Computer modeling of the replacement of "coarse" cement particles by inert fillers in low w/c ratio concretes Hydration and strength

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Computer modeling of the replacement of "coarse" cement particles by inert fillers in low w/c ratio concretes Hydration and strength

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Abstract

In concretes with water-to-cement (w/c) ratios below about 0.38, a portion of the cement particles will always remain unhydrated due to space limitations within the material. Thus, in many of the high-performance concretes currently being produced, cement clinker is in effect being wasted. This communication examines the possibility of replacing the coarser fraction of a cement powder by an inert filler, to conserve cement without sacrificing material performance. Using the NIST CEMHYD3D cement hydration model, it is demonstrated that for "initial" w/c ratios of 0.25 and 0.30, a portion of the coarser cement particles can be replaced by inert fillers with little projected loss in compressive strength development. Of course, the optimal replacement fraction depends on the initial w/c ratio, suggesting that blended portland/inert filler cements need to be produced with the end concrete mixture proportions in mind. This further implies that a cement/inert mixture of specific proportions will only perform optimally in a limited range of concrete mixture proportions.

Keywords: Blended cements; Compressive strength; Hydration; Modeling; Particle sue distribution

1. Xntroduction

Cement manufacturers are being placed under ever more restrictive regulations regarding emissions and the environment. Still, most US plants are producing cement at near capacity due to the large demand by the concrete construction community. Much of this cement is being utilized in the newer high-performance low water-to-cement (w/c) ratio concretes. Unfortunately, as noted by Taylor [1], for w/c ratios below about 0.38, complete hydration of the cement will not occur. In fact, a portion of the relatively costly cement particles will remain unhydrated and thus serve only as reinforcing fillers. Cement is a rather expensive filler material, so it should be of great cost benefit to the industry to find a solution to this problem.

Previously [2,3], it has been suggested that some of the energy costs related to grinding could be saved by using coarser cements in these low w/c ratio high-performance concretes. In this paper, an alternative solution will be explored, namely, the replacement of a fraction of the coarse cement particles by an inert (and inexpensive) filler. Computer modeling studies using the NIST cement hydration and microstructure development model (CEMHYD3D) will be used to contrast the predicted hydration and compressive strength development of systems with filler replacement to those where the complete original cement particle size distribution (PSD) is used (no filler replacement). It should be noted that the technology of manufacturing a cement with only the coarse fraction replaced by limestone (or another basically inert filler) or a cement with a reduced maximum particle size would need to be more fully developed. But, such technology could provide benefits in reduced energy and raw material consumption and reduced emissions of carbon dixoide per ton of concrete binder produced.

2. Modeling approach

All simulations were conducted using version 2.0 of the NIST CEMHYD3D program [4,5] and the new prototype

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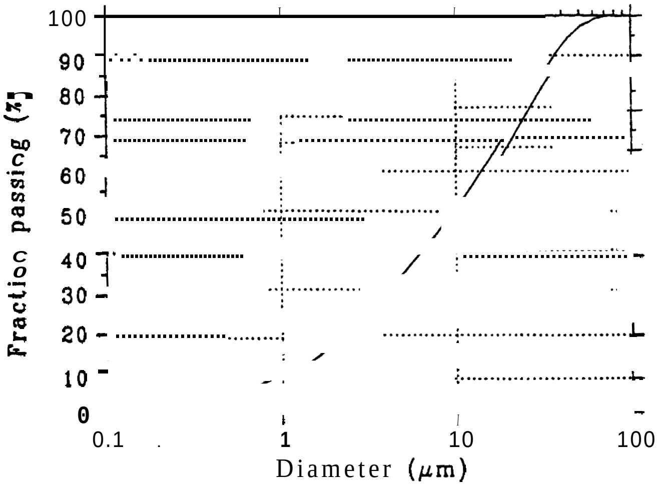

Fig. 1. Measured PSD for Cement 135 used in the computer modeling [7].

Virtual Cement and Concrete Testing Laboratory Web-based interface [6]. Three-dimensional starting microstructures were created based on the measured PSD and phase composition of Cement and Concrete Reference Laboratory proficiency cement sample number 135, issued in January of 2000 [7]. Six different microstructures were examined, three with a water-to-solids (w/s) mass ratio of 0.25 and three others with a w/s of 0.30. For the w/s = 0.30 systems, one system had zero replacement and the other two had the coarsest 14.5% and 22.3% mass fraction of the cement particles replaced by inert fillers, respectively. For the w/s = 0.25, in addition to the base system with no replacement, replacement levels of 20.5% and 30.8% by mass were investigated. The complete measured PSD for Cement 135 is provided in Fig. 1. Typically, we are replacing all the particles larger than 20–27 μm in diameter by inert (non-reactive) particles. All systems were then hydrated for 4000 dissolution/reaction cycles of the hydration model (representing about 200 days of real hydration time) [7]. Comparisons were then made on the basis of the development of degree of hydration with time and compressive strength development predicted using Power's gel–space ratio concept [1,4] with a strength prefactor (the strength achieved for a gel–space ratio of 1.0) of 100 MPa for ASTM C109 mortar cubes [7]. By using a constant strength prefactor, we are implicitly assuming that the contribution of the inert filler to the compressive strength of the composite is the same as that of the unreacted cement particle cores. We will then be evaluating the ability of the smaller cement particles to hydrate more completely to compensate for the original hydration provided by the now missing coarser cement particles. Due to local space limitations within the microstructure (real and computer modeled), the smaller cement particles may not be able to totally compensate far the l of the coarser ones.

3. Results and discussion

The model predictions for the two systems containing filler with w/s = 0.25 are contrasted against those for the system with no filler in Figs. 2 and 3. In both cases, it can be seen that while the systems with the inert filler replacing the

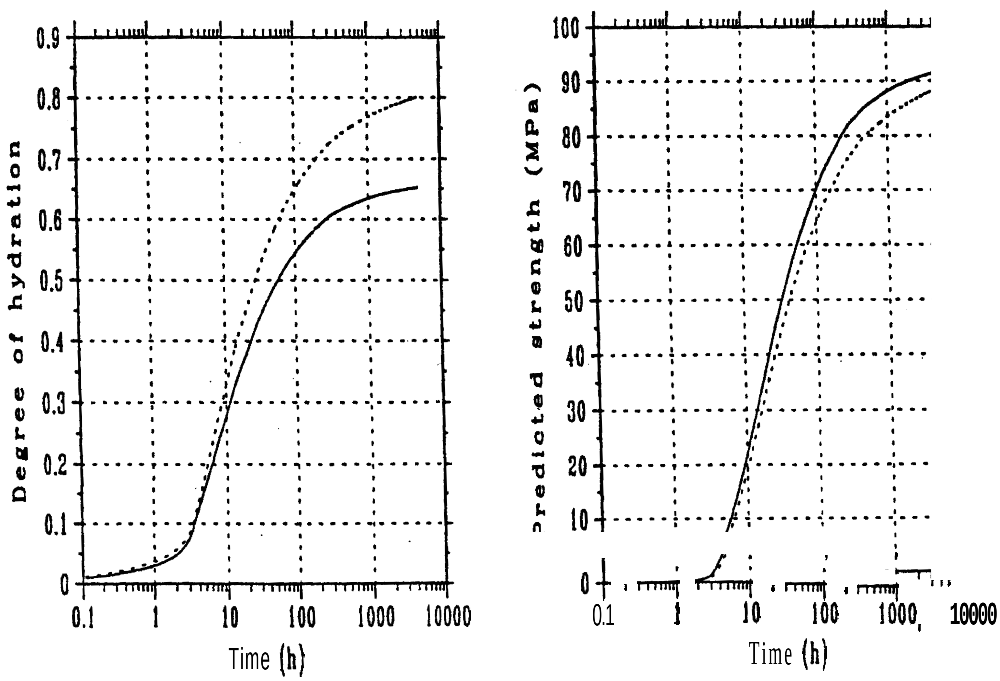

Fig. 2. Predicted degree of hydration and compressive strength development for base w/c = 0.25 system and system with the coarsest 20.5% of cement particles replaced by inert filler. Solid line is the original system and dotted line is the system with 20.5% replacement.

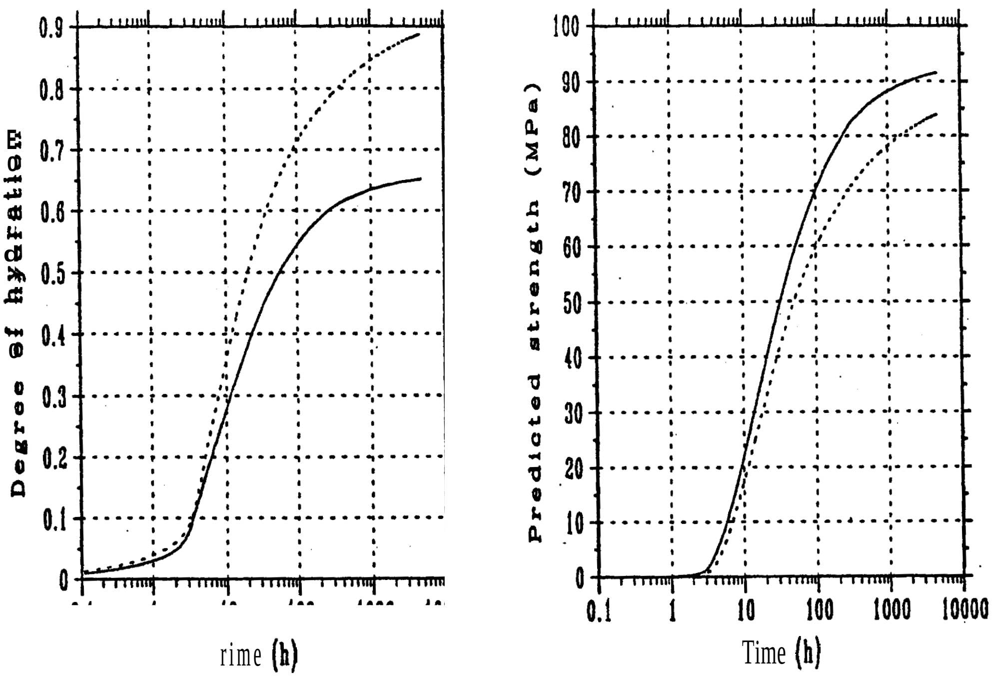

Fig. 3. Predicted degree of hydration and compressive strength development for base w/c = 0.25 system and system with the coarsest 30.8% of cement particles replaced by inert filler. Solid line is the original system and dotted line is the system with 30.8% replacement.

coarser cement particles actually hydrate more completely (due to their higher effective w/c ratio), their compressive strength development is less than that of the control (no filler) system. These strength differences are highlighted in Fig. 4, which shows the projected strength reduction vs. time for the two replacements considered in this study. It is observed that the compressive strength reduction is maximal after about 12 days and then decays towards zero, as the "filled" systems continue to hydrate due to their overall higher w/c ratio. For the 20.5% replacement, the maximum projected reduction is only 6 MPa (or about 7%), which may be quite acceptable from a performance standpoint. After 28 days, the standard age for acceptance testing, the projected reductions are about 5 MPa (6%) and 11 MPa (13%) for the 20.5% and 30.8% replacement levels, respectively.

Similar results were obtained for the w/s = 0.30 systems. Thus, only the strength differential plot is provided here (in Fig. 5). Here, the maximum difference in Compressive strength is observed to occur at a slightly later age, 18 to 40 days, since with a higher w/c ratio, the control system is able to maintain a significant hydration rate for a longer period of time. After 28 days, the projected reductions in compressive strength are about 6 MPa (7%) and 11 MPa (13%) for the 14.5% and 22.3% replacement levels, respec-

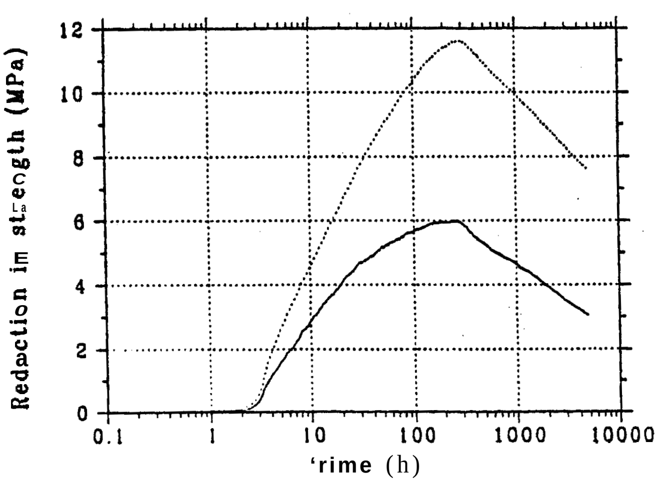

Fig. 4. Predicted reduction in compressive strength due to coarse cement particle replacement for Cement 135 with w/s = 0.25. Solid line is the reduction with 20.5% replacement level and dotted line is the reduction with replacement level of 30.8%.

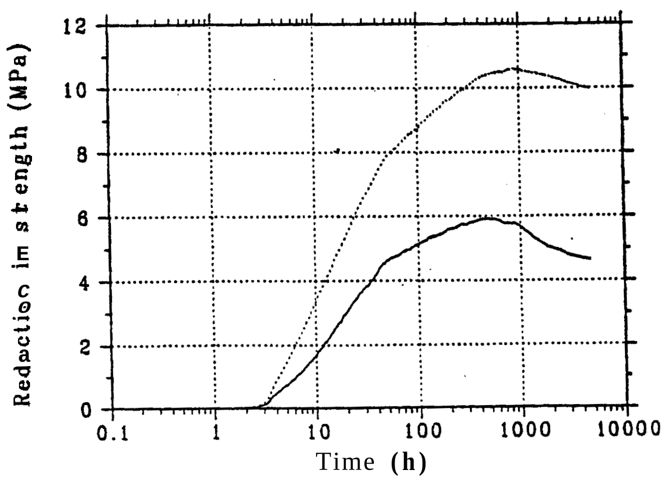

Fig. 5. Predicted reduction in compressive strength due to coarse cement particle replacement for Cement 135 with w/s = 0.30. Solid line is the reduction with 14.5% replacement level and dotted line is the reduction with replacement level of 22.3%.

tively. Therefore, in this case, only a 15% replacement level of the coarsest cement particles may be acceptable. In principle, the lower the "initial" w/c (w/s) ratio, the greater the possible replacement level for the coarse particles without detrimentally reducing the compressive strength. The preliminary results presented here would suggest maximum replacements of 15% and 20% for w/c ratios of 0.30 and 0.25, respectively. Thus, the optimal replacement level is seen to be a strong function of the ultimate concrete mixture proportions. This implies that a given replacement level would only provide "optimal" performance in a limited range of concrete mixture proportions.

Regarding the appropriate filler material to use, coarse limestone particles may offer one possibility. Studies [8,9] have indicated that limestone particles are only mildly reactive within the cement system, producing small amounts of a monocarboaluminate Ah-type reaction product at longer hydration times. With relatively coarse limestone particles in these lower w/c ratio concretes, these long-term reactions may be further limited by the same space limitations that prohibit all of the coarser cement particles from hydrating completely. The incorporation of limestone–cement reactions into the NIST CEMHYD3D computer model is the subject of current research, so that this reactivity will be examined quantitatively by both experiments and computer modeling in the future.

4. Conclusions

It has been demonstrated that in low w/c ratio concrete, replacement of the coarsest cement particles by inexpensive inert fillers should result in only a small (7% or so) reduction in compressive strength development. In concrete with an initial w/c ratio between 0.25 and 0.30, replacement levels are likely limited to about 15% to 20%; for higher replacements levels, substantial (> 10 MPa or 10%) losses in compressive strength were projected. The optimal replacement level will depend on the actual concrete mixture proportions being used in practice. This implies that a blended inert/cement mixture of specific proportions will only be optimal for a finite range of high-performance concrete mixture proportions.

Acknowledgments

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