Proceedings of the Seventeenth International Conference on
Civil, Structural and Environmental Engineering Computing
Edited by: P. Iványi, J. Kruis and B.H.V. Topping
Civil-Comp Conferences, Volume 6, Paper 4.2
Civil-Comp Press, Edinburgh, United Kingdom, 2023
doi: 10.4203/ccc.6.4.2

Application of a Multiscale Model for 3D Printed Concrete

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Abstract

3D printing of concrete is a rapidly growing technology in the construction industry because of its numerous benefits such as reducing wastes, improving material efficiency, and increasing design flexibility. Nonetheless, the 3D printing process and mix design can lead to differences in microstructure, which may have significant implications on its macroscopic mechanical properties. To investigate the relationship between microstructure and mechanical behavior, a multiscale model based on continuum micromechanics was applied to predict the mechanical properties of single-layer 3D printed concrete (3DPC). The computational results demonstrate a correlation relationship between the macroscopic mechanical properties and the volume fraction and morphology of the microstructural constitutions of 3DPC. Furthermore, it is found that some kind of external admixtures can alter the mapping between the mechanical properties and the age of 3DPC, while the mapping between its mechanical properties and hydration degree remains unchanged. These findings highlight the importance of understanding the distinct microstructure of 3DPC and the potential of multiscale modeling in term of predicting its mechanical behavior and enhancing the design of 3D printed structures.

Keywords: 3DPC, hydration degree, compressive strength, continuum micromechanics, multiscale model

1 Introduction

In recent years, 3D printed concrete has emerged as a promising technology for construction due to its numerous benefits such as reduced waste, improved material efficiency, and design flexibility [1,2,3]. However, the unique microstructure resulting from the 3D printing process and the special mix design can lead to differences in microstructure [4,5,6,7] compared to conventional mould-cast concrete. The distinct microstructure of 3DPC has significant implications on its macroscopic mechanical properties [8,9].

To fully understand the relationship between the microstructure and mechanical behaviour of 3DPC, a comprehensive and accurate multiscale modelling approach is necessary. Considering that concrete is a complex heterogeneous composite material and exhibits significant variation in length scales from nanometres to macroscopic decimetres [10], continuum micromechanics provides a powerful framework to effectively address this heterogeneity by equating materials as the collection of "representative volume elements" (RVE) and "equivalent homogeneous media" (EHM) [11]. And the multiscale model that concentrates on cement-based materials has been developed and extensively studied in Refs. [10,12]. This model has been highly effective in accurately characterizing the relationship between mechanical properties and the hydration degree in conventional concrete.

This paper aims to check whether or not this multiscale model is useful for description of the development of the compressive strength of 3DPC. For this purpose,the theoretical basis of the multiscale model was succinctly explicated in Section 2. Subsequently, to ascertain the viability of the model in forecasting the mechanical properties of 3DPC, experimental data from open literatures were employed and corroborated in Section 3, culminating in the discovery of definitive insights in Section 4.

2 Fundamentals of continuum micromechanics

In continuum micromechanics [11], the characteristic length l of RVE needs to fulfill the 'separation of scales', reads as

$$\{L, \lambda\} \gg l \gg d \gg d_0 \tag{1}$$

where L is the characteristic length of the structure containing the RVE, λ denote the characteristic length of the structure excitations, d represents the characteristic dimensions of the considered inhomogeneities within the RVE, and d_0 is lower length bound under which continuum mechanics is no more valid.

Based on matrix-inclusion problems, an estimate for the 'homogenized' stiffness $\mathbb{C}_{est}^{hom}$ of a material reads as [10]

$$\mathbb{C}_{est}^{hom} = \sum_r f_r \mathbb{C}_r : \mathbb{A}_r \tag{2}$$

the f_r and $\mathbb{C}_r$ refer to the volume fraction and stiffness tensor of the r-th phase, the symbol ':' stands for double contraction, the $\mathbb{A}_r$ is the concentration tensor, which has been simplified by C. Hellmich et al. [13]. Given the random microstructure of cement-based materials, it is naturally to consider all phases as isotropic [10]:

$$\mathbb{C}_r = 3k_r\mathbb{J} + 2\mu_r\mathbb{K} \tag{3}$$

where k_r, μ_r, k_0, μ_0 are the bulk moduli and the shear moduli of phase r and of the reference medium, $\mathbb{J}$ is the volumentric part of the fourth-order unit tensor $\mathbb{I}$, $I_{ijkl} = 1/2(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$, $J_{ijkl} = (1/3)\delta_{ij}\delta_{kl}$, δ_{ij} stands for the Kronecker delta, and $\mathbb{K} = \mathbb{I} - \mathbb{J}$ is the deviator part.

According to the study of B. Pichler et al. [12] and M. Königsberger et al. [14], stress peaks govern phase failure, and the cementitious system exhibits linear elastic behavior, provided that the quadratic deviatoric stress averages over each of the hydrate phases (oriented in all space directions φ and ϑ) remain below a critical strength value $\sigma^{dev}_{hyd,crit}$.

3 Application

3.1 Representation of the multiscale microstructure of 3DPC

Following the work by O. Bernard et al. [10], microstructure of 3DPC can be divided into four scale levels:

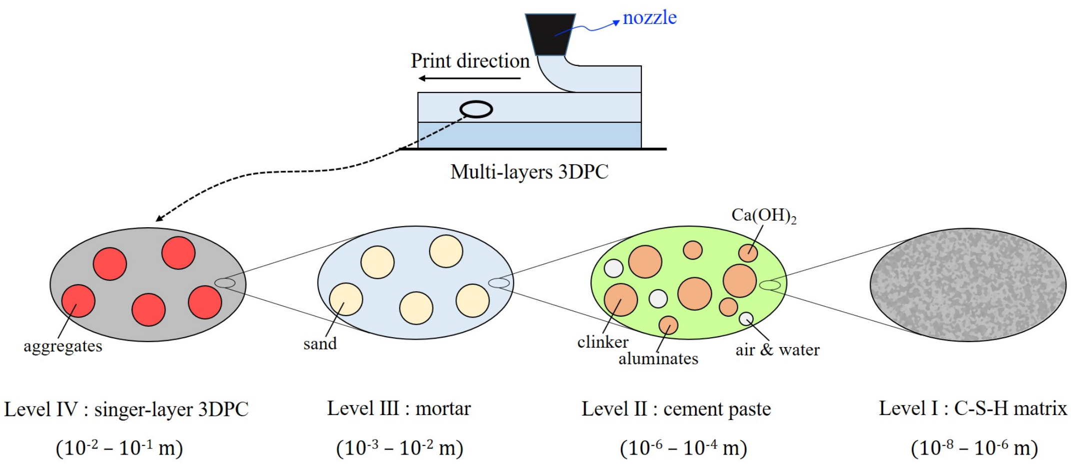

Figure 1: Multiscale microstructure of 3DPC

3.2 Mineralogical composition of cement and mix proportions of 3DPC

Some of the experimental data in open literatures do not explicitly provide the mass fraction of the mineralogical composition of the cement, however, the mineralogical composition can be derived from the mass fractions of the cement oxides based on the chemical reaction of the silicate cement:

$$m_{C_3S} = 4.07m_{CaO} - 7.60m_{SiO_2} - 6.72m_{Al_2O_3} - 1.43m_{Fe_2O_3} - 2.85m_{SO_3} \quad (4)$$

$$m_{C_2S} = 2.87m_{SiO_2} - 0.75m_{C_3S} \quad (5)$$

$$m_{C_3A} = 2.65m_{Al_2O_3} - 1.69m_{Fe_2O_3} \quad (6)$$

$$m_{C_4AF} = 3.043m_{Fe_2O_3} \quad (7)$$

The mineralogical composition of cement in Ref. [15] was provided by manufacturer: $m_{C_3S} = 62.6\%$, $m_{C_2S} = 16.5\%$, $m_{C_3A} = 1.5\%$, $m_{C_4AF} = 13.1\%$. Two sets of mix proportions of 3DPC are listed in Table 1.

Mix	M1	M1-SP
Portland cement (g)	682.75	682.75
Water (g)	236.25	236.25
Sand (g)	850	850
SP (g)	0	1.76

Table 1: Mix proportions of 3DPC

A new generation polyvalent non chlorated acrylic copolymer superplasicizer (SP), SIKA VISCOCRETE TEMPO 11 was used in M1-SP. Considering the effect of water absorption of aggregates on the model, the effective water-cement ratio is defined as:

$$w/c_{eff} = (w/c) - (a/c) * W, \quad (8)$$

where a/c is the aggregate-cement ratio, W is the absorption coefficient.

3.3 Hydration degree and heat

The total heat of hydration when the cement is fully hydrated can be obtained if the mineral composition of the cement is known [16].

$$Q_{max,c} = 510m_{C_3S} + 247m_{C_2S} + 1356m_{C_3A} + 427m_{C_4AF}, \quad (9)$$

where $Q_{max,c}$ is theoretic heat evolution of completely hydrated Portland cement. By means of the heat released, it is possible to determine the hydration degree relative to hydration duration accounding to the equation:

$$\xi(t) = \frac{Q(t)}{Q_{max,c}}, \tag{10}$$

where Q_t is heat evolution at time t. Combining with Eq. 9 and Eq. 10, we can convert the development of hydration with age by fitting the cumulative heat curve. Finally, the mapping relationship between compressive strength and hydration degree could be obtained, see Table 2.

Age (d)	M1		M1-SP	
	ξ (1)	compressive strength (Mpa)	ξ (1)	compressive strength (Mpa)
3	0.555	56.01	0.486	50.79
7	0.677	77.21	0.727	70.07
28	0.724	88.55	0.805	81.41
60	0.735	85.60	0.820	82.20

Table 2: Compressive strength and hydration degree

3.4 Verification

Combined the mineralogical composition of cement and mix proportions, the mapping relationships between the volume fraction of each phase and the hydration degree can be calculated, besed on hydration kinetics [10,17]. These relationships are shown in Fig. 2.

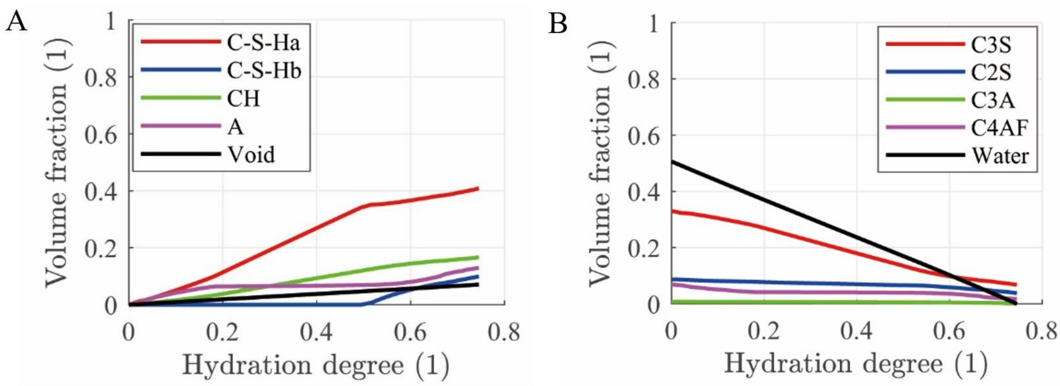

Figure 2: Volum fractions of the phases of M1; (A) products; (B) reactants.

Subsequently, the strength can be obtained by using the following strength criterion [12]:

$$|\Sigma_{11}| \max_{\vartheta,\varphi}[\lim_{f_{hyd}^{\vartheta,\varphi}\to 0} (\frac{\mu_{hyd}^2}{f_{hyd}^{\vartheta,\varphi}} \underline{e_1} \otimes \underline{e_1} : \frac{\partial \mathbb{C}_{\text{hom}}}{\partial \mu_{hyd}^{\vartheta,\varphi}}^{-1} : \underline{e_1} \bigotimes \underline{e_1})^{\frac{1}{2}}] - \sigma_{crit}^{dev} \leqslant 0 \tag{11}$$

These relations give access to an estimate of the macroscopic uniaxial compressive strength, which is equal to the value of $|\Sigma_{11}|$ for which the left-hand sides of Eq.11 become exactly zero [12]. Combining with the section 2, the compressive strength of M1 could be solved. The results obtained from the multiscale model with the experimental results are shown in Figure 3.

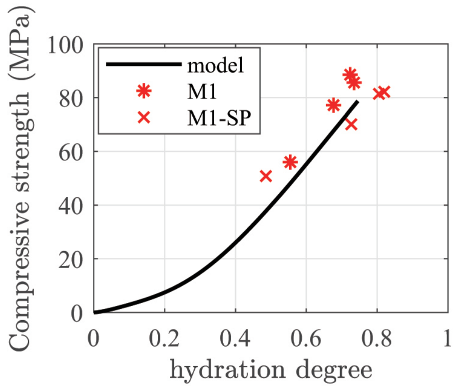

Figure 3: Compressive strength of M1

The model accurately captures the early-age compressive strength of 3DPC. It is interesting to note that the superplasicizer used affect hydration rate [15], but do not affect the mapping relationship between compressive strength and hydration degree.

4 Conclusions

In this study, a multiscale modeling approach based on the principles of continuum micromechanics was applied to predict the mechanical properties of single-layer 3D printed concrete. The model integrated the microstructural features of 3DPC at different length scales and enabled the estimation of macroscopic mechanical properties. The results demonstrated that there is a clear relationship between the macroscopic mechanical properties and the volume fraction and morphology of the microstructure of 3DPC.

Furthermore, the effect of external admixtures on the mechanical properties and age-strength relationship of 3DPC was investigated. The incorporation of some kind of external admixtures into 3DPC changes the mapping between mechanical properties and age, but not the mapping between mechanical properties and hydration degree.

Overall, the findings of this study demonstrate the potential of multiscale modeling in predicting the behavior of single-layer 3DPC and improving the design of 3D printed structures. Future work could extend the multiscale modeling framework to include more complex microstructural features and explore the effect of different printing parameters and layer-to-layer interfaces on the mechanical performance of 3DPC.

Acknowledgements

We gratefully acknowledge the financial support from the National Key R&D Programme Intergovernmental Cooperation on International Science and Technology Innovation (No. 2021YFE0114100), Science and Technology Commission of Shanghai Municipality (No. 21DZ1203505), and Science and Technology Project of Department of Transportation of Jiangxi Province (No. 2021C0008). The authors would like to express their deep appreciation to Professor Bernhard Pichler from TU Wien for his insightful ideas and meaningful inspirations involved in this work.

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