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CIVIL & ENVIRONMENTAL ENGINEERING | RESEARCH ARTICLE

Optimization of ultra-high performance concrete, quantification of characteristic features

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Abstract: An optimization experimental program was designed to identify a desired balance of key mix design parameters for an economical ultra-high-performance concrete (UHPC) mixture. The following mix design parameters were evaluated: superplasticizer content, coarse-to-fine aggregate ratio and steel fiber volume fraction. The values of packing density, water film thickness and excess paste film thickness were calculated considered in the optimization experimental program. The trends in the effects of packing density, water film thickness and excess paste film thickness on compressive strength and fresh mix flow were investigated. The results were used to identify viable ranges of these defining characteristics for the category of UHPC. Response surface analysis of the fresh mix flow and the hardened concrete compressive strength test results led to identification of the optimum values of mix design parameters. The optimum mix was found to produce a desired balance of fresh mix flow and hardened concrete compressive strength.

Subjects: Concrete & Cement; Structural Engineering; Transportation Engineering



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PUBLIC INTEREST STATEMENT

The work reported in this paper focused on the development of ultra-high performance concrete (UHPC) mix designs (Compressive strength more than 150 MPa) incorporating coarse aggregates for achieving improved economics. The UHPC mix designs were described using some alternative parameters, including packing density, water film thickness and excess paste film thickness. A response surface design of experiments was developed for identifying the optimum values of coarse-to-fine aggregate weight ratio, superplasticizer content and steel fiber volume fraction in an UHPC mix with a specific cementitious binder composition, binder content and water-to-binder ratio. Response surface analysis of the fresh mix flow and the hardened concrete compressive strength test results led to identification of the optimum values of mix design parameters. The optimum mix was found to produce a desired balance of fresh mix flow and hardened concrete compressive strength (68 cm and 223 MPa, respectively).

Keywords: ultra-high-performance concrete; mix design; packing density; water film thickness; excess paste film thickness

1. Introduction

Ultra-high-performance concrete (UHPC) with more than 150 MPa compressive strength (Wille, Naaman, & Parra-Montesinos, 2011) generally incorporate relatively high dosages of silica fume, superplasticizer and fiber, with relatively low concentrations of aggregates of small size. Some distinguishing features of UHPC include an optimized gradation of the granular matter for achieving high packing densities, and water-to-cementitious materials ratios of less than 0.25 (Schießl, Mazanec, & Lowke, 2007). The hydrated paste in UHPC has a dense microstructure which provides a distinct balance of strength, impermeability and durability (Graybeal, 2006, Russell & Graybeal, 2013). Plain UHPC is highly brittle; discrete fiber reinforcement is thus an inherent feature of UHPC (Peyvandi et al., 2016, Sbia, Peyvandi, Soroushian, & Balachandra, 2014a, Sbia, Peyvandi, Soroushian, Lu, & Balachandra, 2014b). The superior mechanical and durability characteristics of UHPC have led its use in rehabilitation of concrete structures (Graybeal, 2006, Richard & Cheyrezy, 1995). Recent developments in this field have emphasized broadening of the raw materials selections and use of common concrete production methods in order to facilitate commercial applications of UHPC (Reda, Shrive, & Gillott, 1999, Sbia et al., 2017, Yunsheng, Wei, Sifeng, Chuje, & Jianzhong, 2008).

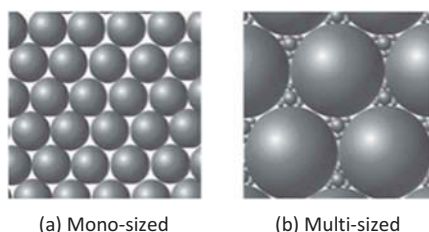
The work reported herein focused on the development of UHPC mix designs incorporating coarse aggregates with reduced cementitious binder contents for achieving improved economics and dimensional stability. The UHPC mix designs were described using some alternative parameters, including packing density, water film thickness and excess paste film thickness (Kwan & Fung, 2012, Kwan, Fung, & Wong, 2010, Li & Kwan, 2011). Higher packing densities of solid raw materials were achieved by refining the gradation of all granular matter. The effects of water on packing density were accounted for, and viable ranges of water and excess paste film thicknesses were identified for achieving desired fresh mix workability and effective binding of aggregates. These criteria provided the basis for developing a systematic approach to UHPC mix design.

1.1. Packing density, water film thickness and paste film thickness

Given a unit volume filled with particles, packing density is defined as the volume of solids in a unit volume; it is equal to one minus the volume occupied by voids. Packing density provides an indication of how efficiently particles fill a certain volume. If a high volume of aggregates is packed in a given volume, the need for binder, which is particularly costly in the case of UHPC, to fill the voids and bind the particles will be decreased (de Larrard & Sedran, 1994, Elrahman & Hillemeier, 2014, Lange, Mörtel, & Rudert, 1997). UHPC achieves high-performance characteristics partly because it has a relatively low porosity. Increasing the packing density of the granular raw materials (aggregates, cementitious materials, etc.) is one step towards lowering the porosity of the hardened material.

In the case of mono-sized spherical particles (Figure 1a), packing density approaches 0.72 (Cumberland & Crawford, 1987). When a proper amount of smaller particles is added to larger particles, the smaller particles would fill the voids between the larger ones, thus increasing the packing density (Figure 1b).

Figure 1. Simplified depiction of the effect of particle size distribution on packing density (Stovall, De Larrard, & Buil, 1986).



Water plays a lubricating role in fresh concrete. All (cement and aggregate) particles in fresh mix should receive a continuous coating of water. The water film thickness formed on particles is a key factor determining the fresh mix workability (Chandrasekhar, Pramada, Raghavan, Satyanarayana, & Gupta, 2002). In normal- and high-strength concrete materials, the available water fills the void space between particles, and also forms a continuous film on the particle surfaces (Figure 2a). This is why the term “excess water thickness” is used. In the case of ultra-high-performance concrete, the calculations conducted in this work indicate that the available water is not adequate to fill the voids between particles. Instead, all water seems to be adsorbed on the hydrophilic surfaces of particles, with the void spaces remaining empty. An optimum water film thickness should provide adequate workability without excessively separating the particles which would increase the porosity of the cementitious binder and thus lower its strength (Kwan & Fung, 2012, Kwan et al., 2010, Li & Kwan, 2011).

Given the brittle nature of the cementitious paste, it needs to fully coat the aggregates in order to render binding effects. The paste should fill the void space between fine and coarse aggregates before it can effectively coat the aggregate particles. The excess paste theory views the thickness of the excess paste beyond that required for filling of voids between fine and coarse aggregates (Figure 2b) as a parameter influencing the fresh mix and the hardened material qualities. The cementitious paste in UHPC can reach higher strength levels than aggregates (Li & Kwan, 2013, Shen & Yu, 2011). This is not generally the case with normal- and high-strength concrete materials prepared with normal-weight aggregates. Therefore, new trends may emerge as far as the relationship between the strength of UHPC and its excess paste film thickness is concerned.

The work reported herein derived viable ranges of the fundamental mix parameters introduced above for ultra-high-performance concrete (UHPC). Achievement of these viable ranges can guide efforts to design UHPC mixtures with locally available materials.

1.2. Calculation of water film thickness and excess paste film thickness

1.2.1. Water film thickness

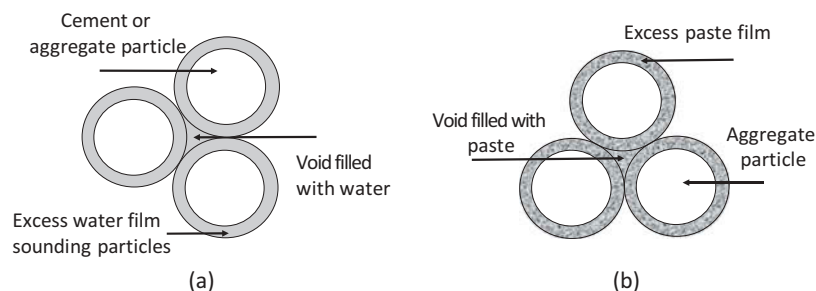
The conventional approach to water film thickness calculates the ‘excess’ water film thickness covering the surfaces of all granular matter, neglecting the amount of water required to fill the voids between the granules (Li & Kwan, 2013, Powers, 1969). For this purpose, the packing density of particles, Φ , needs to be calculated, based on which the void ratio between packed particles, μ , can be calculated as follows (Graybeal, 2011):

$$\mu = \frac{1 - \Phi}{\Phi} \quad (1)$$

The excess water ratio (μ_w'), beyond that required to fill the void space, can thus be calculated as (Yost, Radlinska, Ernst, Salera, & Martignetti, 2013):

$$\mu_w' = \mu_w - \mu \quad (2)$$

Figure 2. The excess water film thickness (a), and the excess paste film thickness (b) principles.



where μ_w is the total volume of water divided by the volume of all solid particles. The excess water film thickness, WFT, can then be calculated as:

$$WFT = \mu_w' / A_s \quad (3)$$

where

$$A_s = \sum_{k=1}^n R_k \cdot A_k \quad (4)$$

k refers to each of the n granular solids in the mix, R_k is the volumetric ratio of the k^{th} granular matter, and A_k is the specific surface area of the k^{th} granular matter.

While the above approach is valid for normal- and high-strength concrete, its application to ultra-high-performance concrete yields negative values of excess water film thickness. This indicates that, considering the very low water content of UHPC, the voids between granular matter cannot be filled with water. Given the energetic preference of water to adsorb onto hydrophilic surfaces, we assumed that water is present only as the film adsorbed on particle surfaces, and does not fill the voids between them. Hence, the water film thickness (WFT) can be calculated as follows for UHPC:

$$WFT = \mu_w / A_s \quad (5)$$

1.2.2. Excess paste film thickness

The excess paste film thickness is calculated as the thickness of the film formed on fine and coarse aggregates after the voids between aggregates are filled with the paste. Considering the maximum wet packing density of aggregates, $\Phi_{a,\max}$, the minimum void ratio between aggregates to be filled with paste is calculated as:

$$\mu_{\min} = (1 - \Phi_{a,\max}) / \Phi_{a,\max} \quad (6)$$

The excess paste ratio μ_p' is then expressed as follows:

$$\mu_p' = \mu_p - \mu_{\min} \quad (7)$$

The excess paste film thickness can then be calculated as:

$$PFT = \mu_p' / A_A \quad (8)$$

2. Material and methods

2.1. Materials

The cementitious binder used in UHPC comprised Type I Portland cement, undensified silica fume, ground granulated blast furnace slag, and limestone powder. The silica fume used in the project had 200nm mean particle size, 15m²/g specific surface area (Blaine fineness), and ≥105% 7-day pozzolanic activity index. The slag had a specific gravity of 2.90 and bulk density of 1275 kg/m³. Figure 3 presents the size distributions of all the powder materials used in the project. Limestone with a maximum particle size of 12 mm was used as coarse aggregate. Two silica sands with different particle size distributions were used as fine aggregates. Figure 4 presents the size distributions of the coarse and fine aggregates. A polycarboxylate-based superplasticizer (Chryso 150 supplied by Chryso with 1.06 specific gravity and 1.8% solid content) and straight (brass-coated) steel fibers of 0.2 mm diameter and 12 mm length (supplied by Bekaert) were also used in UHPC mixtures. Chemical compositions of the Portland cement, slag, silica fume and limestone powder used in this investigation are presented in Table 1.

2.1.1. Mixing procedures

Ultra-high-performance concrete mixtures were prepared in the following steps:

Figure 3. Particle size distributions of Type I Portland cement, limestone powder, slag and silica fume.

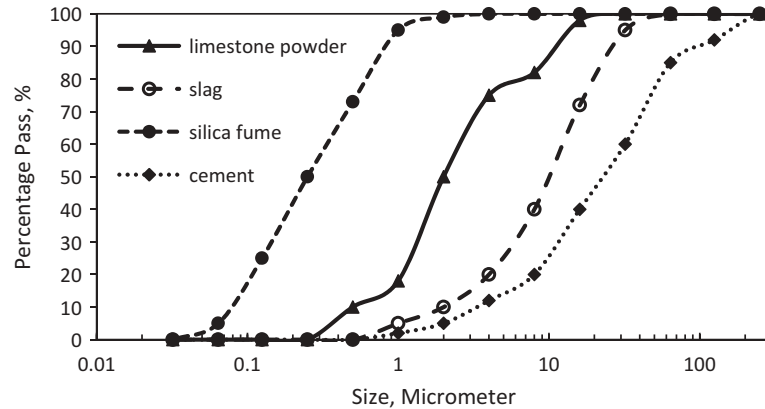


Table 2. The variables and their levels considered in the optimization experimental program

Factor	Level 1	Level 0	Level 1
Coarse to fine aggregate ratio	1.0	1.5	2.0
Superplasticizer ratio	32	34	36
Fiber ratio	0.8	1.0	2.0

2.2. Experimental optimization of mix proportions

A response surface design of experiments was developed for optimizing three primary mix proportioning parameters: (i) coarse aggregate-to-fine aggregate (weight) ratio; (ii) superplasticizer content; and (iii) steel fiber volume fraction. Table 2 presents the three levels of these variables considered in the optimization experimental program. Viable ranges of these parameters were identified through a preliminary investigation. These ranges were 1.0–2.0 for coarse aggregate-to-fine aggregate ratio, superplasticizer content of 32–36 vol.% of mixing water, steel fiber content of 0.8–2.0 vol.% of solid content. The response surface design of experiments for identifying the optimum combination of these variables is presented in Table 3. Besides these parameters, other aspects of the UHPC mix design were kept constant. The cementitious binder comprised Type I Portland cement: limestone powder: silica fume: slag at 48: 17: 24: 11 weight ratios. This composition was selected to provide a desired particle size distribution for achieving a high level of packing density, and was then refined using a trial-and-adjustment approach to produce high strength levels. These cementitious materials were used at a constant dosage of 880 kg/m³ in UHPC. The ratio of water to cementitious materials was also kept constant at 0.124. The fact that only some of the mix parameters were subject of this optimization experimental program implies that the optimum UHPC mix design developed here is valid for the selected values of the mix variables that were kept constant. The optimization experimental program was designed using the Box-Bhenken design procedure in the SYSTAT© statistical software. The fresh mix workability of UHPC was assessed using the flow table test procedure per ASTM C124. Cube specimens of 50 mm dimensions were prepared with each UHPC mixtures using external vibration. They were stored in sealed condition inside molds, and demolded after 24 h. Steam curing of specimens was then accomplished at 90°C over 48 h. The specimens were then allowed to cool down and stored at 50 ± 5% and 22 ± 2°C until 7 days of age when they were subjected to compression testing per ASTM C109. Eight cube specimens were prepared and tested for each mix.

3. Experimental results

Figure 5 presents the compressive strength and workability test results for the UHPC mixes considered in this investigation. The measured values of compressive strength ranged from 160 MPa for Mix 12 to 215 MPa for Mix 1. The fresh mix flows ranged from 55 cm (Mix 7) to 85 cm (Mix 12).

3.1. Effect of the packing density on compressive strength

Figure 6 shows the relationship between compressive strength and packing density for ultra-high-performance concrete. It should be noted that the data points presented in Figure 6 were produced with different superplasticizer and fiber contents (see Table 3), which explains some of the variations observed at similar packing densities. The UHPC packing density is observed to range from 0.825 to 0.855. Within this range, compressive strength tends to increase with increasing packing density. This is the anticipated trend, noting that high superplasticizer contents are used in UHPC mixtures to achieve viable workability levels in spite of their low water contents. The trend in increasing strength with increasing packing density seems to approach a plateau within the range of packing densities considered in this experimental program.

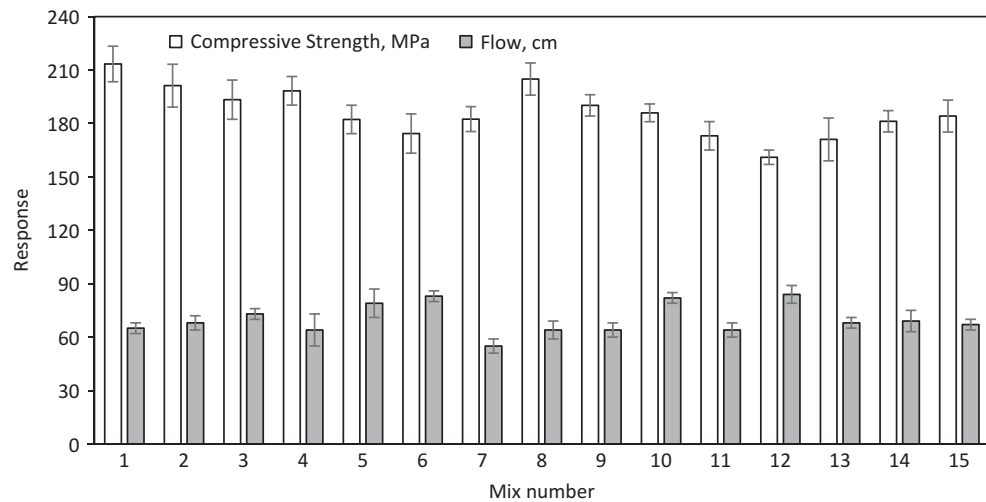
3.2. Effect of the water film thickness on compressive strength

Figure 7 presents the relationship between the water film thickness and the compressive strength of the refined UHPC mix designs. The UHPC mixtures considered here have water film thicknesses

Table 3. The response surface design of experiments for optimization of the UHPC mix proportions

Mix No.	Coarse to fine aggregate ratio	Superplasticizer ratio	Fiber volume fraction, %
1	1.0	32	1.0
2	2.0	32	1.0
3	1.0	36	1.0
4	2.0	36	1.0
5	1.0	34	0.8
6	2.0	34	0.8
7	1.0	34	2.0
8	2.0	34	2.0
9	1.5	32	0.8
10	1.5	36	0.8
11	1.5	32	2.0
12	1.5	36	2.0
13	1.5	34	1.0
14	1.5	34	1.0
15	1.5	34	1.0

Figure 5. Compressive strength and flow table test results for the optimization UHPC mixtures.



ranging from 0.058 to 0.07 μm . Within this range, higher water film thicknesses yield lower values of compressive strength. It is worth mentioning that a minimum water film thickness would be required to lubricate the granular matter and produce a viable fresh mix workability. This minimum was probably exceeded in the UHPC mixtures considered here, which were designed to provide adequate workability. The calculated values of water film thickness for UHPC are lower than those reported for high-strength concrete. The use of relatively large superplasticizer dosages enabled lowering the UHPC water film thickness while still achieving adequate fresh mix workability. It should be noted that some of the variations in compressive strength for similar water film thicknesses can be attributed to the differences in the superplasticizer content and packing density that vary for different data points (see mix designs of Table 3).

Figure 6. The relationship between compressive strength and packing density for UHPC.

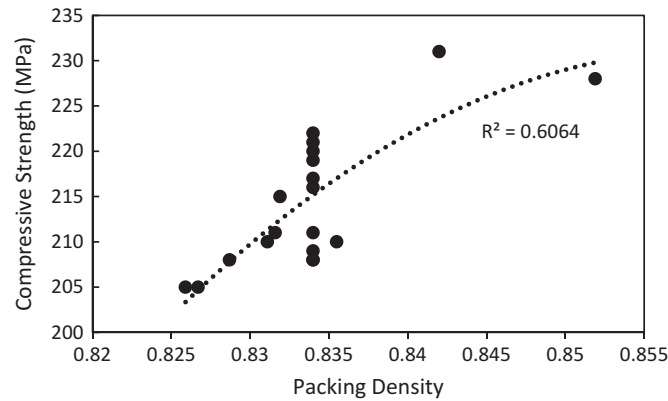
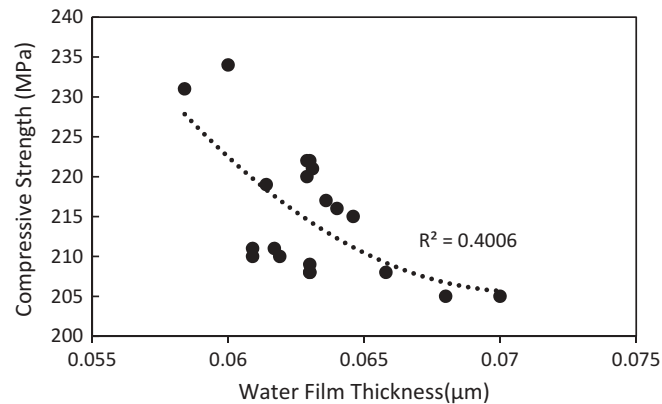


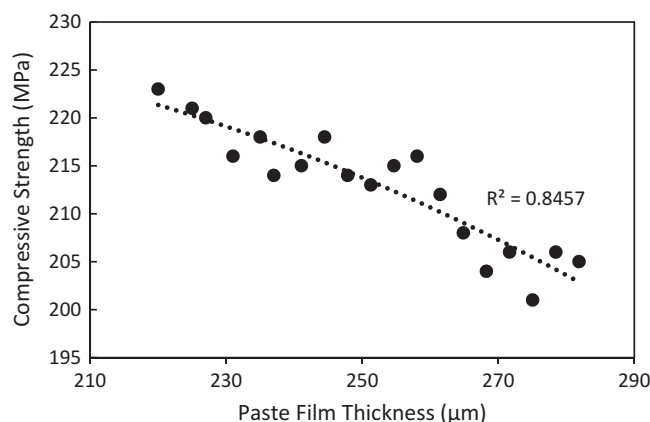
Figure 7. The relationship between the water film thickness and compressive strength of UHPC.



3.3. Effect of the excess paste film thickness on compressive strength

Figure 8 shows the relationship between the UHPC compressive strength and the excess paste film thickness (on fine and coarse aggregates). The excess paste film thickness is observed to range from 220 to 280 μm for the UHPC mixtures considered here. The compressive strength of UHPC is observed to decrease with increasing excess paste film thickness. Similar to water film thickness, a minimum value of excess paste film thickness would be required for achieving a viable level of fresh mix workability. This minimum was probably exceeded in this experimental work which sought to produce UHPC mixtures of adequate workability in fresh state. It should be noted that

Figure 8. The relationship between the excess paste film thickness and the compressive strength of UHPC.



various data points shown in Figure 8 correspond to the mix designs of Table 3 where different mix variables change simultaneously.

The response surfaces developed using the compressive strength and workability test data are presented in Figures 9 and 10, respectively. Response surface (Ridge) analysis of these test results yielded the following optimum levels of the UHPC mix design variables:

Coarse to the fine aggregate ratio: 1.20
 Superplastizer dosage, vol. % 32.7
 Fiber volume fraction, % 1.43

The UHPC mix with the optimum mix design parameters identified above was prepared using the procedures described earlier. Table 4 presents the calculated values of packing density, water film thickness (WFT), and excess paste film thickness (PFT) for the optimum mix; this table also presents the average values and ranges (for eight replicated specimens) of flow and compressive strength. The average values of flow and compressive strength for the optimized mix were 68 cm and 223.6 MPa, respectively, which are within the ranges predicted by response surface analysis of the results of the optimization experimental program. The calculated values of packing density, water film thickness and excess paste film thickness for this optimized mix design are also within the viable ranges for ultra-high-performance concrete introduced earlier.

Figure 9. Response surfaces of the compressive strength test data generated in the optimization experimental program of the UHPC mix.

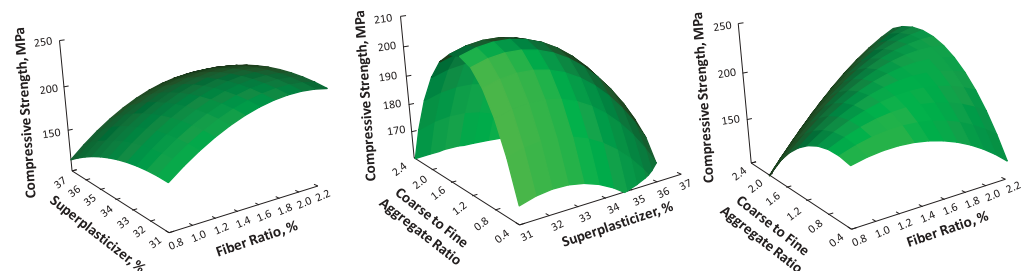


Figure 10. Response surfaces of the workability test data generated in the optimization experimental program of the UHPC mix.

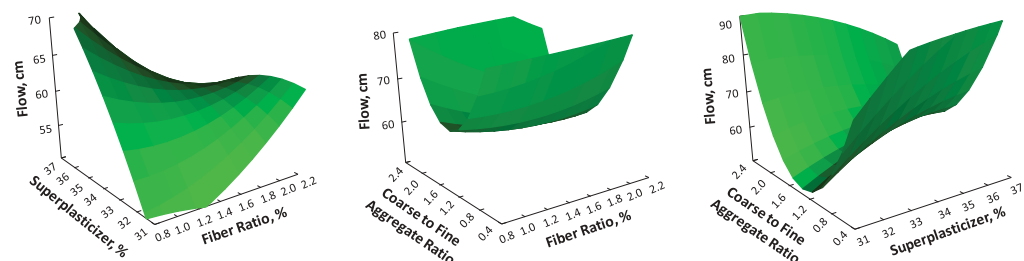


Table 4. The calculated values of packing density, water film thickness and excess paste film thickness, and the measured values of fresh mix flow and hardened concrete compressive strength for the optimized UHPC mix design

Packing density	WFT, μm	PFT, μm	Fresh mix flow, cm	Compressive strength, MPa
0.843	0.053	219	68 ± 4.2	223.4 ± 8.0

4. Conclusions

A response surface design of experiments was developed for identifying the optimum values of coarse-to-fine aggregate weight ratio, superplasticizer content and steel fiber volume fraction in an ultra-high-performance concrete mix with a specific cementitious binder composition, binder content and water-to-binder ratio. The fresh mix flow and the hardened concrete compressive strength were examined. For each UHPC mix design, the values of packing density, water film thickness and excess paste film thickness were also calculated. The following conclusions could be derived from the test results produced for the ranges of variables considered in the experimental program.

- The UHPC packing density ranged from 0.825 to 0.855. Within this range, compressive strength increased with increasing packing density, although compressive strength seemed to approach a plateau for the higher end of the packing densities considered here. It should be noted that the higher packing densities achieved here would probably compromise the fresh mix workability without the high superplasticizer contents used in this UHPC mixture.
- The distinctly low water content of UHPC seems, based on calculations, to produce a film on the surfaces of all particles, but leave the voids formed between particles empty. A water film thickness on particles was calculated based on this assumption. The UHPC mixtures considered in this investigation had water film thicknesses ranging from 0.058 to 0.07 μm . Within this range, higher water film thicknesses produced lower values of compressive strength. A minimum water film thickness would be required to lubricate the granular matter and produce a viable fresh mix workability. This minimum was probably exceeded in the UHPC mixtures considered here, which were designed to provide adequate workability. The calculated values of water film thickness for UHPC are lower than those reported for high-strength concrete. The use of relatively large superplasticizer dosages enabled lowering the UHPC water film thickness while still achieving adequate fresh mix workability.
- The excess paste film thickness for the specific UHPC mixtures considered in this investigation ranged from 220 to 280 μm . The compressive strength of UHPC decreased with increasing values of excess paste film thickness. Similar to water film thickness, a minimum amount of excess paste film thickness would be required for achieving a viable level of fresh mix workability. This minimum was probably exceeded in this experimental work which sought to produce UHPC mixtures of adequate workability in fresh state.
- Response surface analysis of test results yielded, for the specific UHPC mixtures considered in this investigation, optimum values of 1.5% for fiber volume fraction, 32–34% (by weight of water) superplasticizer content, and 1.2–1.4 coarse-to-fine-aggregate ratio. This optimum mix was prepared and tested; it yielded a desired balance of fresh mix flow and compressive strength (68 cm and 223 MPa, respectively). The calculated values of packing density, water film thickness and excess paste film thickness for this optimum mix were 0.843, 0.053 μm and 219 μm , respectively, which occur within the viable ranges identified in the project. The measured values of flow and compressive strength were within the range anticipated through response surface analysis of the results of the optimization experimental program. Given the diversity of the UHPC mix designs, the quantitative information developed in this project should be considered applicable to the particular category of UHPC mix design considered here. The selections of raw materials could also influence these quantitative findings.

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