hydration; the filler effect that accelerates the hydration of Portland Clinker grains [4], the formation of carboaluminate [5,6] and the modification of the microstructure [7].

In this paper, the μic model [9] has been used to simulate the effect of limestone cement on microstructure and hydration products and it will be extended to consider the above influences of limestone fillers on cement hydration [10]. The flexibility of μic model enables the easy inclusion of more cement phases and hydration conditions in the simulation. Therefore, this model is used in this paper to predict the influence of limestone cement on the hydration behavior.

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2. Background of cement hydration models

Researchers have developed many microstructures of models for cement and concrete over the past years. At the level of cement paste, Jennings and Johnson [11] developed a continuum model representation, based on spherical cement (C_3S) particle enveloped by hydration shells of C–S–H gel, whose thickness increases over time. Calcium hydroxide (CH) crystals were nucleated and grown in a continuum pore space. Van Breugel [12] developed a similar microstructure simulation model that is called HYMOSTRUC [13]. As with the Jennings and Johnson model [11], HYMOSTRUC uses various mass and volume balance rules to accommodate microstructural changes due to dissolution and precipitation of various phases. The computer model CEMHYRD3D was originally developed in National Institute of Standard and Technology (NIST) by Bentz and Garboczi [14] to represent the hydration process of Portland cement two-dimensionally. It was later enhanced into a 3-D computer model and the reaction of other cementitious materials, such as fly ash and silica fume are incorporated Bentz [15]. In 2005, this computer program is updated to include the effect of incorporation of different particles such as slag, inert filler, and calcium carbonate on cement hydration process [16]. The recently developed μic (pronounced ''mike'') microstructural modeling platform is derived from an earlier model developed by Navi and Pignat [17]. The new support libraries developed for the platform allow μic to model the hydration of millions of cement particles, needed to realistically represent the particle size distributions of cements, considering neighborhood of each particle into account.

2.1. Advantage of using μic model over other microstructural models

There are several important aspects of cement hydration that are still not well understood. The cement hydration model ''CEMHYD3D'' is a reliable model for cement hydration, this simulation of cement particle (composition and distribution of phases) using the real images of cement and real particle size distribution of cement particles, makes this simulation program a powerful tool for characterization of microstructure development in cement based materials. However, input data for this simulation program require special and very advanced techniques for the measurement of PSD of cement and image analysis of SEM-X-ray images. On the other hand, μic model needs simple experimental procedure to characterize cement particles such as particle size distribution, the kinetic and stoichiometry of cement hydration reaction and it is well suited to investigate various phenomena at the microstructure and it allows user to fully customize the simulation [18,19]. The model was designed to allow users to input and test their own ideas in simulations, making experimentation with the model possible. This unique feature of μic can make it a feasible tool for understanding cement chemistry. Furthermore, the model has been designed in a programmer friendly manner, with object-oriented programming in Java. Java contains all the necessary features and built-in libraries to support advanced development [20]. In this model, particle size distribution and the phase composition of the powder are defined, it can be chosen from library of plugins of the most commonly used models or create external plugin for new models. In order to allow simulation of different types of materials, including cements with different phases; the presence of other materials such as fillers and mineral additives μic allows the definition of different materials for the simulations. All the reactants, products and possible intermediate products are defined as materials. For example, in the system prescribed in Fig. 1, Alite, Aluminate, Limestone, CH, Inner C–S–H, Outer C–S–H and Filler C–S–H are the materials defined. As μic simulates the evolution of the geometry, the proportions of various materials involved in the reactions are defined in terms of volumes. These volumes can be calculated using the stoichiometry of the reaction and the base value of the density of individual materials. Plugins can be used to control the rates of reactions for individual particles. The reaction rate of a particle can depend on its own condition, its neighborhood or global values such as time. Reactions can also be defined to be active only under certain conditions. For example, the reaction of a mineral additive may be defined to occur only after a defined minimum amount of an alite has reacted.

3. Simulation mechanism

The Simulation mechanism is implemented to cover the physical and chemical effect of limestone substitution on cement hydration. The limestone substitution from 5% to 20% is included in μic model, where the filler effect can be evaluated; while, some modification is made on the model to simulate its chemical reactivity, where the AFm can be converted into AFmc in the presence of calcium carbonate, as reported in the literature [8].

3.1. Simulating the filler effect of lime stone

Some researches claimed that the main effects of limestone powder are of physical nature [20–22]. It causes a better packing of cement granular skeleton and a larger dispersion of cement grains. Others concluded that limestone powder acts as the crystallization nucleus for the precipitation of CH. These simultaneous effects accelerate production of the hydration of cement grains [23]. Therefore, the influence of limestone as filler on cement hydration was modeled using μic model as ''fine filler''. Also, the effect of different percent of limestone is varied to cover the range of EN and ES specification, 5%,

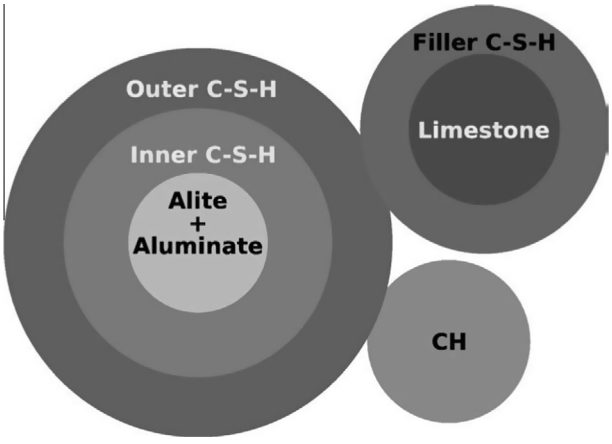

Figure 1 Example of different materials and particle types defined in a simulation.