Construction and Building Materials 166 (2018) 130–140

Contents lists available at ScienceDirect

Construction and Building Materials

journal homepage: www.elsevier.com/locate/conbuildmat

Analysis of hydration and strength optimization of cement-fly ash-limestone ternary blended concrete

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HIGHLIGHTS

- Simulate the hydration of cement-fly ash-limestone ternary blends.
- Consider interactions among cement hydration, fly ash reaction, and limestone reaction.
- Evaluate the strength development of ternary blended concrete.
- Find the optimum combinations of cement, fly ash, and limestone.

ARTICLE INFO

Article history:
Received 25 September 2017
Received in revised form 6 January 2018
Accepted 9 January 2018

Keywords:
Fly ash
Limestone
Hydration
Model
Strength optimization

ABSTRACT

Limestone powder improves concrete early-age strength while fly ash improves concrete late-age strength due to its pozzolanic reaction. The optimal mixture of cement, fly ash, and limestone is crucial for material design of ternary blended concrete. This research presents a simulation program for evaluating the hydration and strength optimization of ternary blended concrete. The simulation program begins with a kinetic hydration model which simulates the hydration of cement-fly ash-limestone ternary blends. The hydration model considers the mutual effects among reactions of cement, fly ash, and limestone by means of the contents of calcium hydroxide and capillary water. The individual reaction degrees of components of ternary blends are calculated from the hydration model. Furthermore, the compressive strength growth of hydrating ternary blended concrete is calculated by means of gel-space ratio and Powers' strength theory. Finally, based on parameter studies, the optimal combinations of cement, fly ash, and limestone at different ages are determined. The proposed numerical procedure is valuable for making composite cements as it pertains to compressive strength and environment regulations.

1. Introduction

Fly ash and limestone are more and more utilized in producing high performance concrete in the modern concrete industry. Fly ash and limestone present different effects on strength development of concrete. Fly ash can enhance the long-term age strength of concrete due to a pozzolanic reaction while limestone can enhance the young-age strength of concrete because limestone can accelerate cement hydration. When limestone and fly ash are used together, due to the synergy effect, the individual deficiencies can be compensated [1].

Abundant experimental and theoretical studies have been performed on cement-fly ash-limestone ternary blended concrete. Weerdt et al. [2] found that the additional aluminum from the fly ash pozzolanic reaction amplified the chemical reaction of limestone powder. Scholer et al. [3] found that a limestone content of 2–5% leads to the stabilization of monocarbonate and ettringite which can increase the volume of hydration products and increase the strength. Bentz et al. [4] found that nano-limestone can accelerate the early age hydration of cement and reduce the setting time of fly ash blended concrete. Thongsanitgarn et al. [5,6] found that cement-fly ash-limestone ternary blended concrete presents higher strength compared to cement-fly ash binary concrete. Limestone with finer particle size is effective to speed up cement-fly ash hydration. Celik et al. [7,8] found that concrete containing high volume fly ash and limestone has high workability, high late age strength, high chloride resistance, and low global warming potential. Ghrici et al. [9] found that natural pozzolana did not change the sulfate resistance of limestone cement, natural pozzolana improved hydrochloric acid resistance, and limestone improved sulfuric acid resistance.

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https://doi.org/10.1016/j.conbuildmat.2018.01.058

Compared with abundant experimental studies of ternary blended concrete [2–9], theoretical studies of ternary blended concrete are relatively limited. Gao et al. [10] put forward an analytical modeling about the hydration of cement-slag-limestone blends. The local water to cement ratio and water transport in the interfacial transition zone was simulated. Maekawa et al. [11] proposed a computational platform which can assess the time-dependent mechanics and durability mechanics of concrete structures. The couplings among hydration, mass transport, and damage evolution were considered. However, Gao et al. [10] and Maekawa et al.'s [11] studies do not consider the chemical reaction of limestone in ternary blended concrete. Bentz [12] proposed a model which simulated the dilution, nucleation, and chemical effects of limestone additions in cement-limestone binary blends. Weerdt et al. [13] made a thermodynamic modeling of hydration of cement-fly ash-limestone ternary blends. The volumetric phase fractions of the hydrating paste were calculated using Gibbs Energy Minimization Software (GEMS) program. However, the thermodynamic modeling in the Weerdt et al. study [13] mainly focuses on the chemical aspects of ternary blended concrete. Regarding the optimal combinations of cement, fly ash, and limestone in ternary blended concrete, current models [10–13] still do not cover this point.

To avoid the flaws of current studies, this research presents a hydration based simulation program to assess the strength growth and optimal combinations of ternary blended concrete. The strength is evaluated considering the influences from reactions of cement, fly ash, and limestone. The optimal combinations are determined based on parameter studies of the hydration-strength integrated model.

2. Simulation of the hydration of cement-fly ash-limestone ternary blends

2.1. Simulation of the hydration of cement-fly ash binary blends

Our previous studies [14–16] presented a kinetic hydration model for concrete containing fly ash. This kinetic hydration model includes three sub-models, i.e. model for hydration of cement, model for reaction of fly ash, and model for mutual effects between reactions of cement and fly ash. The cement hydration model considers the kinetic stages involved in the hydration of cement, such as initial dormant stage, chemical-reaction related stage, and diffusion related stage. The cement hydration model also considers the water withdrawal on account of the lack of capillary water regarding high strength concrete. The equation of cement hydration is simplified and written as follows [14–16]:

$$\frac{d\alpha}{dt} = f(k_d(T), D_e(T), k_r(T), r_0) * C_{w-free} * (S_w/S_0) \tag{1}$$

where $\frac{d\alpha}{dt}$ is rate of hydration, k_d is rate of coefficient in initial dormant stage, T is curing temperature, k_r is rate of coefficient in reaction related stage, D_e is rate of coefficient in diffusion related stage, r_0 is unreacted cement particles radius, S_w means the effective contact area between the surrounding capillary water and cement particles [14–16], S_0 means the total area if cement hydration products progress unconstrained, C_{w-free} is capillary water content ($C_{w-free} = \left(\frac{W_0 - 0.4C_0\alpha}{W_0}\right)^r$ where C_0 is cement content in concrete mixing proportions, W_0 is the content of water in the proportions of concrete mix, r ($r = 2.6 - 4\frac{W_0}{C_0}$) is an empirical factor considering the approachability of capillary water from outer hard shell to inner anhydrous part of cement particles).

The rate coefficients k_d, k_r, and D_e can be determined based on compound compositions of cement [14–16]. The effect of temperature on rate of hydration of cement is recognized as following Arrhenius's law [14–16]. For high strength concrete, degree of hydration is reduced due to the withdrawal of capillary water. The water withdrawal mechanism is considered through (S_w/S_0) and C_{w-free} in Eq. (1). (S_w/S_0) describes the decrease in contact area between cement particle and ambient capillary water, and C_{w-free} describes the decrease in capillary water concentration.

Similarly with hydration of cement, fly ash reaction also consists of three stages [14–16], initial dormant stage, chemical-reaction related stage, and diffusion related stage. In addition, fly ash reaction is dependent on calcium hydroxide content in cement-fly ash binary blends. The equation of fly ash reaction is simplified written as below [14–16]:

$$\frac{d\alpha_{FA}}{dt} = f(k_{dFA}(T), D_{eFA}(T), k_{rFA}(T), r_{FA0}) * \frac{m_{CH}(t)}{P} \tag{2}$$

where $\frac{d\alpha_{FA}}{dt}$ is fly ash reaction rate, k_{dFA} is rate of coefficient in initial dormant stage of fly ash, D_{eFA} is rate of coefficient in diffusion related stage of fly ash, k_{rFA} is rate of coefficient in reaction related stage of fly ash, r_{FA0} is unreacted fly ash particles radius, $m_{CH}(t)$ is the content of calcium hydroxide, P is fly ash content in proportions of concrete mix.

The time-dependent cement or fly ash reaction degrees can be calculated using the cement-fly ash binary hydration model. In addition, the thermal properties, mechanical properties, and durability of fly ash blended concrete can be evaluated using reaction degree of individual component of binders. The cement-fly ash binary hydration model is multiply validated using experimental data for concrete with various proportions of mix and curing conditions. However, because the cement-fly ash binary hydration model does not consider the effect of limestone, binary hydration model cannot analyze the hydration of cement-fly ash-limestone ternary concrete.

2.2. Limestone powder reaction mode

Bentz [12] reported that the addition of limestone presents dilution, nucleation, and chemical effects on cement hydration. The dilution effect happens when limestone substitutes partial cement, cement content decreases and water to cement ratio increases correspondingly. The nucleation effect is the fact that limestone may work as a nucleation site of hydrating cement. Hydration of cement can accelerate due to the nucleation effect. The chemical effect is the formation of monocarboaluminate due to the limestone reaction in preference to a monosulfoaluminate.

In this research, the dilution effect of limestone powder can be considered by $\frac{C_0}{W_0}$ term in C_{w-free} of Eq. (1). Regarding the nucleation effect, Maekawa et al. [11] and Wang [16] proposed that the nucleation effect of limestone relates to the ratio of surface area of cement particles to that of limestone powder. The nucleation effect indicator of limestone powder can be written as follows [16]:

$$L_r = \frac{LS_0 * S_{LS}}{C_0 * S_C} \tag{3}$$

where L_r denotes the indicator of the nucleation effect from limestone addition, LS_0 denotes the limestone mass in proportions of concrete mix, S_{LS} denotes the specific surface (Blaine) of limestone, and S_C denotes the specific surface (Blaine) of cement. Maekawa et al. [11] reported that the nucleation effect of limestone is significant in the reaction related stage and the diffusion related stage. In our former study [16], based on the experimental data of hydration degree of cement in cement-limestone binary blends, Wang [16] proposed that the nucleation effect of limestone powder can described as follows: