Mix design of strain hardening cementitious composites through multiscale and multiphysics models

Li, Junxia

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**NANYANG
TECHNOLOGICAL
UNIVERSITY**

**MIX DESIGN OF STRAIN HARDENING
CEMENTITIOUS COMPOSITES THROUGH
MULTISCALE AND MULTIPHYSICS MODELS**

LI JUNXIA

**Interdisciplinary Graduate School
Residues and Resource Reclamation Center (R3C)
Nanyang Environment & Water Research Institute (NEWRI)**

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LI JUNXIA

**Interdisciplinary Graduate School
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Nanyang Environment & Water Research Institute (NEWRI)**

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Abstract

Strain hardening cementitious composites (SHCC) have been developed and applied in the field, but having no appropriate mix design method constrains its growth significantly. This thesis demonstrates the multiscale and multiphysics philosophy to develop the design method of SHCC.

Two main difficulties have to be overcome in order to come up with a mix design method for SHCC. Firstly, the variability of microstructural properties and the macroscopic composite nature of SHCC have to be considered. Based on the existing deterministic-based micromechanics model of SHCC, a probabilistic-based micromechanics model (PMM) is proposed to perform reliability assessment of the specified mix design with considering all possible variations of micromechanical parameters. Correspondingly, a new model of predicting the tensile properties of SHCC is developed which can take all the variability into account as well. Secondly, it is requisite to relate factors of mix design to micromechanical parameters which makes the mix design method for SHCC become a reality. By virtue of this relationship and the model of tensile properties, factors of mix design can relate to the ultimate composite performance, which means that the ultimate tensile properties can be predicted given the designed mix of the composite.

Consequently, a systematic mix design method for SHCC is proposed involving selection of raw materials, prior prediction of strain hardening behavior and output reliable composite performance of desired mix.

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List of Symbols and Abbreviations

The following list of symbols and abbreviations is provided for ease of reference for those symbols and abbreviations that are most frequently used in this thesis. It is therefore not exhaustive. Nonetheless, all symbols and abbreviations used in this thesis are defined at their first mention in the main text.

Symbols:

J_b'	=	maximum complementary energy
J_{tip}	=	energy of crack initiation and propagation
σ_0	=	maximum bridging strength
σ_{fc}	=	first matrix cracking strength
σ	=	stress
w	=	crack width
ε	=	strain capacity
σ_B	=	fiber bridging stress
δ	=	crack opening
K_m	=	matrix fracture toughness
E_m	=	matrix Young's modulus
K_{tip}	=	composite fracture toughness
c	=	pre-existing internal flaw size
$\sigma_B(\delta)$	=	fiber bridging constitutive law
G_d	=	chemical bond
τ_0	=	interfacial frictional bond
β	=	slip hardening coefficient
f	=	snubbing coefficient
f'	=	strength reduction factor
E_f	=	fiber elastic modulus
L_f	=	fiber length
d_f	=	fiber diameter
σ_{fu}	=	fiber tensile strength
V_f	=	fiber volume
ϕ	=	fiber inclined angle
L_e	=	fiber embedment length
K_L	=	energy produced by applied remote loading
K_B	=	energy absorbed by fiber bridging
σ_{mu}	=	tensile strength of the matrix
ΔL_e	=	elastic deformation
ε_e	=	elastic strain
E_c	=	elastic modulus of the composite
L	=	gauge length of the specimen

δ_{peak}	=	average crack opening
n	=	crack number
x_d	=	minimum distance of stress transfers from fiber to the adjacent matrix
P_f	=	probability of failure
X_i	=	random variables
$G(x), F(x)$	=	limit state surface (performance function)
α	=	reliability index
V_m	=	matrix volume fraction
σ_{ss}	=	stress at steady state
δ_{ss}	=	crack opening at steady state
λ	=	scale parameter
k	=	shape parameter
σ_{cu}	=	ultimate cracking strength
T	=	clamping stress
γ	=	coefficient of friction

Abbreviations:

FRC	=	Fiber reinforced concrete
HPFRCC	=	High performance fiber-reinforced cementitious composites
SHCC	=	Strain hardening cementitious composites
ECC	=	Engineered cementitious composites
PE	=	Polyethylene
PVA	=	Polyvinyl alcohol
PP	=	Polypropylene
PDF	=	Probability density function
PMM	=	Probabilistic-based micromechanics model
MARS	=	Multivariate adaptive regression splines
FORM	=	First-order reliability method
DMM	=	Deterministic-based micromechanics model
BS	=	British Standards
ACI	=	American Concrete Institute
W/C	=	Water-to-cement ratio
S/C	=	Sand-to-cement ratio
ACK	=	Aveston-Cooper-Kelly theory
BFs	=	Basis functions
GCV	=	Generalized Cross-Validation
R^2	=	Coefficient of determination
MSE	=	Mean Squared Error
MAE	=	Mean Absolute Error
ANOVA	=	Analysis of variance
WST	=	Wedge splitting test
CMOD	=	Crack mouth opening displacement
IPKM	=	Integrated particle kinetics model
CSH	=	Calcium Silicate Hydrate

CH	=	Portlandite
NIST	=	National Institute of Standards and Technology
VCCTL	=	Virtual Cement and Concrete Testing Laboratory
MCS	=	Monte Carlo simulation
COV	=	Coefficient of variations
SEM	=	Scanning electron microscope
ITZ	=	Interface transition zone
SCM	=	Supplementary cementitious materials
DOE	=	Design of experiment
OPC	=	Ordinary Portland cement
ANN	=	Artificial neural networks

1 Introduction

1.1 Background

Concrete is the most used man-made material in the world. One major drawback of concrete as a construction material, however, is its high brittleness with low tensile strength and tensile ductility. To overcome this bottleneck, fiber reinforced concrete (FRC) was developed in the 1950s. However, FRC still shows post-cracking tension-softening behavior under uniaxial tensile loading which means the load decreases with the increase of crack opening upon matrix first cracking as depicted in Fig. 1.1. Thereafter, many efforts were placed to develop a new class of cement-based material which exhibits post-cracking tensile strain hardening behavior. High performance fiber-reinforced cementitious composites (HPFRCC) or strain hardening cementitious composites (SHCC) was first introduced by Naaman and Reinhardt [1] and with its macro strain hardening behavior after first cracking under uniaxial tensile loading as shown in Fig. 1.1.

Figure 1.1 The tensile behavior of Concrete, FRC and SHCC

Engineered cementitious composites (ECC) is a unique type of SHCC with extreme tensile strain capacity of 3-5%, whereas the fiber content is only 2% by volume or less [2]. In contrast, Ductal, a commercial version of SHCC, has typical tensile strain hardening capacity of around 0.1% with 2% of steel fiber by volume [3]. Another distinctive product is SIFCON with up to 2% tensile strain capacity, whereas the fiber dosage may range from 8% to over 20% depending on fiber geometry, specimen preparation procedures, and mold size [4].

The ultra-high ductility of ECC, several hundred times that of normal concrete, with low fiber volume is achieved by optimizing the microstructure of the composite employing the micromechanics-based design and tailoring method [5]. This approach can take into account all of the fiber, matrix and interface properties affecting the composite tensile strain hardening behavior. Therefore, ECC is not only a notation of ductile concrete, but also a design philosophy of cementitious materials which elevates the trial-and-error empirical combination of individual constituents to systematic engineered selection.

Fig. 1.2 provides a philosophical underpinning of the bottom-up approach for ECC design. The design process is multilevel in the sense that decisions must be made with respect to the ultimate behavior at each level of material hierarchy. By utilizing this design theory, a strain hardening material can be achieved by exploiting the multiscale linking between composite performance (macroscale), to fiber bridging properties (mesoscale), and to material microstructure, i.e. fiber, matrix, and interface properties (microscale) as shown in Fig. 1.2 [2]. The linkage between the meso level and the macro level is the theoretical steady-state crack analysis represented by two requirements, i.e. the complementary energy J_b' to be equal to or

greater than the matrix crack tip toughness J_{tip} , and secondly, the first cracking strength σ_{fc} must be lower than the maximum fiber bridging strength σ_0 . Detailed description of these criteria are given in Section 2.2.1. The fiber bridging stress-crack opening displacement relation $\sigma_B(\delta)$ is established with respect to micromechanical parameters of the fiber, matrix and interface to link up the micro level with the meso level. All in all, ECC tensile strain hardening behavior is associated with a set of micromechanical parameters which are determined from fiber, matrix, and interface properties. Through proper control of the material microstructure, composite tensile strain hardening behavior can be engineered and achieved.

Figure 1.2 Multiscale linking of ECC design [2]

1.2 Research motivation

The control of material microstructure, i.e. fiber, matrix and interface properties, is realized by properly selecting and tailoring material composition, i.e. types and proportioning of ingredients. Unfortunately, there is no systematic investigation on the correlation between material microstructure and material composition. Current state-of-the-art in controlling microstructure remains empirical and is through

numerous experiments or reasonable assumptions. To the best of the author's knowledge, no available mix design method could be used to predict the tensile strain hardening behavior of SHCC from the initial material composition.

In addition, satisfying the strain hardening criteria, i.e. $J_b' \geq J_{tip}$ and $\sigma_0 \geq \sigma_{fc}$, does not necessarily mean saturated multiple cracking thus high ductility, due to the heterogeneous nature of any fiber-reinforced material. The heterogeneity originates from the variation of properties of ingredients such as the fiber diameter, the random distribution of flaw size, the fiber orientation and the fiber dispersion in matrix. Generally, large margins between J_b' and J_{tip} , σ_0 and σ_{fc} are necessary to ensure high ductility. These margins are highly empirical and vary in different ECC systems [5], e.g. polyethylene (PE) fiber reinforced ECC with $J_b'/J_{tip} > 3$ and $\sigma_0/\sigma_{fc} > 1.2$ to produce saturated strain hardening behavior, while σ_0/σ_{fc} is to be larger than 1.45 for polyvinyl alcohol (PVA) fiber reinforced ECC. However, this deterministic safety factor is empirical and supported by limited data, and its aim is to achieve saturated multiple cracking with high ductility, whereas different applications have various requirements of materials.

So, these two issues are identified as knowledge gaps for the further development of SHCC.

1.3 Research goal and objectives

To fill these two research gaps, an extended scale linking design philosophy, where the material composition (nanoscale) is added below the material microstructure, is proposed in this research as depicted in Fig. 1.3. Once the link

between the material composition and the material microstructure is established, the composite tensile strain hardening behavior can be now associated with the material composition, e.g. proportioning of ingredients, directly through a chemistry-based cement hydration model. On the other hand, the heterogeneity introducing the uncertainty of tensile strain hardening behavior, will be described by considering micromechanical parameters as random variables through probabilistic-based design approach.

Figure 1.3 Extended multiscale linking of SHCC design

The ultimate goal of this research is to develop a mix design method for SHCC which relates material properties with the material composition through multiscale and multiphysics models. To achieve this goal, three specific objectives are defined in this thesis as follows:

- 1) To develop probabilistic-based strain hardening criteria and micromechanical model which links material microstructure with heterogeneity to composite tensile strain hardening behavior and therefore uncertainty of ingredients and processing can be taken into consideration for SHCC mix design; and

- 2) To conduct a systematic investigation on the correlation between the material microstructure and the material composition of SHCC; and
- 3) To propose an SHCC mix design method based on the relations between the mix proportions and the ultimate mechanical behavior involving the compressive strength and tensile strength.

1.4 Research methodology

Fig. 1.4 is the conceptual framework of this research. Material properties, such as 2% in tensile strain capacity, can be specified by the end user as the design target. As expected, material properties are largely controlled by material microstructures. In the development of SHCC, micromechanics serves as a useful tool to link the material microstructure to the composite tensile strain hardening behavior. Besides the material microstructure, the heterogeneity introduces large uncertainty and has significant impact to the resulting material properties. One way to consider this uncertainty due to processing and variation of properties of ingredients in design is to extend current deterministic-based micromechanics model into a probabilistic-based model by considering micromechanical parameters, e.g. interfacial chemical bond, frictional bond, as random variables. A probability density function (PDF) can be used to describe the uncertainty of each variable and the PDF of each variable can be acquired from literature and/or experiments. Probabilistic-based strain hardening criteria can also be developed through the same manner.

In the lower triangle, the material microstructure can be associated with the material composition including types and proportioning of ingredients and maturity which is a function of age and curing method. Cement hydration model combined

with experimental investigation is engaged to relate the material composition and the maturity with the material microstructure. Focus is placed on relating each micromechanical parameter to material composition and maturity through literatures, cement hydration model, and/or experiments. This methodology represents a multiscale (from nanometer to centimeter) and multiphysics (including probabilistics, mechanics and chemistry) material design approach which is innovative and holistic.

Figure 1.4 Methodology of SHCC design

1.5 Research tasks

Fig. 1.5 shows the roadmap of this proposed research. Detailed research tasks are as follows,

Task 1: To develop the probabilistic-based micromechanics model (PMM)

Probability density function (PDF) can be used to describe the uncertainty of each micromechanical parameter. Thus, the strain hardening criteria can be translated into mathematical probability model with limit state surfaces (performance function). The pivotal step in developing the PMM is the explicit expression of performance index. An easy-to-interpret method called multivariate adaptive regression splines (MARS) is used to derive the prediction model of the performance index. After obtaining the performance functions, probabilistic assessment approaches such as first-order reliability method (FORM) can be used to assess the probability of failure P_f to predict the strain hardening behavior of the composites.

Task 2: Modeling the crack process and tensile ductility of SHCC

The strain hardening behavior of SHCC is governed by the number of sequential multiple cracking and the opening of cracks. The number of cracks is determined based on the distribution of the matrix cracking strength and the stress transfer distance between the fiber and the matrix. And the magnitude of the crack opening is distributed among cracks in the composite due to the randomness of the fiber dispersion as well as variations of interfacial properties. By considering the heterogeneity of the fiber, the interface and the matrix, a holistic method which connects the micromechanical parameters with composite properties is developed here. This method is numerically realized to model all the tensile properties involving distributed crack opening, distributed crack spacing, the crack evolution process, the first cracking strength and the ultimate tensile strength.

Task 3: To relate the material microstructure with the material composition and

maturity

In this research task, the effects of the material composition on each micromechanical parameter will be evaluated through experimental and/or numerical methods. Major factors of material composition (type and proportion) will be studied including fiber type, water-to-cement ratio, and sand-to-cement ratio. Experimental methods will be engaged in the investigation, such as single fiber pullout test, single fiber in-situ strength test, and wedge splitting test. In the numerical simulation, a cement hydration model will be contributed to reveal the mechanism of the microstructure in terms of chemical and physical properties of the hydration process.

Task 4: To develop mix design method for SHCC

Due to the existence of multivariate in the mix design and micromechanical parameters, an appropriate methodology is needed to link the mix composition with the ultimate composite performance. This methodology is proposed based on the requisite relation of mix composition and micromechanical parameters (Task 3) and the modeling of tensile stress-strain behavior using the micromechanical parameters as inputs (Task 1 and Task 2). It is not a direct way to acquire the designed mix composition with targeted performance, but a refined way of selecting the mix composition to achieve the target. For this method, the first step is to select the initial trial mix mainly based on compressive strength. After assessing the reliability of the trial mix, the designer can output the tensile behavior with satisfied performance, or conduct tailoring of the mix if the performance is not satisfied. The methodology is more like an easy-to-use engineering tool to facilitate the design process by the engineer.

Figure 1.5 Research roadmap

1.6 Layout of the thesis

The present thesis is intended to develop a mix design method for SHCC starting from the deterministic-based micromechanics model (DMM). In order to find an available and applicable design method, the variability of micromechanical parameters is considered in the micromechanics model as well as the prediction of ultimate composite performance. In addition, the requisite relation of mix design factors with micromechanical parameters is build up. This thesis consists of seven chapters.

Chapter 1 presents the background, motivation, objectives, methodology, and specified tasks and layout of this thesis.

Chapter 2 gives a condensed review of current design methods of cementitious materials as well as the state-of-the-art of SHCC design theory. Basics of probabilistic analysis are also introduced. In addition, some of the important experimental and numerical methods to relate the micromechanical parameters to the mix composition are reviewed as well.

Chapter 3, Chapter 4, Chapter 5 and Chapter 6 report the completion of the four tasks in sequence.

Overall conclusions from this study are summarized in Chapter 7, and some future works worthy of further investigations are outlined.

2 Literature Review

In this chapter, mix design methods for concrete, fiber reinforced concrete (FRC) and strain hardening cementitious composites (SHCC) are firstly discussed. Then the state-of-the-art of SHCC are reviewed, including the basics of engineered cementitious composites (ECC) design theory, the variability of micromechanical parameters and the modeling of the tensile stress-strain relation. In order to adopt the concept of probability, the probabilistic-based analysis methods are briefly introduced. Lastly, the methods to relate the mix composition and micromechanical parameters are illustrated, involving the experimental method as well as the information about cement hydration models.

2.1 Mix design methods for concrete, FRC and SHCC

Concrete mix design is the process of selecting suitable ingredients of concrete and determining their relative quantities, aiming to produce the most economical concrete while retaining the specified minimum properties such as strength, durability, and consistency. The following basic data is required for concrete mix proportioning:

- (i) Grade designation: It gives characteristic compressive strength of concrete.
- (ii) Type of cement;
- (iii) Maximum nominal size of aggregate;
- (iv) Maximum water-to-cement (w/c) ratio;
- (v) Minimum cement content;

- (vi) Workability;
- (vii) Exposure conditions;
- (viii) Type of aggregate;
- (ix) Use of admixtures.

The mix design procedure of British Standards (BS) method [6] and American Concrete Institute (ACI) method [7] provide a first approximation of the proportions and must be checked by trial batches. Taking the ACI method as example, the procedure to get the approximate mix proportion is shown in Fig. 2.1 [7]. Firstly, the amount of water and air is selected according to the workability and durability consideration. Secondly, water-to-cement (W/C) ratio is governed by desired compressive strength and limited by durability requirements. The rest should be simple manipulation with diagrams and tables based on large numbers of trial mixes, which allow an estimate of the required mix proportions for various conditions and permit predetermination on small unrepresentative batches.

In summary, the BS method (BS EN 206-1) and ACI method (ACI 211) of concrete mix design are mostly based on empirical relations, charts, graphs, and tables developed through extensive experiments and investigations using their own locally available materials. Both methods in general follow the same basic principles in selection of mix design parameters, but some procedural differences exist in each of these methods. As a result, the selected mix design parameters would be different as well.

Figure 2.1 The flowchart of ACI mix design of concrete [7]

For fiber reinforced concrete (FRC) that exhibits strain softening behavior, a similar mix design method for ordinary concrete is used to get the first trial mix with fibers being considered as coarse aggregate. Next, different approaches have been

proposed by the technical committees to optimize the FRC design. The proposals can be classified into two basic approaches, the σ - ε method where testing yields a load–deflection [8] and the σ - w method where testing yields a load–crack [9]. These approaches are based on simplified mechanics and geometry in meso level, which is distinct with the micromechanical model for SHCC.

Some technical committee claimed that the same method as FRC can be extended to apply into designing SHCC. Yet there is no formatted document reporting the validity of this kind of method and other applicable design method except the experimental method [10]. Whereas the micromechanical model of ECC pushes one step further to build up the mix design of SHCC by linking the micromechanical parameters to fiber bridging properties.

2.2 Current design theory of SHCC

2.2.1 Micromechanics-based design theory

ECC design philosophy-multiscale linking is demonstrated in Fig. 1.2, in which a micromechanical model links microscale parameters to fiber bridging behavior in the mesoscale, and the steady state crack analysis controls the fiber bridging property to achieve tensile strain hardening at the macroscale. The strain hardening behavior of ECC is achieved by sequential development of matrix multiple cracking. There are two fundamental requirements for multiple cracking. First for all, the steady-state flat crack extension can prevail under tension, which requires the crack tip toughness J_{tip} to be less than or equal to the complementary energy J_b' as Eqn. 2.1. J_{tip} stands for the energy to initiate a crack and the crack propagation, J_b' is the

maximum complementary energy to bridge the crack and can be calculated from the bridging stress σ_B versus crack opening δ curve, as illustrated in Fig. 2.2 [11].

Figure 2.2 σ - δ curve [11]

$$J_{tip} \leq \sigma_0 \delta_0 - \int_0^{\delta_0} \sigma(\delta) d\delta = J'_b \quad (2.1)$$

$$J_{tip} = \frac{K_{tip}^2}{E_m} \approx \frac{K_m^2}{E_m} \quad (2.2)$$

σ_0 is the maximum bridging strength corresponding to the opening δ_0 . K_m is the matrix fracture toughness, and E_m is the matrix Young's modulus. For small fiber volume fraction, K_{tip} can be simplified as the matrix toughness K_m . The other condition for the multiple cracking is that the first matrix cracking strength σ_{fc} must not exceed the maximum fiber bridging strength σ_0 .

$$\sigma_{fc} \leq \sigma_0 \quad (2.3)$$

where σ_{fc} is determined by the matrix fracture toughness K_m , pre-existing internal flaw size c and the fiber bridging constitutive law $\sigma_B(\delta)$. Eqn. 2.1 governs the crack propagation mode, while Eqn. 2.3 controls the initiation of cracks. Satisfactory of both Eqns. 2.1 and 2.3 is necessary to achieve the strain hardening behavior. Details of micromechanical model can be found in Yang et al. [12]. In some literature, the

investigation of first cracking strength also has been conducted [13, 14]. Here, both of the two issues are summarized as follows.

1) Fiber bridging model

Obviously, $\sigma_B(\delta)$ which describes the relationship between the bridging stress σ_B across the crack and the crack opening δ , is the key to establish the micromechanical model. Analytical tools of fracture mechanics, micromechanics and probabilistics are used to derive $\sigma_B(\delta)$. As a result, the $\sigma_B(\delta)$ curve is expressible as a function of micromechanical parameters listed in Fig. 2.3. In total, there are thirteen parameters in this model: five parameters describe fiber properties alone; for the matrix, there are three factors considered here and the interface properties are expressed by the chemical bond G_d , the interfacial frictional bond τ_0 and the slip hardening coefficient β . In addition, the snubbing coefficient f and the strength reduction factor f' are introduced to account for the interaction between fiber and matrix as well as the reduction of fiber strength when pulled at an inclined angle.

Figure 2.3 Micromechanical parameters of ECC

Due to the complexity of mathematical form of the $\sigma_B(\delta)$ relationship, the

numerical procedure is developed by Yang et. al as the flow chart in Fig. 2.4 [12]. It constructs starting from modeling a single fiber pullout behavior against the surrounding matrix. The $\sigma_B(\delta)$ relationship can then be obtained by averaging the contributions from fibers with different embedment length and orientation across the crack plane. For special fiber type like PVA fiber, two-way fiber debonding-pullout due to a slip-hardening interfacial bond is considered. Finally, matrix micro-spalling as well as Cook-Gordon effect are considered to refine the model.

Figure 2.4 Flow chart of the numerical procedure for computing $\sigma_B(\delta)$

2) The first cracking strength

The first cracking strength σ_{fc} has been theoretically clarified in the Reference [13, 14] for fiber pull-out type SHCC and the Reference [15] for fiber rupture type SHCC. In these literature, a simple penny shape flaw involved in the composite body, which is bridged by short random fibers as illustrated in Fig. 2.5. The fundamental notation was based on the equilibrium equation that the stress intensity factor due to applied remote loading K_L and fiber bridging K_B must balance the crack tip fracture toughness K_{tip} when the crack occurs:

$$K_L + K_B = K_{tip} \quad (2.4)$$

where K_L is expressed by hypothesizing a penny shaped crack in an infinite composite body subjected to remote loading σ ,

$$K_L = 2\sigma\sqrt{\frac{c}{\pi}} \quad (2.5)$$

K_B is obtained by integrating closure pressure due to fiber bridging over the crack profile.

$$K_B = -2\sqrt{\frac{c}{\pi}} \int_0^c \frac{\sigma_B[\delta(c)]}{\sqrt{c^2 - x^2}} dx \quad (2.6)$$

Figure 2.5 Flaw model for cracking strength estimation

The crack profile is assumed to be a half parabolic shape as

$$\delta = \frac{1}{2} \sqrt{c(1 - R^2)} \quad (2.7)$$

Finally, σ_{fc} is estimated by substituting Eqn. 2.5 and 2.6 into Eqn. 2.4.

$$\sigma_{fc} = \frac{1}{2} \sqrt{\frac{\pi}{c}} K_{tip} + \int_0^c \frac{\sigma_B[\delta(c)]}{\sqrt{c^2 - x^2}} dx \quad (2.8)$$

Note that σ_{fc} in Eqn. 2.8 is numerically calculated using the fiber bridging model $\sigma_B(\delta)$, which can be used in both fiber pullout type composites and fiber rupture type composites. Here, c is estimated assuming a penny-shaped flaw in an infinite composite, similar to derive K_L in Eqn. 2.5.

$$c = \left(\frac{\sqrt{\pi}}{2} \frac{K_m}{\sigma_{mu}} \right)^2 \quad (2.9)$$

where σ_{mu} is the tensile strength of the matrix.

The above theories for the fiber bridging properties and the first cracking strength are essential in this research, especially in modeling the tensile properties of SHCC.

2.2.2 Variability of macroscopic composite and microstructure

The design of structures composed of SHCC should be based on the statistical consideration of the properties. The stochastic properties of SHCC include:

- Compressive strength
- Young's modulus
- Tensile ultimate strength
- Tensile ultimate strain
- Crack spacing
- Crack opening

To illustrate, Fig. 2.6 shows an extreme case of tensile strain variability. The crack spacing of the multiple cracks is directly linked to the tensile strain capacity since the inelastic deformation derives from the opening magnitude and the number of multiple cracks in a representative volume element. A typical pattern of unsaturated multiple cracking can be seen from Fig. 2.7, showing a wide distribution of crack spacing. Normal, lognormal, and Weibull distributions were generally selected as potential distribution models that could represent the material property distribution [16]. Each of the distribution types has been used in various statistical studies on material properties [17-20].

Figure 2.6 Tensile behavior of SHCC samples from the same batch

Figure 2.7 Unsaturated multiple cracking of SHCC

Generally, the variability of SHCC is strongly influenced by the fabrication process, curing condition and testing, for example, the constraint mold size and the degree of compaction causes preferred orientation of the fibers in the composite. Telling from the mechanism, the statistical variability sourcing from the variation of all relevant micromechanical parameters include:

- 1) Variations of fiber properties (E_f , L_f , d_f , σ_{fu}) due to manufacturing or batching;
- 2) Variations in the concentration of fibers as Fig. 2.8 which influences the distribution of V_f .

Figure 2.8 SEM photo of an SHCC section (black dots are fibers) [21]

- 3) Variability in the interfacial bond properties (G_d , τ_0 , β); f and f' are varied with different fiber type.
- 4) Variation in initial flaw size (c) as Fig. 2.9 or matrix cracking strength (σ_{mu}) due to processing as well as cracks generated by shrinkage or other environmental effects at the time of testing.

Figure 2.9 Voids with various sizes in four SHCC sections sampled from a coupon specimen [21]

- 5) The matrix toughness K_m can fluctuate within a given member, although this may be difficult to measure directly.

The distribution of some micromechanical parameters was also discussed in the literature, such as normal distribution of d_f [22], normal distribution of L_f [23], Weibull distribution of σ_{mu} [24].

2.2.3 Modeling of the tensile stress-strain relation

Since the emergence of SHCC, many studies have been conducted on modeling the multiple cracking sequence and strain capacity. The uniqueness of SHCC exhibiting strain hardening behavior includes the co-existence of the progressively developed matrix damage and successive activation of bridging fibers across the cracks in the composite prior to final failure. There are mainly two ways to simulate the tensile ductility, namely, numerical modeling using finite element method [25-27] as well as analytical modeling based on relevant mechanics [28-30]. In this thesis, focus is placed on analytical analysis of multiple cracking mode as Fig. 2.10.

Figure 2.10 The photo and sketch of multiple cracking mode

The strain capacity of SHCC can be deduced using Eqns. 2.10 ~ 2.13 as follows,

$$\varepsilon = \frac{\Delta L}{L} = \frac{\sum_{i=1}^n \delta_i + \Delta L_e}{L} = \frac{\sum_{i=1}^n \delta_i}{L} + \varepsilon_e \quad (2.10)$$

$$\Delta L = \sum_{i=1}^n \delta_i + \Delta L_e \quad (2.11)$$

where δ_i is the cracking width; L is the gauge length of the specimen; ΔL_e is the elastic deformation; ε_e is the elastic strain which is negligible in most cases, e.g. $\sigma = 4 \text{ MPa}$, $E_c = 20 \text{ GPa}$, $\varepsilon_e = 0.02\%$; E_c is the elastic modulus of the composite; thus,

$$\varepsilon = \frac{\sum_{i=1}^n \delta_i}{L} \quad (2.12)$$

Assuming that the composite achieves full saturation of multiple cracking and uniform matrix strength, the average crack spacing is denoted as x and the average crack width as δ_{peak} , consequently,

$$\varepsilon = \frac{n\delta_{peak}}{nx} = \frac{\delta_{peak}}{x} \quad (2.13)$$

while $x \in (x_d, 2x_d)$, x_d is the minimum distance of fiber bridging stress in the existing crack transfers to the adjacent matrix to activate a new crack, the average crack

spacing was derived as $1.337x_d$ [31] based on the analogy with minimum average spacing between cars of length x_d and parked randomly along an infinite line, so

$$\varepsilon = \frac{\delta_{peak}}{1.337x_d} \quad (2.14)$$

For simplicity, the first approach is to use Eqns. 2.13 or 2.14 to estimate the strain capacity by early researchers. Aveston et al. [32] first proposed the conditions for multiple cracking in continuous aligned fiber reinforced brittle matrix composites, laying the foundation of subsequent research [28, 33]. In those models, identical flaw size in the matrix was assumed, and thereby deterministic composite strength during the multiple cracking was predicted. Regarding the nature of the distribution of crack spacing in composites, Wu and Li (1995) [28] studied the stochastic process of multiple cracking in fiber composites by a Monte Carlo simulation with an assumed Weibull-type function. A good agreement of composite strength and average crack spacing between experimental data and simulation results is found for PE fiber reinforced cement paste ($V_f = 2\%$). However, the observed crack width distribution was not considered in calculating the strain capacity. Suwannakarn (2009) [33] proposed a model based on a combination of composite mechanics and experimental observations to predict the stress-strain response of fiber reinforced cement composites. However, the prediction equations for average crack spacing and average crack width for SHCC reinforced with several types of fibers were simply derived with the function of the fiber volume only.

On the basis of the micromechanical composite design methodology of SHCC by Li and Leung [14], the mechanism of multiple cracking sequence and saturation is clarified in the Reference [34] by recognizing that SHCC must have variations in initial matrix flaw size and fiber bridging properties. At that stage, Kanda and Li

[11] suggested two performance indices, J_b'/J_{tip} and σ_0/σ_{fc} prompted by the two criteria of ECC design, correlating to the ultimate tensile strain with saturated multiple cracking. Subsequently, Kanda and Li [29] proposed a modeling method of the tensile stress-strain relation employing crack spacing modified by a probabilistic description of initial flaw size distribution, crack interaction, crack characteristic and fiber volume fraction. However, many parameters are required from experimental observations and need to be known to calibrate the model. They also suggested that the actual crack spacing should be higher than the crack spacing obtained from the modified Aveston-Cooper-Kelly theory (ACK) [35]. In conclusion, they suggested that it is possible to predict the crack spacing reasonably accurately.

The second way is to use more accurate calculation with Eqn. 2.12 involving two unknowns, the crack number n and the width of individual crack δ . The crack number can be determined based on the transfer distance x_d . Lu and Leung (2016) [30] adopted this concept to come up with a new analytical model which takes into consideration the effects of non-uniform matrix strength, the post-cracking increase in fiber bridging stress and fiber rupture on stress transfer. Yet, the crack width distribution was not considered in the model, which was still taken as constant among all cracks at each stress level. Nonetheless, it renders a good way to model the cracking process and tensile ductility of SHCC with full account of variations of the matrix and fiber distribution for further study.

2.3 Basics of probabilistic analysis

2.3.1 Probabilistic approach

A probabilistic approach provides an organized and systematic means by quantifying the uncertainties and their influences on the response. Fig. 2.11 illustrates a 3D joint probability density function (PDF) of the load S and the resistance R , with mean values denoted by m_s and m_R , respectively [36, 37]. First of all, a limit state of one situation that separates the desired states has to be defined. Considering two criteria of SHCC as mentioned in Section 2.2.1, two limit states are inferred to be satisfied coincidentally in order to achieve strain hardening behavior. It is usual to write the limit state surface (performance function) as

$$g(X) = R(X_1, \dots, X_j) - S((X_{j+1}, \dots, X_n)) = 0 \quad (2.15)$$

where X_i are random variables. Mathematically, $R > S$ or $g(x) > 0$ denote the ‘safe’ domain, while $R < S$ or $g(x) < 0$ denote the ‘failure’ domain. The probability of failure P_f is the integral of the PDF over the failure domain as indicated by the volume $abcd$ in Fig. 2.11.

Figure 2.11 3D Joint PDF

To express the relationship in terms of probability, the design formula becomes

$$P\{R - S < 0\} < P_{acc} = \phi(-\alpha) \quad (2.16)$$

where P is the probability that the failure event occurs; P_{acc} is the accepted value of the probability of failure; ϕ is the distribution function of the standard normal distribution; α is the reliability index.

2.3.2 Methods to obtain limit state functions

Multivariate adaptive regression splines (MARS) is a nonparametric regression method to model the nonlinear responses between input variables and output introduced by Friedman in 1991 [37]. The main advantages of MARS are of its capacity to deal with high dimensional data and easy to interpret the model. Extensive applications of MARS include estimating the deformation of asphalt mixtures, analyzing shaking table tests of reinforced soil wall and analysis of geotechnical engineering systems [38-40]. MARS attempts to approximate complex relationships by taking the form of linear combination of basic functions (BFs) and their interactions expressed as

$$f(x) = c_0 + \sum_{i=1}^M c_i BF_i(x) \quad (2.17)$$

where x is an independent variable, the coefficient c is the constant estimated by the least-squares method, $BF_i(x)$ is a basis function (BF). BFs are piecewise linear or piecewise cubic functions. For simplicity, only piecewise linear is expressed here, which is of the form $\max(0, x - t)$ or $\max(x - t, 0)$ with t being the knot schematically expressed in Fig. 2.12.

Figure 2.12 Basis function (BF)

The knot t marks the end point of data of each region and the starting of another, and its determination is the key challenge addressed by MARS search algorithm. The MARS model is a data-driven process, mixing up the paired types of BFs and coming up with appropriate values of c by searching in a stepwise manner.

MARS builds a model in two phases: the forward and the backward stage. The forward stage repeatedly adds BFs in pairs to the model until the change in residual error is too small or the maximum number of BFs is reached, which often results in an over-fitted models. Then the backward stage prunes the model by removing BFs one by one until the process finds the best sub-model using the Generalized Cross-Validation (GCV) criterion described below. The loss of GCV is the measure to assess the importance of the removed BFs associated with a variable.

$$GCV_{\lambda} = \frac{\frac{1}{N} \sum_{i=1}^N [y_i - f_{\lambda}(x_i)]^2}{\left[1 - \frac{M_{\lambda}}{N}\right]^2} \quad (2.18)$$

$$M_{\lambda} = M + d \times (M - 1)/2 \quad (2.19)$$

where λ is the optimal model term, N is the number of observations, $f_{\lambda}(x_i)$ denotes the predicted values of the best estimation model, M_{λ} is the effective number in the

model which is expressed in terms of the number of BFs denoted as M and the number of knots $(M - 1)/2$ and d is the penalizing parameter. Other measures of goodness of fit listed in Table 2.1 can be used to assess the accuracy of the regression model in contrast to the “true” function or data points.

Table 2.1 Measures of goodness of fit

Measure	Calculation formulas
Coefficient of determination (R^2)	$R^2 = 1 - \frac{\frac{1}{n} \sum_{i=1}^n (y_i - f(x_i))^2}{\frac{1}{n} \sum_{i=1}^n (y_i - \bar{y})^2}$
Mean Squared Error (MSE)	$MSE = \frac{1}{n} \sum_{i=1}^n (y_i - f(x_i))^2$
Mean Absolute Error (MAE)	$MAE = \frac{1}{n} \sum_{i=1}^n y_i - f(x_i) $

n is the number of data points in the selected dataset; $\bar{y}$ is the mean value of all the data points y_i ; $f(x_i)$ is the prediction value of MARS model.

The adaptive regression splines toolbox for Matlab is used to build the MARS model [41]. Fig. 2.13 illustrates a typical example of how MARS would attempt to fit data, in a three dimensional space as the following two-variable function

$$y = \sin(0.83\pi x_1) \cos(1.25\pi x_2) \quad (2.20)$$

It can be approximated using 45 BFs of linear splines with high R^2 values of 0.9976.

Figure 2.13 Surface fitting using MARS with 45 BF's of linear splines

Based on the optimal MARS model, the procedure known as analysis of variance (ANOVA) decomposition can be used to assess the contributions of input variables in the model. In this thesis, the performance indices J_b' and σ_0 of the micromechanical model will be conducted by MARS fitting instead of the numerical solution.

2.4 Methods to relate micromechanical parameters with mix composition

2.4.1 Experimental determination

All micromechanical parameters of SHCC were independently measured or deduced. Among them, fiber parameters E_f , L_f , and d_f are measurable with good accuracy with a single fiber test. The apparent fiber strength σ_{fu} and fiber strength reduction coefficient f' are measured by a single fiber in-situ strength test [42]. The interface properties τ_0 , G_d , β can be measured by single fiber pullout test. Matrix Young's modulus E_m is determined from the compressive strength and fracture

toughness K_m also can be measured experimentally.

1) Fracture toughness K_m

For the determination of matrix properties, four main techniques are recommended including a three-point bending test on a notched beam, single or double notched plate tensile test, compaction tension test on cubical specimens, and wedge splitting test on cubical or cylindrical specimens [43-45]. For the bending test, although the self-weight effect is considered to do correction, it may overestimate the fracture energy due to the crushing near the supports. While direct tensile tests are not easy to carry out. The drawback of the compact tension test is the difficulty to capture the crack opening displacement and the post peak behavior.

The wedge splitting test (WST), originally introduced by Linsbauer and Tschegg in 1986 [46] and improved by Brühwiler and Wittmann [47] is a suitable method for obtaining the fracture energy and fracture toughness. The method has been proved to be reliable for the determination of fracture properties of concrete [48], high-strength concrete [49, 50], and fiber reinforced concrete [51], among others. Zhao et al. [52] highly recommended this technique after working on the fracture energy and the fracture toughness of concrete specimens of various sizes, and pointed out that a significant size effect exists. But the initial notch length was incorrectly regarded as the critical crack length during the calculation. So Kim and Kim [50] verified the validity of a crack mouth opening displacement (CMOD) calibration technique by comparisons with other methods in order to get correct critical crack length.

In this research, the WST method is used for the matrix toughness based on the specimen size in the Reference [52] with its interpretation formulas as Eqns. 2.22 ~

2.24 and the critical crack length procurement from CMOD in the Reference [53] as Eqn. 2.21. Fig. 2.14 shows the typical curve from a mortar matrix fracture test.

Figure 2.14 Typical curve from a mortar matrix fracture test

$$\text{CMOD}_c = \frac{P_c}{BE} \left[11.56 \left(1 - \frac{a_c}{D} \right)^{-2} - 9.397 \right] \quad (2.21)$$

$$K_{ic} = (K_m) = \frac{P_c}{B\sqrt{D}} F(\alpha) \quad (2.22)$$

$$F(\alpha) = 29.6\alpha^{0.5} - 185.5\alpha^{1.5} + 665.7\alpha^{2.5} - 1017.0\alpha^{3.5} + 638.9\alpha^{4.5} \quad (2.23)$$

$$\alpha = \frac{a_c}{D} \quad (2.24)$$

where B is the thickness of the specimen; D is the depth of specimen; a_c is the effective crack length. E is the elastic modulus of the matrix; P_c and CMOD_c are the critical (peak) load and critical CMOD which are recorded by the test.

2) Interfacial properties G_d, τ_0, β

A variety of fiber pull-out models [54-56] are available to interpret the experimental data into interface bond properties. In the present research, bond properties of polyvinyl alcohol (PVA) fibers in a mortar matrix were investigated

with the simplified model of Lin et al. [57]. The derivation included in the present study is only an approximate solution to this complicated problem, based on simplified force and energy balance. The attempt has been made to capture the physical essence of the interfacial parameters in a simple, easy-to-use formulation without getting into complex mathematics. In the existing micromechanics model, the fiber dispersion effect and the statistical distribution of fiber strength are not included.

The pull-out behavior of an embedded fiber from the matrix can be divided into the debonding process and the pullout process. The former process is controlled by chemical bond and frictional bond, the latter process is governed by frictional bond only. The interface chemical bond energy G_d , frictional bond strength τ_0 , and slip-hardening coefficient β , can be calculated from the load-displacement curve recorded during the test (Fig. 2.15).

$$G_d = \frac{2(P_a - P_b)^2}{\pi^2 E_f d_f^3} \quad (2.25)$$

$$\tau_0 = \frac{P_b}{\pi d_f l_e} \quad (2.26)$$

$$\beta = \frac{d_f}{l_e} \left(\frac{1}{\tau_0 \pi d_f} \frac{\Delta P}{\Delta S'} \Big|_{s' \rightarrow 0} + 1 \right) \quad (2.27)$$

Figure 2.15 General profile of a single fiber pullout curve

2.4.2 Modeling of cement hydration

In order to look into the relationship between the mix composition and the microstructure of SHCC, cement hydration is intermediate media. From the view of microstructure formation, the fracture of the matrix and the interfacial bond of fiber are highly related to the chemical reaction of constituents in nature. Therefore, cement hydration is the original and paramount process needed to be studied. Comprehensive effort has been put to study the cement hydration in concrete, both experimentally and numerically. Numerical modeling provides a useful tool to describe the hydration reactions.

In the late 1980s, Johnson and Jennings simulated the cement hydration based on nucleation and growth of spherical particles in 3D space [58]. HYMOSTRUC built by van Breugel [59] is the representative model of the former principle. The emphasis of this kind of model is on the formation of the microstructure and the physical properties related to the bulk, while the evolution of hydrated products is

less focused. Integrated particle kinetics model (IPKM) [60] and μic [61] are improved models that assume that the Calcium Silicate Hydrate (CSH) deposits on the surface of cement particles and the formation of Portlandite (CH) takes place in pores. Their drawbacks are low efficiency and small number of particles as a result of explicit calculation of all possible interactions.

Afterwards, discretization approach was extensively studied and applied in the numerical simulation. Bentz and Garboczi [62] launched a new model called CEMHYD3D with cellular automata rules applied to digital images. It can accurately represent the microstructure, but little or no kinetic information and is rule-based to mimic reaction and diffusion. A new model called HydratiCA [63] has been developed by National Institute of Standards and Technology (NIST), in which microstructure and chemistry are being simultaneously simulated.

2.5 Summary

SHCC has been applied in a few infrastructures owing to its excellent tensile behavior but comparable compressive strength with normal concrete. It is a promising material for application, especially with respect to potentially reducing the maintenance cost and the repair expense; thereby the life cycle cost will be reduced for infrastructures. The new added functions of SHCC are also used to improve the safety, durability, and sustainability of infrastructure systems. While the micromechanics model of ECC represents the state-of-the-art design approach of SHCC, no systematic investigation on the correlation between material microstructure and material composition exists. Controlling microstructure through ingredients selection and component tailoring remains empirical. Thus, there is a

need to develop a mix design method for SHCC.

ECC design theory adopts a multiscale linking approach from micro level to macro level which can be extended for SHCC mix design if the following two research objectives are fulfilled.

- 1) Considering the heterogeneity of the composite involving the variation of fiber properties, the fiber distribution and the flaw size distribution, the cracking process and tensile ductility of SHCC should be modelled deliberately with certain confidence levels using the probabilistic-based approach.
- 2) To understand the correlation between mix composition and micromechanical parameters through experimental methods as well as numerical tools like Virtual Cement and Concrete Testing Laboratory (VCCTL) software.

3 Probabilistic-based Micromechanics

Model based on Multivariate Adaptive

Regression Splines (MARS)

3.1 Introduction

In this chapter, a novel and holistic probabilistic-based micromechanics model (PMM) is proposed for evaluating the strain hardening behavior of SHCC, in which the failure domain is defined as the prevailing of strain softening failure mode when Eqns. 3.1 and/or 3.2 are/is violated. The boundary separating the safe and failure domain is the limit state surface (performance function) [36] defined as:

$$G(x) = J_b' - J_{tip} = 0 \quad (3.1)$$

$$F(x) = \sigma_0 - \sigma_{fc} = 0 \quad (3.2)$$

where x denotes random variables. Mathematically, $J_b' > J_{tip}$ and $\sigma_0 > \sigma_{fc}$ or $G(x) > 0$ and $F(x) > 0$ denote the ‘safe’ domain, while $J_b' < J_{tip}$ and $\sigma_0 < \sigma_{fc}$ or $G(x) < 0$ and $F(x) < 0$ denote the ‘failure’ domain. For ECC, the limit state surfaces $G(x)$ and $F(x)$ are not known explicitly because performance indices J_b' and σ_0 are known only implicitly through a numerical procedure in Section 2.2.1. Thus, closed-form limit functions of J_b' and σ_0 are necessarily constructed using a regression method. The more advanced regression method called multivariate adaptive regression splines (MARS) is adopted here.

After obtaining the performance functions, probabilistic assessment approaches such as first-order reliability method (FORM) [64] can be used to

calculate the failure probability P_f of the composite to predict the strain hardening behavior. The calculation of P_f includes the determination of joint probability distribution of performance indices (J_b , J_{tip} and σ_0 , σ_{fc}) given the distribution of random variables and the integration of probability density function (PDF) over the failure domain. In FORM, random variables are assumed as standard normal distributions, then P_f can be calculated by

$$P_{f1} = P \{G(x) < 0\} \approx \phi(-\alpha_1) \quad (3.3)$$

$$P_{f2} = P \{F(x) < 0\} \approx \phi(-\alpha_2) \quad (3.4)$$

where P is the probability that the failure event occurs; ϕ is the distribution function of the standard normal distribution; and α is the reliability index computed as

$$\alpha = \min \sqrt{\left(\frac{x_i - \mu_i}{\sigma_i}\right)^T [R]^{-1} \left(\frac{x_i - \mu_i}{\sigma_i}\right)} \quad (3.5)$$

where x_i is the random variable; μ_i and σ_i are the mean value and the standard deviation of the random variable, respectively; and R is the correlation matrix.

In conclusion, the design framework of the probabilistic-based micromechanics model (PMM) is depicted stepwise as Fig. 3.1. It consists of three steps and reaches the goal of reliability analysis of the specific composite. In step I, since a multivariate regression method is used to build up the prediction model for J_b and σ_0 , sufficient amount of data is prerequisite which can be acquired using the existing deterministic-based micromechanics model as described in Section 3.2. For step 2, a Matlab/Octave toolbox named ARESLab is applied for building the MARS model, outputting the prediction model in Section 3.3. Finally, eleven cases sourced from the previous literature are used to conduct the probabilistic analysis to relate the strain capacity and the failure probability in Section 3.4.

Figure 3.1 Framework of probabilistic-based micromechanics model (PMM)

3.2 Create database for J_b' and σ_0

In search of explicit prediction models for J_b' and σ_0 , a sound and large enough database is created using the deterministic-based micromechanics model of Section 2.2.1. In this existing model, each group of micromechanical parameters for each SHCC mixture is treated as inputs into the numerical procedure as Fig. 2.4 and it outputs the corresponding values of performance index J_b' and σ_0 . A number of groups of inputs and outputs are acquired for further conducting the establishment of the prediction model by regression fitting method. In this study, ten relevant micromechanical parameters (denoting x_1 to x_{10} as input variables) and two performance indexes (denoting y_1 and y_2 as outputs) are shown in Table 3.1, the selected values are typical ones in PE fiber [65], PVA fiber [66] and polypropylene (PP) fiber reinforced cementitious composites [5]. All combinations of input variables are used as input groups to get corresponding outputs, except that some outliers which may lead to a crude model, are removed using the residual analysis.

Thereof, 527 groups (75%) of the observations were randomly selected for training and the remaining 175 groups (25%) used as testing data.

Table 3.1 Summary of input variables and output

Inputs and outputs	Parameters		Observations		
			PE	PVA	PP
Input variables	x1	E_f (GPa)	120	22, 42.8	11.6
	x2	L_f (mm)	12.7, 19	10	8, 19
	x3	d_f (μm)	20, 38	40	16.6
	x4	σ_{fu} (MPa)	2700	1060, 1620	400, 928
	x5	V_f (%)	0.5, 1, 1.5, 2	1, 2, 3	2, 4, 6
	x6	G_d (J/m ²)	0	0.5, 2.5, 5.0	0, 1.5
	x7	τ_0 (MPa)	0.3, 0.6, 0.9, 1.5	0.5, 1.5, 3, 5	0.5, 1, 3
	x8	β	0	0.05, 0.5, 5	0.005
	x9	f'	0.5	0.3	0.1
	x10	f	0.5, 0.8	0.2, 0.5	0.39
Outputs	y1	J_b' (J/m ²)			
	y2	σ_0 (MPa)			

3.3 The prediction model of performance indices J_b' and

σ_0

Based on the MATLAB platform, two sets of program code for MARS model of J_b' and σ_0 are written using ARESLab toolbox as Appendix I. Table 3.2 lists the MARS model of J_b' and σ_0 . Piecewise linear and piecewise cubic basis functions (BFs) with the maximum interaction of 2 are applied. By comparison, a piecewise linear function is selected for the following studies because it can reach high accuracy with less complexity and computational time. High R^2 approaching 1 and low GCV are obtained as a result of the large database though high dimensions. A summary of basis functions (BFs) and the final model of J_b' and σ_0 is listed in Table

3.3 and 3.4. Using the final model, the prediction for training data and testing data is graphically illustrated in Figs. 3.2 and 3.3, a good agreement is achieved as can be seen from high R^2 values.

Table 3.2 MARS model to predict J_b' and σ_0

Outputs	MARS model			
	J_b'		σ_0	
Type of BFs	Piecewise	Piecewise	Piecewise	Piecewise
No. of BFs	63	63	51	51
CPU time (s)	83.9	84.8	28.5	29.2
Max interaction	2	2	2	2
GCV	196.537	207.266	0.156	0.169
R^2 of training data	0.963	0.961	0.993	0.993
R^2 of testing data	0.960	0.960	0.993	0.993
MSE of training data	97.403	102.720	0.090	0.098
MSE of testing data	154.447	156.825	0.097	0.094
MAE of training data	7.495	7.793	0.206	0.218
MAE of testing data	9.149	9.138	0.226	0.226

Table 3.3 Basis functions and corresponding equations of MARS model for J_b'

Basis function	Equation	Basis function	Equation
BF1	$\max(0, x4 - 1620)$	BF32	$\text{BF8} * \max(0, x7 - 3)$
BF2	$\max(0, 1620 - x4)$	BF33	$\text{BF8} * \max(0, 3 - x7)$
BF3	$\max(0, x1 - 22)$	BF34	$\max(0, 2 - x5) * \max(0, x7 - 1.5)$
BF4	$\max(0, 22 - x1)$	BF35	$\text{BF9} * \max(0, x4 - 928)$
BF5	$\max(0, x7 - 1.5)$	BF36	$\text{BF9} * \max(0, 928 - x4)$
BF6	$\max(0, 1.5 - x7)$	BF37	$\max(0, x6 - 0.5)$
BF7	$\max(0, x10 - 0.5)$	BF38	$\text{BF6} * \max(0, x2 - 10)$
BF8	$\max(0, 0.5 - x10)$	BF39	$\text{BF6} * \max(0, 10 - x2)$
BF9	$\max(0, x5 - 2)$	BF40	$\text{BF13} * \max(0, 2 - x5)$
BF10	$\text{BF6} * \max(0, x8 - 0.05)$	BF41	$\text{BF14} * \max(0, x7 - 3)$
BF11	$\text{BF6} * \max(0, x4 - 1060)$	BF42	$\text{BF37} * \max(0, 3 - x5)$
BF12	$\text{BF6} * \max(0, 1060 - x4)$	BF43	$\max(0, 3 - x7)$
BF13	$\max(0, x8 - 0.5)$	BF44	$\text{BF5} * \max(0, x1 - 22)$
BF14	$\max(0, 0.5 - x8)$	BF45	$\text{BF8} * \max(0, 0.5 - x8)$
BF15	$\text{BF14} * \max(0, x7 - 1.5)$	BF46	$\text{BF6} * \max(0, 3 - x5)$
BF16	$\text{BF14} * \max(0, 1.5 - x7)$	BF47	$\text{BF43} * \max(0, x4 - 1060)$

BF17	BF6 * max(0, 0.5 - x10)	BF48	BF43 * max(0, 1060 - x4)
BF18	max(0, 2 - x5) * max(0, x4 - 1620)	BF49	BF3 * max(0, x8 - 0.5)
BF19	max(0, 2 - x5) * max(0, 1620 - x4)	BF50	max(0, 0.5 - x6) * max(0, x7 - 0.9)
BF20	BF2 * max(0, x1 - 22)	BF51	max(0, 0.5 - x6) * max(0, 0.9 - x7)
BF21	BF2 * max(0, 22 - x1)	BF52	BF9 * max(0, 1 - x7)
BF22	BF8 * max(0, x4 - 1060)	BF53	BF6 * max(0, x6 - 1.5)
BF23	BF2 * max(0, x7 - 1.5)	BF54	BF43 * max(0, x2 - 10)
BF24	BF2 * max(0, 1.5 - x7)	BF55	BF43 * max(0, 10 - x2)
BF25	BF2 * max(0, 0.5 - x8)	BF56	max(0, 2 - x5) * max(0, 12.7 - x2)
BF26	BF3 * max(0, x7 - 3)	BF57	BF37 * max(0, 3 - x7)
BF27	BF3 * max(0, 3 - x7)	BF58	BF37 * max(0, x2 - 8)
BF28	BF8 * max(0, 2 - x5)	BF59	BF2 * max(0, x2 - 8)
BF29	BF3 * max(0, x5 - 2)	BF60	max(0, 0.5 - x6) * max(0, 19 - x2)
BF30	BF3 * max(0, 2 - x5)	BF61	BF43 * max(0, x6 - 2.5)
BF31	BF3 * max(0, 0.8 - x10)	BF62	BF43 * max(0, 2.5 - x6)

$$\begin{aligned}
J_b' = & 168.93 + 0.25021 * BF1 - 0.1852 * BF2 - 5.4929 * BF3 + 147.13 \\
& * BF4 - 26.599 * BF5 - 141.44 * BF6 - 452.17 * BF7 \\
& + 208.36 * BF8 + 24.914 * BF9 + 8.0609 * BF10 - 0.13195 \\
& * BF11 - 1.5583 * BF12 + 4.7813 * BF13 - 185.62 * BF14 \\
& + 87.388 * BF15 + 143.55 * BF16 - 330.29 * BF17 \\
& - 0.12054 * BF18 + 0.063491 * BF19 + 0.0036486 * BF20 \\
& - 0.2108 * BF21 + 0.27334 * BF22 + 0.022747 * BF23 \\
& + 0.13338 * BF24 + 0.11329 * BF25 - 2.1056 * BF26 \\
& + 1.7412 * BF27 - 92.018 * BF28 - 0.68224 * BF29 \\
& + 1.0456 * BF30 - 4.3893 * BF31 - 20.231 * BF32 \\
& + 46.105 * BF33 + 8.7863 * BF34 + 0.021826 * BF35 \\
& - 0.036856 * BF36 - 32.695 * BF37 + 9.5053 * BF38 \\
& + 72.135 * BF39 - 3.6065 * BF40 - 72.808 * BF41 \\
& + 1.7067 * BF42 - 249.29 * BF43 + 2.484 * BF44 - 90.034 \\
& * BF45 + 22.907 * BF46 + 0.026139 * BF47 + 1.4257 \\
& * BF48 - 0.095552 * BF49 + 122.48 * BF50 - 172.35 \\
& * BF51 + 16.932 * BF52 - 16.461 * BF53 - 8.7344 * BF54 \\
& - 73.274 * BF55 - 24.45 * BF56 + 134.24 * BF57 + 14.183 \\
& * BF58 - 0.019171 * BF59 - 28.279 * BF60 - 134.48 \\
& * BF61 + 135.19 * BF62 \quad (3.6)
\end{aligned}$$

Table 3.4 Basis functions and corresponding equations of MARS model for σ_0

Basis function	Equation	Basis function	Equation
BF1	$\max(0, x5 - 3)$	BF26	$\max(0, 0.05 - x8) * \max(0, 0.6 - x7)$
BF2	$\max(0, 3 - x5)$	BF27	$BF16 * \max(0, x5 - 2)$
BF3	$\max(0, 1.5 - x7)$	BF28	$BF16 * \max(0, 2 - x5)$
BF4	$\max(0, x4 - 1620)$	BF29	$BF16 * \max(0, x7 - 3)$
BF5	$\max(0, 1620 - x4)$	BF30	$\max(0, 0.5 - x8)$
BF6	$\max(0, x7 - 1.5) * \max(0, x5 - 3)$	BF31	$BF3 * \max(0, x10 - 0.5)$
BF7	$\max(0, x7 - 1.5) * \max(0, 3 - x5)$	BF32	$BF3 * \max(0, 0.5 - x10)$
BF8	$\max(0, x8 - 0.05)$	BF33	$\max(0, 0.39 - x10)$
BF9	$BF5 * \max(0, x7 - 1)$	BF34	$BF2 * \max(0, 0.39 - x10)$
BF10	$BF5 * \max(0, 1 - x7)$	BF35	$BF2 * \max(0, x2 - 12.7)$
BF11	$BF2 * \max(0, x7 - 0.5)$	BF36	$BF2 * \max(0, 12.7 - x2)$
BF12	$BF2 * \max(0, 0.5 - x7)$	BF37	$BF30 * \max(0, 1.5 - x7)$
BF13	$BF2 * \max(0, x4 - 1620)$	BF38	$BF4 * \max(0, x7 - 0.9)$
BF14	$BF2 * \max(0, 1620 - x4)$	BF39	$BF4 * \max(0, 0.9 - x7)$
BF15	$\max(0, x7 - 1.5) * \max(0, x10 - 0.2)$	BF40	$BF30 * \max(0, 2700 - x4)$
BF16	$\max(0, x3 - 20)$	BF41	$BF3 * \max(0, x6 - 1.5)$
BF17	$BF2 * \max(0, x8 - 0.05)$	BF42	$BF30 * \max(0, 3 - x7)$
BF18	$BF2 * \max(0, 0.05 - x8)$	BF43	$\max(0, x10 - 0.39) * \max(0, x8 - 0.5)$
BF19	$\max(0, x2 - 12.7)$	BF44	$\max(0, x1 - 11.6)$
BF20	$\max(0, 12.7 - x2)$	BF45	$\max(0, x10 - 0.39) * \max(0, 1620 - x4)$
BF21	$BF5 * \max(0, x8 - 0.05)$	BF46	$BF44 * \max(0, 1.5 - x7)$
BF22	$BF5 * \max(0, 0.05 - x8)$	BF47	$BF16 * \max(0, x7 - 0.6)$
BF23	$\max(0, x7 - 1.5) * \max(0, x8 - 0.05)$	BF48	$BF16 * \max(0, 0.6 - x7)$
BF24	$\max(0, x7 - 1.5) * \max(0, 0.05 - x8)$	BF49	$BF2 * \max(0, 3 - x7)$
BF25	$\max(0, 0.05 - x8) * \max(0, x7 - 0.6)$	BF50	$BF5 * \max(0, x5 - 4)$

$$\begin{aligned}
\sigma_0 = & 13.7 + 2.8519 * BF1 - 3.1749 * BF2 - 5.0982 * BF3 + 0.0032472 \\
& * BF4 - 0.0064076 * BF5 + 0.95632 * BF6 + 1.491 * BF7 \\
& + 0.52096 * BF8 - 0.00042556 * BF9 + 0.0076495 * BF10 \\
& - 1.6037 * BF11 + 6.7053 * BF12 - 0.0018135 * BF13 \\
& + 0.0021424 * BF14 - 0.35353 * BF15 - 0.1511 * BF16 \\
& - 0.1168 * BF17 + 31.133 * BF18 + 0.38676 * BF19 \\
& + 0.33325 * BF20 - 0.00021301 * BF21 - 0.069562 * BF22 \\
& - 0.057197 * BF23 - 132.39 * BF24 + 94.849 * BF25 \\
& - 278.23 * BF26 - 0.069113 * BF27 + 0.064422 * BF28 \\
& - 0.016687 * BF29 - 2.9675 * BF30 + 1.3719 * BF31 \\
& - 4.5199 * BF32 + 6.2698 * BF33 - 1.8568 * BF34 \\
& - 0.13507 * BF35 - 0.13896 * BF36 + 3.0939 * BF37 \\
& - 0.0055437 * BF38 + 0.0037122 * BF39 + 0.0018169 \\
& * BF40 - 0.27539 * BF41 - 1.2099 * BF42 - 0.67765 \\
& * BF43 - 0.0064915 * BF44 + 0.0042706 * BF45 \\
& - 0.016604 * BF46 + 0.046666 * BF47 + 0.094019 * BF48 \\
& + 0.16612 * BF49 - 0.0011965 \\
& * BF50
\end{aligned} \tag{3.7}$$

Figure 3.2 MARS prediction for J_b' of: (a) training data and (b) testing data

Figure 3.3 MARS prediction for σ_0 of: (a) training data and (b) testing data

The MARS model can automatically prune the model by removing the extraneous variables with the lowest contribution and the relative importance assessment of all variables is processed using the ANOVA procedure. Table 3.5 displays the ANOVA decomposition of the built MARS model for J_b' and σ_0 . The first column lists the ANOVA function number. The second column gives an indication of the importance of the corresponding ANOVA function, by listing the GCV score for a model with all BFs corresponding to that particular ANOVA function removed. This GCV score can be used to evaluate whether the ANOVA function is making an important contribution to the model, or whether it just marginally improves the global GCV score. The third column gives the particular input variables associated with the ANOVA function. Fig. 3.4 gives the plots of the

relative importance of the input variables for the two MARS models. It can be observed that variable 1 (E_f) and variable 7 (τ_0) are the two most important parameters to affect the maximum complementary energy J_b' of fiber bridging. Variable 5 (V_f), variable 4 (σ_{fu}), variable 3 (d_f) and variable 7 (τ_0) are significantly important in determining the fiber bridging strength σ_0 .

Table 3.5 ANOVA decomposition of MARS model

Function	J_b'		σ_0	
	GCV	Variable(s)	GCV	Variable(s)
1	440106	x1	0.32	x1
2	36530	x4	2.48	x2
3	1019	x5	13.16	x3
4	13670	x6	17.77	x4
5	344792	x7	36.26	x5
6	7851	x8	11.19	x7
7	5945	x10	4.72	x8
8	751525	x1, x4	1.04	x10
9	3021	x1, x5	0.73	x1, x7
10	48959	x1, x7	0.81	x2, x5
11	218	x1, x8	1.79	x3, x5
12	4300	x1, x10	8.15	x3, x7
13	3892	x2, x4	5.53	x4, x5
14	2680	x2, x5	2.99	x4, x7
15	13134	x2, x6	1.03	x4, x8
16	5943	x2, x7	0.18	x4, x10
17	4935	x4, x5	7.69	x5, x7
18	182513	x4, x7	2.60	x5, x8
19	901	x4, x8	0.30	x5, x10
20	831	x4, x10	0.19	x6, x7
21	262	x5, x6	2.26	x7, x8
22	1045	x5, x7	0.39	x7, x10
23	249	x5, x8	0.18	x8, x10
24	413	x5, x10		
25	330745	x6, x7		
26	3678	x7, x8		
27	758	x7, x10		
28	234	x8, x10

Figure 3.4 Relative importance of the input variables selected in the MARS model:

(a) J_b' ; and (b) σ_0

3.4 Reliability analysis of strain hardening behavior of SHCCs

3.4.1 First order reliability method (FORM)

To perform the reliability assessment, the FORM for simplicity is selected to assess the failure probability of both criteria of Eqns. 3.1 and 3.2. In the FORM procedure, the performance functions and MARS models are incorporated into an

EXCEL spreadsheet using the approach developed by Low and Tang [67]. Fig. 3.5 illustrates the analysis procedure with FORM.

In the Distribution column, many options can be selected such as Normal, Lognormal, Uniform, Weibull, Gamma and so on. The Para 1 and Para 2 column list the relevant parameters to describe the distribution type, taking Normal distribution for example, they are the mean value and standard deviation of variables. The built MARS models for J_b' and σ_0 in Eqns. 3.6 and 3.7 are formatted into MARS column as Fig. 3.5 (a) and 3.5 (b). The design point (x_i^*) was obtained using Microsoft EXCEL's built-in optimization routine SOLVER with minimizing α in cell X2 and W2, subject to the constraint of the performance functions of $G(x)$ and $F(x)$ in Eqns. 3.1 and 3.2. The iterative numerical search for x_i^* is automatic starting from the mean values of the original random variables by setting $n_i = 0$ initially, whereby x_i^* is a function of n_i . P_{f1} and P_{f2} are the failure probability of the two criteria.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y		
1	Distribution	Para1	Para2	x_i*	MARS					Correlation matrix [R]													n_i	G(x)	α₁	P_{f1}	
2	Uniform	<i>E_f</i>	41.1	41.1	41.1	BF1=	0	BF32=	0	1	0	0	0	0	0	0	0	0	0	0	0	0	-5E-07	-2E-08	1.8898	2.94%	
3	Normal	<i>L_f</i>	10	2	10	BF2=	550	BF33=	0	0	1	0	0	0	0	0	0	0	0	0	0	0	-5E-07	<div>$G(x) = J_{\delta'} - J_{tip}$<div><div></div><div></div></div><div>Eqn. 2.2</div><div>Predicted MARS model as Eqn. 3.6</div></div>			
4	Normal	<i>d_f</i>	44	2	44	BF3=	19.1	BF34=	0	0	0	1	0	0	0	0	0	0	0	0	0	0	-5E-07				
5	Uniform	<i>σ_{fu}</i>	1070	1070	1070	BF4=	0	BF35=	53.3	0	0	0	1	0	0	0	0	0	0	0	0	0	-5E-07				
6	Normal	<i>V_f</i>	2	0.2	2.376	BF5=	0.88	BF36=	0	0	0	0	1	0	0	0	0	0	0	0	0	0	1.8784				
7	Uniform	<i>G_d</i>	0.19	0.19	0.19	BF6=	0	BF37=	0	0	0	0	0	1	0	0	0	0	0	0	0	0	-5E-07				
8	Uniform	<i>τ_θ</i>	2.38	2.38	2.38	BF7=	0	BF38=	0	0	0	0	0	0	1	0	0	0	0	0	0	0	-5E-07				
9	Uniform	<i>β</i>	0.28	0.28	0.28	BF8=	0	BF39=	0	0	0	0	0	0	0	1	0	0	0	0	0	0	-5E-07				
10	Uniform	<i>f'</i>	0.30	0.3	0.3	BF9=	0.376	BF40=	0	0	0	0	0	0	0	0	1	0	0	0	0	0	-5E-07				
11	Uniform	<i>f</i>	0.50	0.5	0.5	BF10=	0	BF41=	0	0	0	0	0	0	0	0	0	1	0	0	0	0	-5E-07				
12	Normal	<i>E_m</i>	20.00	2	20	BF11=	0	BF42=	0	0	0	0	0	0	0	0	0	0	1	0	0	0	-2E-04				
13	Normal	<i>K_m</i>	0.61	0.2	0.568	BF12=	0	BF43=	0.62	0	0	0	0	0	0	0	0	0	0	0	1	0	-0.208				
14						BF13=	0	BF44=	16.8																		
15						BF14=	0.22	BF45=	0																		
16						BF15=	0.194	BF46=	0																		
17						BF16=	0	BF47=	6.2																		
18						BF17=	0	BF48=	0																		
19						BF18=	0	BF49=	0																		
20						BF19=	0	BF50=	0.46																		
21						BF20=	10505	BF51=	0																		
22						BF21=	0	BF52=	0																		
23						BF22=	0	BF53=	0																		
24						BF23=	484	BF54=	0																		
25						BF24=	0	BF55=	0																		
26						BF25=	121	BF56=	0																		
27						BF26=	0	BF57=	0																		
28						BF27=	11.84	BF58=	0																		
29						BF28=	0	BF59=	1100																		
30						BF29=	7.175	BF60=	2.79																		
31						BF30=	0	BF61=	0																		
32						BF31=	5.73	BF62=	1.43																(a)		

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X		
1	Distribution	Para1	Para2	x_i^*	MARS					Correlation matrix [R]													n_i	F(x)	α_2	P_{f2}
2	Uniform	E_f	41.1	41.1	41.1	BF1=	0.000	BF26=	0.000	1	0	0	0	0	0	0	0	0	0	0	-5E-07	-3E-07	1.2292	10.95%		
3	Normal	L_f	10	2	10.27	BF2=	1.034	BF27=	0.000	0	1	0	0	0	0	0	0	0	0	0	0.1331	<div>$F(x) = \sigma_s - \sigma_{fc}$ Eqn. 2.8 Predicted MARS model as Eqn. 3.7</div>				
4	Normal	d_f	44	2	44.09	BF3=	0.000	BF28=	0.815	0	0	1	0	0	0	0	0	0	0	0	0.0462					
5	Uniform	σ_{fu}	1070	1070	1070	BF4=	0.000	BF29=	0.000	0	0	0	1	0	0	0	0	0	0	0	-5E-07					
6	Normal	V_f	2.0	0.2	1.966	BF5=	550.000	BF30=	0.220	0	0	0	0	1	0	0	0	0	0	0	-0.169					
7	Uniform	G_d	0.19	0.19	0.19	BF6=	0.000	BF31=	0.000	0	0	0	0	0	1	0	0	0	0	0	-5E-07					
8	Uniform	τ_o	2.38	2.38	2.38	BF7=	0.910	BF32=	0.000	0	0	0	0	0	0	1	0	0	0	0	-5E-07					
9	Uniform	β	0.28	0.28	0.28	BF8=	0.230	BF33=	0.000	0	0	0	0	0	0	0	1	0	0	0	-5E-07					
10	Uniform	f'	0.30	0.3	0.3	BF9=	759.000	BF34=	0.000	0	0	0	0	0	0	0	0	1	0	0	-5E-07					
11	Uniform	f	0.50	0.5	0.5	BF10=	0.000	BF35=	0.000	0	0	0	0	0	0	0	0	0	1	0	-5E-07					
12	Weibull	σ_{mu}	1.10	2.4	4.87	BF11=	1.944	BF36=	2.516	0	0	0	0	0	0	0	0	0	0	1	1.2094					
13						BF12=	0.000	BF37=	0.000																	
14						BF13=	0	BF38=	0																	
15						BF14=	568.604	BF39=	0.000																	
16						BF15=	0.264	BF40=	358.600																	
17						BF16=	24.092	BF41=	0.000																	
18						BF17=	0.238	BF42=	0.136																	
19						BF18=	0.000	BF43=	0.000																	
20						BF19=	0.000	BF44=	29.500																	
21						BF20=	2.434	BF45=	60.500																	
22						BF21=	126.500	BF46=	0.000																	
23						BF22=	0.000	BF47=	42.885																	
24						BF23=	0.202	BF48=	0.000																	
25						BF24=	0.000	BF49=	0.641																	
26						BF25=	0.000	BF50=	0.000														(b)			

Figure 3.5 FORM for: (a) energy criterion; (b) strength criterion

3.4.2 Probabilistic distribution of micromechanical parameters

To better illustrate the variation of micromechanical parameters of SHCCs, a

typical SHCC specimen under direct tension is shown in Fig. 3.6 with n parallel cracking planes. Fiber properties (E_f , L_f , d_f , σ_{fu}) and the interface properties (G_d , τ_0 , β , f' , f) are considered as the (in-plane) random variables which vary along each individual cracking plane, while the fiber volume V_f and the matrix properties (E_m , K_m , c) are considered as the (out-of-plane) random variables which vary from one cracking plane to another along the loading axis.

Figure 3.6 Variability of parameters in SHCC system

Consequently, the distribution of each micromechanical parameter should be determined. The effect of fiber diameter variation on composite properties was discussed in the Reference [22], demonstrating that the variation could be properly described by a normal probability function. It concluded that variation of fiber diameter has minimal effect on the fracture energy and tensile strength. In this study, d_f would be treated as uniform distribution. The effect of fiber length variation also investigated using different types of carbon fiber [23], in which quite different

distribution of fiber length was measured before and after mixing with cementitious materials. And it drew a conclusion that fibers with a lower diameter, low strain capacity, higher modulus and longer length tend to suffer more breakage during mixing. For the following studies, L_f also can be considered as constant value according to the experimental results in the Reference [23] due to the larger fiber diameter, high modulus, high strength and short length.

Unfortunately, no studies on the variation of elastic modulus and tensile strength of fibers using in fiber reinforced cementitious composites can be found so far. In the present investigation, E_f and σ_{fu} are assumed to vary according to a normal probability distribution as shown in Fig. 3.7 and Eqn. 3.8. Using the above-mentioned in Section 3.4.1, the influence of the variation of E_f and σ_{fu} on the strain hardening criteria is investigated.

Figure 3.7 The normal probability distribution of the variable x

$$p(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right] \quad (-\infty < x < +\infty) \quad (3.8)$$

where μ and σ are the mean and standard deviation of the distribution, respectively; x can be E_f or σ_{fu} .

Actual fiber modulus and fiber strength variation depends upon fiber type and manufacture route, and is usually less than $\pm 30\%$ which is a conservative value used here. It is well known that 99.97% of the area of a normal probability distribution curve can be described within $\pm 3\sigma$ from the mean value. Then 3σ can be evaluated by equating it to the difference between the smallest and the mean value, which is the variation value multiple the mean value μ as Table 3.6 and Table 3.7. In Table 3.6, two mean values of E_f (20 GPa and 40 GPa) are used here. As can be seen from the resulting reliability index α_1 and α_2 with the same mean value of E_f , the variation of E_f has more significant effect on the energy criterion, but barely influence on the strength criterion. Comparing α_1 derived from the mean E_f of 20 GPa and 40 GPa with different variability, it presents that E_f is an important parameter to affect the maximum complementary energy J_b' and has minimal effect on fiber bridging strength σ_0 . This observation is in agreement with the conclusions drawn from the ANOVA analysis in Section 3.3 as shown in Fig. 3.4. It is therefore necessary to conduct further investigation to reveal the distribution of E_f .

Table 3.6 The influence of E_f variation on the strain hardening criteria

μ (GPa)	E_f		α_1	α_2	P_{f1} (%)	P_{f2} (%)
	σ (MPa)	Variation				
20	0.7	$\pm 10\%$	23.2	1.23	0	10.8
	1.3	$\pm 20\%$	12.5	1.23	0	10.8
	2	$\pm 30\%$	8.1	1.23	0	10.8
40	1.3	$\pm 10\%$	2.9	1.2	0.2	11.6
	2.7	$\pm 20\%$	1.4	1.2	8.4	11.6
	4	$\pm 30\%$	0.9	1.2	17.6	11.6

In Table 3.7, two mean values of σ_{fu} (1070 MPa and 600 MPa) are used. From derived α_1 with the same mean value of σ_{fu} , it indicates that the variation of σ_{fu} has more significant effect on the energy criterion, but little influence on the strength criterion. Comparing α_1 and α_2 derived from σ_{fu} of 1070 MPa and 600 MPa with different variability, it presents that σ_{fu} is affecting both the maximum complementary energy J_b' and the fiber bridging strength σ_θ . This observation is again in agreement with the conclusions drawn from the ANOVA analysis in Fig. 3.4. More research is needed to reveal the variation of σ_{fu} in the future.

Table 3.7 The influence of σ_{fu} variation on the strain hardening criteria

μ (MPa)	σ_{fu} σ (MPa)	Variation	α_1	α_2	P_{f1} (%)	P_{f2} (%)
1070	36	$\pm 10\%$	24	1.4	0	7.9
	71	$\pm 20\%$	12	1.4	0	7.9
	107	$\pm 30\%$	8.3	1.4	0	8
600	20	$\pm 10\%$	8.6	0.86	0	19.6
	40	$\pm 20\%$	7.6	0.86	0	19.6
	60	$\pm 30\%$	5.6	0.85	0	19.7

The volume of fiber V_f is a parameter due to the non-uniform fiber dispersion like fiber bundling due to the processing. It varies from one cracking plane to another along loading axis. No existing literature reports the stochastic properties of V_f among different cracking plane. According to the ANOVA analysis, V_f is the paramount variable to affect the fiber bridging strength. The ultimate tensile strength of SHCC closely depends on the fiber bridging strength of the cracking plane with the lowest fiber volume. In this research, V_f is assumed to be the normal distribution with $\pm 30\%$ variation.

The micromechanical parameters of interfacial properties (G_d , τ_0 , β) are derived from the single fiber pullout test. So far, there is no literature discussed about the distribution. Here, the distribution of all parameters attained from experiments are assumed as normal distribution with mean value and standard deviation.

f is the snubbing friction coefficient describing the additional frictional force due to the interaction of the misaligned fiber with the matrix at the exit of fiber [68, 69]. It can be determined for a particular fiber/matrix interface by conducting a series of single fiber pullout tests at different angles ranging between 0° and 90° , then plotting the maximum load P_{max} versus the different angle Φ and fitting the curve to an equation of the form $P_{max} = P_{max}(\Phi=0)e^{f\Phi}$, where f is the snubbing coefficient. f' is the fiber strength reduction coefficient and can be investigated through pull-to-rupture tests, in which one end of a single fiber is embedded in a matrix foundation and the other end is pulled to rupture the fiber [70, 71]. Similar to f , it is determined by the curve fitting of the test results obtained from specimens with different Φ . Reference values are listed in Table 3.8.

Table 3.8 Reference values of f and f'

Fiber type	σ_{fu} (MPa)	f	f'	Reference
Polyvinyl alcohol (PVA)	1666	0.5	0.3	Kanda and Li 1999 [70]
Polypropylene (PP)	400	0.39	0.1	Yang and Li 2010 [5]
Polyethylene (PE)	2400	0.8	0	Kanda and Li 1999[70]

The parameters describing matrix properties E_m and K_m can be achieved by the compressive test and the matrix toughness test. They are also assumed as normal distribution along the volume here. The flaw size c and the matrix strength σ_{mu} has direct relation as given by Eqn. 2.9. In the literature, σ_{mu} is assumed to follow the

two-parameter Weibull distribution [30]. Weibull analysis is a widely-used statistical tool for describing the strength behavior of brittle materials, which is based on the assumption that failure at the most critical flaw leads to total failure of the specimen. Weibull distribution is easy to interpret and very versatile. The cumulative distribution function for the Weibull distribution is

$$F(x, k, \lambda) = 1 - e^{-\left(\frac{x}{\lambda}\right)^k} \quad (3.9)$$

where k is the shape parameter, λ is the scale parameter, which determines the varying range of the variable. Thus, σ_{mu} is used to perform analysis in the following section.

3.4.3 Reliability assessment

Due to the variation of micromechanical parameters, the possibility of strain hardening behavior can be assessed using FORM. Different SHCC mixtures with strain capacity below 1% up to above 4% are selected from literature [29, 72, 73]. The first group of mixtures is a type of lightweight SHCC using cenosphere as well as slag and fly ash in order to achieve high ductility, and PVA fiber with 1.2% coating is used in these mixtures [72]. The second group consists of cement, sand, water and PVA fibers with different coating of 0.3%, 0.5%, 0.8%, and 1.2% [73]. In the third group, PE fiber with different fiber volume of 0.5%, 0.75%, 1% and 1.25% is applied into the normal matrix [29]. All the relevant micromechanical parameters for each group are listed in Table 3.9. For conservative estimation, $\pm 30\%$ variability is assumed and used to calculate the standard deviation for the parameters without reporting the standard deviation.

Table 3.9-1 Distributions and values of all micromechanical parameters

Parameters	Distribution	Values of each cases			
		SHCCs 1, 2, and 6 [72]			
E_f (GPa)	Normal	42 ± 4.2			
L_f (mm)	Uniform	12			
d_f (μm)	Uniform	39			
σ_{fu} (MPa)	Normal	1070			
V_f (%)	Normal	2 ± 0.2			
G_d (J/m ²)	Normal	0.83 ± 0.37	1.48 ± 0.74	0.62 ± 0.22	
τ_0 (MPa)	Normal	2.34 ± 0.42	2.33 ± 0.46	3.04 ± 0.75	
β	Normal	0.37 ± 0.17	0.45 ± 0.23	0.41 ± 0.19	
f'	Uniform	0.3^a			
f	Uniform	0.5^a			
E_m (GPa)	Normal	20 ± 2^a			
σ_{mu} (MPa)	Weibull	$2.4 / 1.1^a$			
K_m (MPa·m ^{1/2})	Normal	0.51 ± 0.05	0.5 ± 0.05	0.40 ± 0.04	

a: assumed

Table 3.9-2 Distributions and values of all micromechanical parameters

Parameters	Distribution	Values of each cases			
		SHCCs 5, 7, 9, and 11 [73]			
E_f (GPa)	Normal	42.8 ± 4.3			
L_f (mm)	Uniform	12			
d_f (μm)	Uniform	39			
σ_{fu} (MPa)	Normal	1092 ± 109			
V_f (%)	Normal	2 ± 0.2			
G_d (J/m ²)	Normal	$3.16 \pm$	$2.96 \pm$	$2.18 \pm$	1.61 ± 0.6
τ_0 (MPa)	Normal	$2.15 \pm$	$2.14 \pm$	$1.98 \pm$	$1.11 \pm$
β	Normal	$2.31 \pm$	$1.82 \pm$	$1.18 \pm$	$1.15 \pm$
f'	Uniform	0.3^a			
f	Uniform	0.5^a			
E_m (GPa)	Normal	20 ± 2			
σ_{mu} (MPa)	Weibull	$2.4 / 1.1^a$			
K_m	Normal	0.33 ± 0.03^a			

a: assumed

Table 3.9-3 Distributions and values of all micromechanical parameters

Parameters	Distribution	Values of each cases			
		SHCCs 3, 4, 8, and 10 [29]			
E_f (GPa)	Normal	117 ± 11.7			
L_f (mm)	Uniform	19.1			
d_f (μm)	Uniform	38			
σ_{fu} (MPa)	Normal	2400			
V_f (%)	Normal	0.5 ± 0.05	0.75 ± 0.07	1.0 ± 0.1	1.25 ± 0.12
G_d (J/m ²)	Normal	0			
τ_0 (MPa)	Uniform	0.62			
β	Normal	0			
f'	Uniform	0			
f	Uniform	0.8^a			
E_m (GPa)	Normal	23 ± 2.3			
σ_{mu} (MPa)	Weibull	$2.4 / 1.1^a$			
K_m (MPa·m ^{1/2})	Normal	0.33 ± 0.03^a			

a: assumed

Using FORM as Section 3.4.1, the failure probability of strain hardening behavior for these cases is calculated and listed in Table 3.10. P_{f1} and P_{f2} denote the failure probability of the energy criterion and the strength criterion, respectively. Lower P_{f2} such as SHCCs 1 and 2 indicates that the respective composite has the high potential to produce more cracks and the fiber bridging strength is sufficient to take the ambient load once cracks occur. Higher P_{f1} means high possibility of local failure with Griffith crack mode instead of steady state cracking mode for corresponding mixtures. Because the two criteria of strain hardening behavior are a pair of complementary criteria which must be simultaneously satisfied for multiple cracking to occur, a higher value of P_{f1} and P_{f2} is taken as the failure probability P_f of the composite. As can be seen from Table 3.10, P_f decreases with increasing strain capacity, which means that the level of failure probability can reflect the magnitude of strain capacity. There is a clear distinction of P_f corresponding to strain capacity

below and above 1%. If the strain capacity is below 1%, a very high P_f of more than 30% is observed. A P_f of 10% is appropriate to achieve the medium strain capacity between 1% and 4%, and a P_f below 5% is aiming for SHCC with high strain capacity of above 4%. Therefore, the strain hardening behavior can be assessed with the proposed probabilistic-based micromechanics model (PMM).

Table 3.10 The failure probability of strain hardening behavior for typical cases

SHCC	Strain capacity	P_{f1}	P_{f2}	P_f
1	0.48	31.3	0	31.3
2	0.63	33.4	0	33.4
3	0.73	3.5	34.7	34.7
4	1.40	4.6	13.0	13.0
5	1.55	15.1	0	15.1
6	1.71	13.7	0	13.7
7	2.73	13.3	0	13.3
8	3.80	6.2	3.5	6.2
9	3.81	6.8	0.6	6.8
10	4.00	7.8	0.7	7.8
11	4.88	4.7	0.1	4.7

ε	P_f
< 1%	~ 30%
1% ~ 3%	~ 13%
3% ~ 4%	~ 7%
> 4%	< 5%

3.5 Summary

In order to consider the heterogeneity of fiber distribution and flaw size distribution in SHCC, a novel probabilistic-based micromechanics model (PMM) by introducing the probability concept is proposed, instead of the deterministic safety factors of energy performance index J_b'/J_{tip} and strength performance index σ_0/σ_{fc} . In PMM, the critical process is to explicitly express the performance indices J_b' and σ_0 using the MARS method. A database containing 702 groups of data with a total of ten variables is adopted to develop the MARS model. It provides an insight and understanding of underlying micromechanical parameters which can deliver the

information to guide mix design of SHCC. E_f and τ_0 are the most two important parameters to affect the maximum complementary energy to bridge the crack J_b' . V_f , σ_{fu} , d_f and τ_0 are significantly important in determining the fiber bridging strength. Based on the built MARS model, reliability analysis can be conducted by minimizing the reliability index subject to the constraint of the performance function. Lower probability of failure is expected to attain high strain hardening behavior of SHCC. It indicates that P_f below 10% may ensure the strain capacity above 1%, providing practical guidance for the engineer to design desirable mix of SHCC.

4 Stochastic Modeling of SHCC Tensile Properties Considering Microstructure Variability

4.1 Introduction

As described in Section 2.1, the micromechanics-based strain hardening model links material microstructures and composite behavior. Considering the random nature of fiber, fiber/matrix interface and matrix properties in cement composites, a probabilistic micromechanics-based model (PMM) is developed in Chapter 3 to assess the reliability of strain hardening behavior of the composite. But using this model, the level of strain hardening behavior still cannot be determined. To quantify the strain hardening behavior, relevant models have been reviewed in Section 2.2.3. The main drawback of those models based on micromechanics is that they do not consider all the variability of the microstructure, forfeiting correct simulation of significant tensile characteristics. For example, the most up-to-date model [30] can predict the cracking process and tensile ductility considering the matrix cracking distribution, but the crack opening is assumed as constant among all cracks violating experimental observation. It impels the motivation to develop a stochastic model for SHCC tensile properties by taking into account of all the variability of the microstructure. Multiscale linkage from micro level to macro level is requisite with probabilistic considerations as shown in Fig. 4.1.

Figure 4.1 Mutiscale variability of SHCC

At micro level, all the variability of the microstructure is expressible by random variables in terms of fiber, fiber/matrix interface and matrix properties. As discussed in Section 3.4.2, fiber properties ($E_f, L_f, d_f, \sigma_{fu}$) and the interface properties ($G_d, \tau_0, \beta, f', f$) are considered as the (in-plane) random variables which vary along each individual cracking plane, while the fiber volume V_f and the matrix properties (E_m, K_m, c) are considered as the (out-of-plane) random variables which vary from one cracking plane to another along the loading axis.

At meso level, the variability is related to the variation of fiber bridging property and matrix cracking property. The varying fiber bridging property in the form of $\sigma_B(\delta)$ or J_b' , and matrix cracking property in the form of σ_{fc} or J_{tip} are expressed along the loading axis. The first cracking strength σ_{fc} is obviously determined by matrix cracking strength σ_{mu} and contribution of fiber bridging property.

At macro level, the crack opening δ can be determined by the fiber bridging property of each crack. The crack spacing x is defined according to the distribution

of the first cracking strength σ_{fc} and the stress transfer distance x_d from the fiber to the matrix, while the stress transfer distance x_d also can be derived by the fiber bridging property and the matrix cracking strength σ_{mu} . To clarify, the crack spacing x is the distance between two cracks, and the stress transfer distance x_d is the minimum required distance to initiate a new crack. The strain capacity ε can be calculated using the crack opening δ and the number of cracks. The ultimate tensile strength σ_u is determined by the section with the weakest fiber bridging.

In this chapter, the whole framework for simulating SHCC tensile properties is illustrated in Fig. 4.2. Firstly, the crack evolution process and crack saturation in SHCC are clarified in Section 4.2 based on the experimental observations and the theoretical background summarized in Section 2.2.1. Secondly, a parallel computing method is used to simulate the distribution of the fiber bridging property as described in Section 4.3 based on the numerical solution of the fiber bridging model starting from the simulation of a single fiber pullout behavior against the surrounding matrix. Its inputs are all the micromechanical parameters related to the properties of each fiber and the interface. So the variation of fiber bridging property can be described inputting different micromechanical parameters for different sections along the length of a sample. In addition, the simulation of a single fiber pullout facilitates and promotes a new method for the stress transfer distance from fiber to the adjacent matrix in order to obtain the crack spacing as described in Section 4.4. Finally, the tensile properties of SHCC are simulated considering the statistical nature of matrix cracking strength and fiber bridging properties together with the complementary dual-criteria. Different from the capability of existing model for SHCC tensile behavior, the stochastic model can comprehensively present all the tensile characteristics in line with reality, involving distributed crack opening, distributed

crack spacing, the crack evolution process, the first cracking strength and the ultimate tensile strength.

Figure 4.2 The framework of Chapter 4

4.2 Multiple cracking process and saturation in SHCC

Consideration of the above dual-criteria of strain hardening behavior for SHCC, together with the statistical nature of fiber bridging property and matrix cracking strength as described in Chapter 3, provides the foundation for understanding the sequential nature of multiple crack development and the saturation level of multiple cracks. Under displacement controlled deformation, the tensile stress-strain relation for a SHCC sample is characterized by three stages as illustrated in Fig. 4.3.

Figure 4.3 Representative tensile stress-strain relation

- 1) Elastic stage. In the elastic stage, the composite exhibits linear elastic behavior with an elastic modulus E_c equivalent to that of the uncracked composite.
- 2) Multiple cracking stage. Initial damage including pores and cracks in the composites become activated to grow at various external loads. The first crack forms at the lowest strength $\min\{\sigma_{fc}\}$ in the composite, representing the starting point of the strain hardening behavior. After the first crack is formed, the elastic modulus of the uncracked composite is replaced by the fiber bridging relation, i.e. $\sigma_B(\delta)$. Accordingly, the load drops suddenly due to force equilibrium between the cracked section and the adjacent uncracked composite section. The load again increases gradually with an increase of deformation until the induced stress reaches a sufficient level to cause the formation of another crack in the composite. This process is continued until the induced stress reaches the lowest peak bridging stress $\min\{\sigma_{\theta}\}$.
- 3) Damage localization stage. When one of the cracks bridged by fibers reaches

its maximum bridging strength σ_0 , the critical crack opens while other cracks close up. So the stress-cracking opening relation $\sigma_B(\delta)$ of the critical crack should be used in this stage. Based on the two strain hardening criteria, the crack evolution process described above suggests three scenarios for composites which develop unsaturated multiple cracking. Suppose the first $(n-1)$ cracks in a specimen satisfy both of the two criteria. After the formation of these multiple cracks, for the n^{th} crack plane, it may have one of the following three characteristics:

- (i) Energy criterion satisfied / strength criterion not satisfied
- (ii) Energy criterion not satisfied / strength criterion satisfied
- (iii) Energy criterion satisfied / strength criterion satisfied, but $\sigma_{fc}^n > \sigma_B^i$

For cases (i) and (ii), failure must occur immediately on the n^{th} cracking plane. This means the failure crack is the n^{th} crack. For case (iii), formation of multiple cracking continues to the n^{th} crack, but failure occurs at one of the existing crack i because the applied stress is larger than the fiber bridging capacity of crack i . The three scenarios (i)-(iii) represents that saturation of multiple cracking can be prematurely terminated, resulting in unsaturated cracking state of SHCC.

4.3 The distribution of fiber bridging properties

The fiber bridging property $\sigma_B(\delta)$ for in-plane section is calculated using the procedure in Fig. 2.4, with modeling of single fiber behavior and averaging of fiber randomness for in-plane section. As shown in Fig. 4.2, the fiber bridging properties are different for out-of-plane sections due to the variation of micromechanical

parameters. To calculate the distribution of fiber bridging properties, the previous numerical procedure for in-plane fiber bridging property is needed to modify to multiple array instead of single array of inputs (micromechanical parameters) and outputs $\sigma_B(\delta)$. As Fig. 4.4, the inputting sets of data is obtained using Monte Carlo simulation (MCS) according to the distribution of micromechanical parameters. Then for each set of the input, the $\sigma_B(\delta)$ is calculated one by one using the procedure as Fig. 2.4.

Figure 4.4 Modified model of Fiber bridging property $\sigma_B(\delta)$

Based on the modified model of fiber bridging property $\sigma_B(\delta)$, parametric studies are conducted on the micromechanical parameters in Table 4.1. For each parameter, 100 sets of inputs are got using Monte Carlo simulation (MCS) with the respective probabilistic distribution. The distributions of parameters related to fiber properties have been discussed in Section 3.4.2, using the same variation $\pm 30\%$ for E_f , L_f , d_f , σ_{fu} and V_f with the purpose of comparing their relative importance. For the

interface parameters of G_d , τ_0 and β , a large variation of $\pm 90\%$ is assumed with keeping the minimum values above 0. The effects of micromechanical parameters distribution on the fiber bridging properties $\sigma_B(\delta)$ are shown in Fig. 4.5. The resulting crack opening, the fiber bridging strength and the complementary energy are distributed with different variations.

Table 4.1 Micromechanical parameters used as model input

Matrix type	Fiber				Interface				
	E_f (GPa)	L_f (mm)	d_f (μm)	σ_{fu} (MPa)	f	f'	G_d (J/m ²)	τ_0 (MPa)	β
2.0 vol.% PVA	22	12	39	1060	0.2	0.33	1.08	1.31	0.58

Figure 4.5 Effects of μ -parameters distribution on fiber bridging property $\sigma_B(\delta)$

The relative importance of micromechanical parameters influencing these factors are varied, the coefficient of variations (COV) are presented in Fig. 4.6. As can be seen from fiber properties, V_f and σ_{fu} are significantly important in determining the fiber bridging strength σ_0 , σ_{fu} and E_f are major influence parameters for the complementary energy J_b' which fit well with the conclusion in Section 3.3. In order to control the crack opening, it is crucial to select suitable parameters of σ_{fu} and d_f . In terms of interfacial properties, τ_0 is the principal parameter to determine the crack opening, fiber bridging strength, and the complementary energy. The effects of critical parameters influencing δ , σ_0 and J_b' are shown in Table 4.2. Increasing σ_{fu} can lead to higher J_b' and higher fiber bridging strength σ_0 which are favorable for the strain hardening behavior, but can result in larger crack opening

which is generally unexpected. Lower E_f and higher V_f are preferable to achieve high strain hardening behavior. In order to limit the crack opening, lower d_f can be used. With respect to the interfacial properties, moderate frictional bond τ_0 is expected because too low τ_0 also can lead to lower complementary energy J_b' as well as fiber bridging strength σ_0 , as can be seen from Fig. 4.5. In order to develop desired SHCC, this information plays an importance guidance role of selecting different fiber types and tailoring the interface properties.

Figure 4.6 Coefficient of variation for: a) δ , (b) σ_0 and c) J_b' Table 4.2 Effects of critical parameters influencing δ , σ_0 and J_b'

Factors	Fiber	Interface
Crack opening δ (μm)	$\delta \downarrow \rightarrow \sigma_{fu} \downarrow$ $d_f \downarrow$	$\tau_0 \uparrow$
Fiber bridging strength σ_0 (MPa)	$\sigma_0 \uparrow \rightarrow \sigma_{fu} \uparrow$ $V_f \uparrow$	$\tau_0 \uparrow$
Complementary energy J_b' (J/m ²)	$J_b' \uparrow \rightarrow \sigma_{fu} \uparrow$ $E_f \downarrow$	$\tau_0 \downarrow$

4.4 Analytical model and numerical procedure of the transfer distance x_d

With understanding of the mechanism of multiple cracking process, the stress transfer distance x_d is needed to identify the occurrence of multiple cracks. The calculation of x_d is according to the analysis of the equilibrium state of the matrix between two cracks. In order to deduce the analytical model, the simulation of single fiber pullout behavior plays as the basis which facilitates to integrate all bearing forces of matrix transferred from each fiber. This basis promotes the numerical realization of modeling x_d , similar to the numerical procedure for computing $\sigma_B(\delta)$ [12].

4.4.1 Analytical model and numerical procedure of stress transfer distance x_d

The stress transfer distance x_d was first derived by Aveston et al. [32] for continuous aligned fibers and then developed for random distributed short fibers. In the analysis, when a crack occurs, the applied load is carried by the bridging fibers across the crack plane. With increasing load, the fiber stress is then transferred back to the matrix through: 1) interfacial friction along the fiber, 2) and pulley force at the exit point of inclined fibers as shown in Fig. 4.7.

Figure 4.7 The equilibrium state of the matrix

To the matrix, the equilibrium state along x axis can be expressed by

$$\sum F_{pulley-x} + \sum F_{friction-x} = \sigma_{mu} V_m \quad (4.1)$$

$$F_{friction-x} = \pi d_f \tau_0 x_d \quad (4.2)$$

where σ_{mu} is the matrix strength, V_m is the matrix volume fraction, $F_{friction}$ represents the load vector pre unit area of the matrix transferred from the fiber interface by friction, which is a function of transfer distance x_d from the existing crack plane as Eqn. 4.2 with assumed constant frictional bond τ_0 , F_{pulley} represents the load vector per unit area of the matrix resulted from the inclined fiber at the crack plane as Fig.

4.8. Σ is the sum up of all fiber contribution over the existing crack plane.

Figure 4.8 Illustration of F_{pulley}

Thus,

$$F_{pul-x} = P(\delta)e^{f\phi} - P(\delta)\cos\phi \quad (4.3)$$

To substitute Eqns. 4.2 and 4.3 into Eqn. 4.1, then

$$\sigma_{mu}V_m = \int \pi d_f \tau_0 k dL_e d\phi + \int (P(\delta)e^{f\phi} - P(\delta)\cos\phi) dL_e d\phi \quad (4.4)$$

$$k = \min\{L_e \cos\phi, x_d\}$$

k is a parameter to facilitate to differentiate cases with different embedment length

L_e bigger or smaller than transfer distance x_d as shown in Fig. 4.9.

Figure 4.9 Two cases of fibers divided by embedment length

According to Eqn. 4.4, the key is to determine the matrix cracking σ_{mu} and the fiber bridging stress $P(\delta)$ which has been reviewed in Chapter 2. The flow chart of the numerical procedure for computing the stress transfer distance can be found in Fig. 4.10. By virtue of this method, effects of two-way fiber pullout, the chemical bond, and the slip-hardening have been considered but have not been investigated in previous studies on calculating the stress transfer distance [29, 30].

Figure 4.10 Flow chart to determine the stress transfer distance x_d

4.4.2 Parametric studies on factors influencing the transfer distance x_d

From Eqn. 4.4, main factors affecting the transfer distance x_d are listed as

follows:

- 1) With the fiber bridging stress σ_B increasing significantly beyond the first cracking strength, the transferred pulley force F_{pulley} is also increased. Subsequently, the transfer distance x_d is also changed.
- 2) With increasing crack opening δ of the existing crack, fiber pullout totally and rupture would occur, which can significantly reduce the transferred friction force $F_{friction}$ as a result of changing x_d .
- 3) As the matrix strength is not uniform along the member, the method should consider the strength variation of the matrix, σ_{mu} , as well.

With the micromechanical parameters in Table 4.1, the transfer distance is calculated with crack opening following the flow chart in Fig. 4.10 in order to explain the effects of the above three factors. First to demonstrate the relation of x_d with increasing σ_B and δ , the matrix strength is assumed constant as 5 MPa as Fig. 4.11, the fiber bridging stress σ_B along with crack opening δ is calculated following the flow chart Fig. 2.4. For the initial stage with crack opening below 20 μm , no x_d can be determined because F_{pulley} is too small and the required transferred distance of the friction exceeds the fiber length ($x_d > L_f$). With the crack opening from 20 μm to 88 μm , x_d decreases because F_{pulley} increases with σ_B and $F_{friction}$ decreases given constant σ_{mu} . In the stage from 88 μm to 132 μm , x_d increases. Here, F_{pulley} increases resulting in decreasing $F_{friction}$ correspondingly. According to Eqn. 4.4, $F_{friction}$ is mainly influenced by the number of fibers and the stress transfer distance x_d . However, the number of fibers decreases with increasing crack opening due to fiber pullout or rupture, leading to gradually increasing x_d . This also can be seen from the stage after 132 μm , fiber rupture continues significantly resulting in increasing x_d .

Figure 4.11 x_d vs. δ and σ_B vs. δ with $\sigma_{mu} = 5$ MPa

Therefore, the effects of the fiber bridging stress and the crack opening counteract each other on the transfer distance x_d . At early stage, the fiber bridging stress leading to increasing F_{pulley} dominates the decreasing trend of x_d , when fibers rupturing become more and more, the crack opening takes an advantage to control the increase of transfer distance due to the losing integration fibers number in calculating the $F_{friction}$. Over 132 μm , more and more fibers rupture, the bridging stress drops gradually. Meanwhile the calculating procedure of x_d still can get values until it exceeds the fiber length. However, in reality, the upward stage of x_d would not occur because new cracks have been activated following the downward stage.

In summary, the first factor of fiber bridging stress and the second factor of crack opening counteract to affect the transfer distance x_d , while the third factor of the matrix strength takes effect independently. In the following, effects of matrix strength, two-way fiber pullout, fiber/matrix interfacial chemical bond, slip hardening effect, and fiber inclination are discussed.

Matrix strength

Fig. 4.12 illustrates the variation of x_d with the matrix strength σ_{mu} . To this

group of micromechanical parameters, σ_{mu} is assumed as 3.5 MPa and 5 MPa. Obviously, with lower matrix strength, the required transfer distance reduces. The inflection points of $x_d(\delta)$ curve are the same at 88 μm , which indicates more fibers rupture with the increasing crack opening only relating to the fiber bridging properties. The distribution of the matrix strength in SHCC samples will be considered in the Section 4.5.

Figure 4.12 x_d vs. δ with $\sigma_{mu} = 3.5$ MPa and 5 MPa

Two-way fiber pullout

The effect of two-way pullout is discussed because it is a prominent phenomenon in PVA fiber reinforced cementitious composites and it has not been considered by other models in calculating x_d . In PVA-SHCC, the chemical bond and slip-hardening phenomena of fiber/matrix interface are also apparent properties which have not been investigated for their effects of x_d . In addition, fiber rupture is an important mechanism to affect x_d , so the fiber inclination effect is shown in the following. Here, the micromechanical parameters in Table 4.1 are used, and the matrix strength is assumed as 5 MPa.

For many types of fibers with no significant slip hardening response, i.e. β

approaches 0 or even negative like PE fiber, after complete debonding of the short embedment side, the long embedment side remains anchored since the load begins to drop. In this case, one-way pullout is suitable to simulate the single fiber pullout behavior as in Fig. 4.13. However for PVA fiber, the pullout load can be much higher than the load after completed debonding of the short embedment side. As a result, the long embedment side can continue debonding and eventually enter the pullout stage such that two-way pullout occur. Then the contribution of slip displacement from both sides should consider the crack opening δ .

Figure 4.13 Single fiber pullout behavior

The possibility of two-way fiber pullout was originally suggested by Wang et al. [74] and modeled by Yang et al. [12]. In this research, two-way fiber pullout is considered to derive the fiber bridging properties which affect the transfer distance x_d . As shown in Fig. 4.14, a one-way fiber pullout model underestimates both the maximum fiber bridging strength and the maximum crack opening. Consequently, the transfer distance x_d is also underrated indicating that less cracks may be predicted.

Figure 4.14 x_d vs. δ and σ_B vs. δ considering one-way and two-way pullout

Fiber/matrix interfacial chemical bond

For PVA fiber, the chemical bond G_d is also a significant factor to affect the single fiber behavior and the fiber bridging properties as illustrated in Section 2.4.1. As can be seen from Fig. 4.15 (a), x_d drops with increasing G_d , which is as a result of increasing F_{pulley} with increasing fiber bridging stress at early stage as Fig. 4.15 (b). However, the fiber rupture space does not change greatly due to varying G_d , showing similar maximum crack opening and the maximum fiber bridging strength in Fig. 4.15 (b). So x_d is similar at a later stage before the minimum transfer distance is achieved due to similar fiber rupture space. In general, G_d is not a critical factor in the transfer distance within typical values reported.

Figure 4.15 Chemical bond effect on (a) x_d vs. δ , and (b) σ_B vs. δ

Slip hardening effect

Slip hardening response is observed for PVA fibers due to an abrasion and jamming effect during sliding of the fiber in the matrix tunnel. As can be seen from the curve of $\sigma(\delta)$ with $\beta = 0$ in Fig. 4.16 (b), the fiber rupture is not significant after the maximum bridging stress, the crack opening can be quite large with applied stress. Correspondingly, small F_{pulley} leads to large x_d as shown in Fig. 4.16 (a). From the curve of $\sigma(\delta)$ with $\beta = 0.58$ and 2, it indicates that the slip hardening effect can increase the fiber bridging stress on one hand, on the other hand, it increases the possibility of fiber rupture at lower crack opening. These two mechanisms can lead to lower x_d as shown in Fig. 4.16 (a).

Figure 4.16 Slip hardening effect on (a) x_d vs. δ , and (b) σ_B vs. δ

Fiber inclination effect

The relationship between the snubbing coefficient f and x_d is investigated here. Misaligned fibers are subjected to additional frictional force due to the interaction with matrix at the exit of fiber, which may result in significant fiber rupture at the crack plane. The snubbing coefficient f is used the recommended value between 0.2 and 0.8 as discussed in Section 3.4.2. Along with the increasing f , the decrease of x_d becomes shaper as shown in Fig. 4.17 (a) due to fiber rupture at smaller crack opening which can be told from the decreasing trend of $\sigma_B(\delta)$ in Fig. 4.17 (b).

Figure 4.17 Fiber inclination effect on (a) x_d vs. δ , and (b) σ_B vs. δ

4.5 Stochastic Modeling of SHCC Tensile Properties

4.5.1 Stochastic Model for SHCC Tensile Properties

According to the elaboration of multiple cracking process and saturation in SHCC as Section 4.2, the model of tensile properties can be derived based on the following information,

- 1) the fiber bridging model $\sigma_B(\delta)$ as Fig. 4.4;
- 2) the first cracking strength σ_{fc} as Eqn. 2.8;
- 3) the transfer distance x_d as Fig. 4.10; and
- 4) the two criteria as Eqns. 2.1 and 2.3.

For the elastic stage, the ultimate strain ε_e can be calculated by

$$\varepsilon_e = \frac{\min\{\sigma_{fc}\}}{E_c} \quad (4.5)$$

The point $(\varepsilon_e, \min\{\sigma_{fc}\})$ is the starting point of the multiple cracking stage. In this stage, both the first cracking strength σ_{fc} and the transfer distance x_d control the occurrence of the cracks. It is because of the two mechanisms leading to new cracks

as stepwise explained in Fig. 4.18, in which the black solid line denotes the new crack and the blue dotted line refers to the inactivated crack. The inactivated crack is the section with specified first cracking strength σ_{fc} equaling to the applied stress, but a crack would not occur.

Figure 4.18 Illustration of multiple cracking sequence

As Fig. 4.18, when the first crack occurs in the composite, the applied stress is transferred to the fiber, then the fiber would transfer the stress back to the adjacent matrix. In the adjacent matrix under certain applied stress, the stress transfer distance x_d is the minimum distance to initiate a new crack, so if the distance between the crack section and the section with specified cracking strength is less than x_d , the potential crack would not occur (called the inactivated crack). In the sections far from the existing crack, the matrix and the fiber take the applied stress as a whole, so that the cracking strength determines the crack occurrence. Therefore, in each applied stress, two judgements have to be conducted in each step in order to detect new cracks. The first is to find out all sections with specified first cracking strength σ_{fc} equal to the applied stress as potential cracks. Second, the potential cracks in the sections adjacent to all existing cracks are needed to check the occurrence or not; if yes, the potential crack should be marked as new cracks and vice versa. And the left

potential cracks are marked as new cracks.

Meanwhile in each step, each new crack is needed to check whether it satisfies the two criteria for multiple cracking; if no, the simulation has to be stopped with final failure of the composite. Under the condition that the two criteria can be met, the previous process can repeatedly occur until the applied stress achieves the $\min\{\sigma_0\}$. So the saturation of multiple cracking in SHCC is determined by the two criteria. Based on this process, the crack number can be counted at any step, meanwhile, the crack opening can get using $\sigma_B(\delta)$ curve. Hereto, the strain can be derived using Eqn. 2.12 at any step.

The final failure occurs at the section with $\min\{\sigma_0\}$, the strain at this state is calculated by the crack opening of this section. The whole process is programed followed the flow chart as Fig. 4.19. It mainly involves three parts,

- 1) division of sampling sections and determination of micromechanical parameters;
- 2) determination of properties for each sampling section;
- 3) detection of cracks and calculation of tensile properties.

Figure 4.19 Flow chart for computing tensile properties

4.5.2 Illustration of modeling SHCC tensile properties

1) To divide the sampling sections and determine micromechanical parameters

One mix from Yang and Li [5] is selected to illustrate the whole process to calculate the tensile properties of SHCC and compare with the experimental results.

The length of the simulated sample is 150 mm according to the gauge length of the

specimen used in the direct tension test, and it is divided into 300 sections with each section width of 0.5 mm. Observed from experiments, the saturated average multiple cracking interval is generally 1 mm, so 300 sampling sections are enough to detect all the cracks.

The micromechanical parameters are listed in Tables 4.2 and 4.3. As classification of the micromechanical parameters in Section 3.4.2, the fiber volume V_f and the matrix properties (E_m , K_m , c) are to present the statistical properties along the overall volume. To calculate the strain capacity along the sample volume, other parameters should be taken as average values of one section. E_m and K_m are taken as constant, the distribution of σ_{mu} and V_f are assumed as Weibull distribution as shown in Fig. 4.20 and normal distribution, respectively. λ is scale parameter, k is shape parameter. For V_f , the average value is 2% and a relative low standard deviation of 0.1% is selected to simulate the tensile properties as a result of the good fiber dispersion. The first cracking strength is calculated from the theory for steady state cracking to occur [75]:

$$\sigma_{ss}\delta_{ss} - \int_0^{\delta_{ss}} \sigma_c(\delta)d\delta = J_{tip} \quad (4.6)$$

In this equation, σ_{ss} and δ_{ss} stand for the stress and crack opening at steady state. For the first crack, its result is 3.6 MPa using the micromechanical parameters in Table 4.2 and Table 4.3 with fiber volume of 2%.

Table 4.3 Micromechanical parameters used as model input

Fiber				Interface		Matrix		
E_f (GPa)	L_f (mm)	d_f (μm)	σ_{fu} (MPa)	f	f'	E_m (GPa)	σ_{mu} (MPa)	K_m (MPa·m ^{1/2})
42.8	8	39	1070	0.5	0.32	20	Weibull ($\lambda = 1.1$, $k = 2.4$)	0.33

Table 4.4 Interfacial properties of SHCC

$V_f(\%)$	$G_d \text{ (J/m}^2\text{)}$	$\tau_0 \text{ (MPa)}$	β
Normal distribution ($\mu = 2.0, \sigma = 0.1$)	1.61	1.11	1.15

Figure 4.20 Probability density for fiber volume V_f

2) To determine the properties of each sampling section

Based on given micromechanical parameters, the properties of each section involving $\sigma_B(\delta)$, σ_{fc} , J_b' , J_{tip} can be derived. Fig. 4.21 is the derived $\sigma_B(\delta)$ of three sections with the fiber volume 1.7%, 2% and 2.3%. The maximum fiber bridging strength increases along with increasing fiber volume, but the maximum crack opening remains the same due to the single variation of fiber volume. Since the final failure occurs at $\min \{\sigma_0\}$ which is located in the section with minimum fiber volume, the crack openings of other sections can be obtained as the dotted red line.

Figure 4.21 The fiber bridging curve $\sigma_B(\delta)$ with V_f of 1.7%, 2% and 2.3%

Selected values of J_b' , J_{tip} , σ_0 , σ_{fc} in each sampling section from section 1 to section 151 are shown in Fig. 4.22. In this example, J_b' is much larger than J_{tip} which is good for achieving strain hardening behaviour. And most of σ_0 is also larger than σ_{fc} , indicating that the composite should have excellent tensile properties.

Figure 4.22 (a) J_b' , J_{tip} ; and (b) σ_0 , σ_{fc} of each sampling section

3) To calculate the tensile properties of the composite

Finally, the tensile properties can be calculated using the flow chart as Fig. 4.19, and the stress-strain curve is shown in Fig. 4.23 compared with experimental results. The strain is achieved using the sum of all different crack opening divides the sample length as well as the elastic deformation of the uncracked portion. As can be seen from the comparison, the simulated strain capacity is comparable with the experimental results. Typical tensile properties of this composite are summarized in Table 4.5 involving the average cracking opening and cracking interval. The resulted average crack opening is calculated as 68 μm , which is smaller than the experimental result of 88 μm . Once again, it indicates that the assumed distribution of V_f cannot reflect the true case in the experiment, and other variation of micromechanical parameters along the sample volume should be considered. The first cracking strength from simulation is quite larger than the experiment, but the crack number is similar. It indicates that the prediction method of first cracking strength and the assumed distribution of matrix cracking strength are also needed to refine in the future.

Figure 4.23 The simulated tensile stress-strain curve

Table 4.5 Tensile properties of experimental and simulated results

	σ_{fc} (MPa)	σ_{cu} (MPa)	ε (%)	δ (μm)	N
Experiment	2.92	4.41	4.88	85	88
Simulation	3.6	4.5	4.5	68	98

Table 4.6 lists the section No. of potential crack, new cracks and inactivated crack, in which the potential crack is the section with cracking strength equal to the applied stress, the inactivated crack is the section within x_d distance relative to the existing crack, and the new crack is the potential crack by removing the inactivated crack. It essentially proves that the cracking sequence is controlled by the transfer distance x_d and the cracking strength of the composite jointly. With increasing number of cracks, x_d becomes more prominent to control the occurrence of new cracks, thus proving that the method of the transfer distance x_d is effective and valid. Consequently, the applicability of the complicated model for SHCC tensile properties is proved. The cracking state first three and final step are shown in Fig. 4.24.

Table 4.6 Lists of Section No. of potential cracks and new cracks in the three steps

Loading step	Section No. of potential cracks ($\sigma = \sigma_{fc}$)	Section No. of new cracks	Inactivated crack
1	16, 44, 120, 155, 208	16, 44, 120, 155, 208	-
2	2, 66, 105, 151 , 180, 188, 198, 221, 233, 249, 261, 264, 271, 278, 279, 281, 295	2, 66, 105, 180, 188, 198, 221, 233, 249, 261, 264, 271, 278, 279, 281, 295	151
3	71, 116, 121 , 134, 136, 170, 194 , 195 , 200 , 203, 209 , 235 , 254	71, 116, 134, 136, 151, 170, 203	121, 194, 195, 200, 209, 235, 254

Figure 4.24 Cracking state at different step

4.6 Summary

In this chapter, multiple cracking sequence and saturation of SHCC are discussed. The cracking strength of the composite and the stress transfer distance x_d

are shown to determine the cracking sequence as well as cracking number. The modified fiber bridging model based on single fiber pullout simulation is used to calculate the crack opening. The new model for x_d is also achieved based on the single fiber pullout simulation, which is one of the novelties of this research. By consideration of the slip hardening criteria of SHCC, the tensile stress-strain curve can be derived with the clarified mechanism of multiple cracking occurrence. Moreover, this comprehensive and holistic process can treat all the micromechanical parameters as variables, which is another novelty of this research.

This model is not perfect, but aiming to show the feasibility of simulating the multiple cracking sequence and tensile stress-strain property of SHCC with considering the variation of both fiber distribution and matrix.

5 The Relation of Mix Composition and Micromechanical Parameters

5.1 Introduction

While the micromechanical model provides linkage between composite behavior and material microstructural properties through a set of micromechanical parameters, the determination of those micromechanical parameters are often through various microscale tests (Section 2.4.1) and the control of microstructure through ingredients selection and component tailoring are largely empirical and very little effort was made to understand the correlation between mix proportion and micromechanical parameters. As a result, proportioning SHCC mixes is never straightforward and method of SHCC mix design has not been proposed thus far. There is a need to find the relation between factors of mix design and micromechanical parameters as shown in Fig. 5.1.

Figure 5.1 Factors of mix design and micromechanical parameters

To build up this relationship, microscale tests are still main approaches to

adopt, including the single fiber pullout test, matrix toughness test and SEM technique. As can be seen from Fig. 5.1, the relationship is not one-to-one, but many-to-many. In the event of revealing the mechanism of microstructural properties with respect to cement chemistry or physical properties of the microstructure, it can contribute to simplify the complex many-to-many relationship which is similar to the relation between compressive strength and gel/space ratio. A number of numerical models (Section 2.4.2) are available and applicable to acquire the physical and chemical properties of cement hydration.

In this chapter, effects of three key mix design parameters of fiber type, water-to-cement ratio (W/C) and sand-to-cement ratio (S/C) on the micromechanical parameters are investigated for purpose of illustration and not limitation. To have the complete understanding of the correlation between mix composition and micromechanical parameters, other mix design factors such as cement type, aggregate type, and curing conditions should be examined in future study. As shown in Fig. 5.2, fiber type determines most of the fiber related micromechanical parameters and greatly influences the interface related micromechanical parameters. Most SHCC mixes exclude the use of coarse aggregates, and therefore water-to-cement (W/C) ratio and sand-to-cement (S/C) ratios represent the most important matrix design factors which influence both the interface and matrix related micromechanical parameters.

Figure 5.2 The scope of this chapter

5.2 Materials

Three types of fibers are studied in current study, i.e. polyethylene (PE) fiber, and polyvinyl alcohol (PVA) fiber without coating and with hydrophobic oiling agent of 1.2% coating by weight. Detailed properties of these fibers are summarized in Table 5.1. Ordinary Portland cement (ASTM C150 Type I) is used in this study. The chemical admixture used for good workability is a superplasticizer (W.R. Grace, ADVA 181) commercially available in Singapore.

Table 5.1 Properties of PE and PVA fibers

Fiber type	Diameter d_f (mm)	Tensile strength σ_t (MPa)	Elongation ε_f (%)	Young's modulus E_f (GPa)
PE	0.044	1640	5.3	41.1
PVA	3000	3000	2.9	103

Two different mix compositions of matrix are designed as shown in Table 5.2. The first group is to understand the effect of water-to-cement ratio on the microstructural properties, and three fiber types are used to investigate the influence of fiber type on the interface related micromechanical parameters. The second group is intended to evaluate the influence of sand content with sand-to-cement ratio up to 1.2 and only PVA fibers with 1.2% coating is used to investigate the interfacial properties.

Table 5.2 Mix proportions

Mix	Cement	Water	Sand	SP
G1: W/C	1.0	0.25	0	0.22
	1.0	0.30	0	0.17
	1.0	0.35	0	0.12
	1.0	0.40	0	0.02
	1.0	0.45	0	0
G2: S/C	1.0	0.35	0.2	0.05
	1.0	0.35	0.4	0.08
	1.0	0.35	0.6	0.10
	1.0	0.35	0.8	0.12
	1.0	0.35	1.0	0.20

5.3 Test methods

5.3.1 Wedge splitting test

The loading device with specimen is displayed in Fig. 5.3. The loading machine used in the present study is INSTRON 5569 uniaxial testing system with the capacity of 50 kN. It is controlled by extension with constant speed at 0.2 mm/min. The splitting force is applied onto the specimen through pulley wheels which are required to be frictionless. A single central line support on the bottom of the specimen is selected to resist the vertical force component because it is concluded that the influence of various supports is not significant [76]. Crack mouth opening displacement (CMOD) was measured using a special clip gauge with ± 4 mm travel and fixed at the same height as the roller center.

The geometry and size of the cube specimen follow the Reference [52]. The initial notch that simulates the crack was made by inserting a steel plate of 1 mm thickness in the specimen during casting and taken out after one day curing after

curing. The notch depth was constant at 90 mm. Thereafter, all specimens were cured in open air under humidity of 65% RH and temperature of 28°C conditions on average for 28 days.

Figure 5.3 Test setup of the wedge splitting test

5.3.2 Single fiber pullout test

The single fiber pullout test was conducted on an MTS Acumen™ testing machine at a speed of 0.1 mm/min. The whole setup is divided into four parts as can be seen from Fig. 5.2. From the bottom, an X-Y table with ± 25 mm travel in two directions was fixed on the base of the machine in order to assure the accuracy of the alignment of the fiber. A 10 N load cell with 0.0001 N accuracy was used to measure the pulling force for the fiber. Samples were connected to the load cell through a sample holder with flat top surface to glue samples and a T bar to screw into the load cell. Note that it should be avoided to glue the embedded end of the fiber to the sample holder since the pullout force would augment in that case. Due to the limited ability of the gripper, an aluminum plate was clamped first, on which

the free end of the fiber was stuck on. The fiber-free length was kept at a maximum of 1 mm so as to adjust the inclination of the fiber. The embedment length of fiber was chosen to be around 1 mm to ensure full debonding. All specimens were cured in open air under humidity of 65% RH and temperature of 28°C conditions on average for 28 days.

Figure 5.4 Test setup of the single fiber pullout test

5.3.3 SEM technique

A scanning electron microscope (FESEM 6340F) was used to study the fiber surface and the matrix tunnel. Scanning electron microscope (SEM) images were taken for two cases, one case is the tip of fibers being pull out, the other is fibers peeled off from the matrix and the corresponding groove of the matrix as illustrated in Fig. 5.5.

Figure 5.5 Schematic illustration of specimens for microstructural observation

5.3.4 Cement hydration model

In this study, the software called Virtual Cement and Concrete Testing Laboratory (VCCTL) was selected to assist in revealing the mechanism of the microstructural properties. The software is a standalone application that runs on desktop or laptop computers and can be downloaded as a single executable installer. It is a virtual lab simulating all the processing steps of mixing and hydrating of the cement composite in the actual lab. Four main steps are involved:

- To prepare the lab materials made with cements, slags, fly ashes, fillers and aggregates, meaning to input all the properties of the materials;
- To create the mix by specifying the mix proportions of the solid portion of the binder with water and aggregate and specifying the system size and other miscellaneous simulation parameters;
- To hydrate the mix under a variety of curing conditions based on 3D digital images of cement particle microstructure created as previous step;
- To measure cement/concrete properties by calculating the linear elastic properties, compressive strength and transport properties as a function of the curing conditions.

Outputs from the simulation, such as the volume fraction of Portlandite (CH) and Calcium Silicate Hydrate (CSH), as well as the porosity, together with microstructure observation may help to reveal the underlying mechanisms of the correlation between mix composition and micromechanical parameters.

5.4 Results and discussion

5.4.1 Effect of fiber type

In SHCC mix design, to select fiber type is the paramount step as per the specific application, the cost of construction, and its local availability. Besides fiber properties that are different among different fiber types as included in Table 5.1, the interfacial properties between fiber and matrix are distinct as shown in Table 5.3. Apparently for PE fiber, negligible chemical bond and slip hardening response are observed. For the frictional bond, it is much lower for PE fiber than PVA fiber for the same mix design.

Table 5.3 The interfacial properties for different fiber types (W/C=0.4)

	G_d (J/m ²)	τ_0 (MPa)	β
0% PVA	1.55 ± 0.65	1.13 ± 0.09	0.37 ± 0.11
1.2% PVA	1.31 ± 0.6	1.07 ± 0.24	0.31 ± 0.09
PE	0	0.67 ± 0.22	0

Chemical bond is due to the intrinsic hydrophilic property of PVA fiber, while PE fiber shows hydrophobic behavior. In the production of PVA fiber, PVA is hydrolyzed by treating it with an alcoholic solution in the presence of an aqueous acid or alkali, which consists of repeating structural units of $[-CH_2-CH(OH)-]_n$ as

Fig. 5.6. OH groups therein present are capable of forming hydrogen bonds between the fiber surface and the hydration products, CH and CSH [77-79], as shown in Fig. 5.7.

Figure 5.6 Chemical formula of PE and PVA

Figure 5.7 Build-up of CH and CSH at the PVA fiber surface

The SEM images of PE and PVA fiber before pullout from matrix as Figs. 5.8 (a) and (b) demonstrate the distinct phenomenon, showing a layer of matrix on the surface of non-coated PVA fiber with chemical bond in the interface of fiber/matrix. The slip hardening response of PE fiber can be observed by Figs. 5.8 (c) and (d). After being pullout from the matrix, PE fiber is intact in diameter, while PVA fiber has a sharp tip with reduced diameter which is scraped by the matrix.

Figure 5.8 SEM images of PE, PVA fiber before and after pullout from the matrix

5.4.2 Effect of water-to-cement (W/C) ratio

1) Matrix toughness K_m

The matrix toughness is the essential characteristic only associated with the matrix resisting cracking propagation. Fig. 5.9 illustrates the effect of W/C ratio on matrix toughness of cement paste. As can be seen, there is a linear decreasing trend of matrix toughness in cement paste along with increasing W/C and lower matrix toughness is in favor of strain hardening behavior.

From literatures, the matrix toughness of cement paste is dependent on the microstructure involving the fracture toughness of binding phase, e.g. Calcium Silicate Hydrate (CSH) [80] and the porosity [81-83]. Fracture toughness of CSH

should remain largely the same while the porosity is greatly influenced by the W/C ratio. Fig. 5.10 shows the correlation between fracture toughness measured from the experiments and the porosity calculated from the cement hydration model.

Figure 5.9 Matrix toughness vs. W/C ratio

Figure 5.10 Matrix toughness vs. porosity of cement paste

2) Chemical bond G_d

As discussed in Section 5.4.1, the PVA fiber possesses the chemical bond due to the intrinsic hydrophilic property. The effects of the oil content of fiber [73] and fly ash volume in the matrix [84] on the chemical bond has been investigated. In these literatures, the W/C ratio was kept in a higher level of above 0.45, but lower W/C ratio is also desirable for developing high strength SHCC. To date, no

integrative study about the effects of W/C and S/C on the interfacial properties can be found. So it is necessary to investigate the effects W/C and S/C on micromechanical parameters.

Fig. 5.11 shows the relationship between the chemical bond G_d and W/C for PVA fibers without any oil coating, presenting that it increases along with increasing W/C. It can be explained using SEM images of fibers and matrix grooves as shown in Fig. 5.12. The fibers were peeled off from the matrix before any testing. The symbol x%-y-z represents the oil coating percentage, W/C ratio, and surface (either fiber (F) or matrix (M)). Obviously observed from Figs. 5.12 (a), (c), and (e), amount of matrix debris attached to the fiber surface, and porosity of interface transition zone (ITZ) are increased with increasing W/C as can be seen in Figs. 5.12 (b), (d), and (f). This indicates that fiber debonding is inclined to occur in the ITZ and the debonding path is tortuous within different thickness of ITZ as illustrated in Fig. 5.13. And the debonding thickness increases along with the porosity of the ITZ as seen in Fig. 5.13 which can be calculated by the cement hydration model. The debonding path represents a mixed fracture mode I and II of ITZ, mainly the fracture toughness of model II gives the main contribution to resist the debonding. But there are no studies on the effect of W/C on matrix toughness of mode II which might show an increasing trend. From the Reference [85], it can be concluded that the trend of mode II toughness is different from the model I toughness. Because fly ash addition in concrete increased the matrix toughness of model II, while it reduced the matrix toughness of model I [86].

Figure 5.11 G_d vs. W/C for PVA fiber without coating

Figure 5.12 SEM images of the fiber surface and the matrix groove

Figure 5.13 Illustration of the location of fiber debonding

For PVA fiber with 1.2% coating used in cement paste, the relation of the chemical bond G_d with W/C is shown in Fig. 5.14. The aim of coating of 1.2% is to reduce the bond of fiber and matrix, so the debonding locations of samples with W/C of 0.25 to 0.45 inclined to occur at the fiber surface as Fig. 5.16, all fibers are after testing being pullout from the matrix. When 1.2% oiling is applied, the delamination effect almost disappeared, allowing the full embedment length to slide out with little damage. As above explained in Section 5.4.1, OH groups present in PVA fiber are capable of forming hydrogen bonds between the fiber surface and the hydration products, CH and CSH. As Fig. 5.15, the volume fraction of CH and CSH calculated from the cement hydration model reduces with increasing W/C ratio which shows the same trend as the chemical bond.

Figure 5.14 G_d vs. W/C for PVA with 1.2% coating

Figure 5.15 Volume fraction of CH and CSH in cement paste

Figure 5.16 SEM images of fibers after being pullout

From the microstructure findings, two different patterns of bond failure are identified for different fiber reinforced systems as summarized in Table 5.4, the debonding occur at interface transition zone (ITZ) for non-oil coating PVA fiber and at the fiber surface for PVA fiber with 1.2% coating. It is concluded that the hydrogen

bond between the fiber surface and the matrix competes with the properties of ITZ related to the porosity or the irregular debonding thickness, which jointly determined the debonding mechanism. Thus, further studies are necessary to quantify the relation of the hydrogen bond or porosity with the chemical bond G_d .

Table 5.4 Summary of fiber debonding condition

W/C	0% PVA		1.2% PVA	
	Debonding location	G_d (J/m ²)	Debonding location	G_d (J/m ²)
0.25	ITZ	0.2	Surface	1.8
0.3	ITZ	0.5	Surface	2.0
0.35	ITZ	0.8	Surface	1.8
0.4	ITZ	1.2	Surface	1.5
0.45	ITZ	1.5	Surface	1.0

3) Frictional bond τ_0

The frictional bond was reported that it increases along with W/C due to the densification of particle packing [87]. It concluded that from only two types of W/C other than full range, so it is necessary to investigate larger range of W/C to understand the mechanism of the frictional bond.

Fig. 5.17 is the relation of the frictional bond τ_0 and W/C for PE fiber, showing it decreases with increasing W/C. Debonding of PE fiber from the surrounding matrix should occur only along the fiber/matrix interface because there is no chemical bond between the PE fiber and the matrix. From literatures, lateral stresses and strains at the fiber/matrix interface are expected to have considerable influence on the frictional bond [77]. The most important lateral effect is the contraction of the matrix around the fiber due to autogenous shrinkage, which generates a clamping stress by a mechanism which is sometimes referred to as the fiber/matrix misfit as

Fig. 5.18 [88]. As reported in the Reference [77], Stang estimated the frictional bond strength values considering the clamping stress and coefficient of friction. The clamping stress comes from the autogenous shrinkage, which decreases along with W/C as Fig. 5.19 [89]. The statement can well explain the decreasing trend of the frictional bond τ_0 with increasing W/C. The other affecting factor is the coefficient of friction which is controlled by the surface roughness of fiber, which can be taken as the slope of the trend curve.

Figure 5.17 τ_0 vs. W/C for PE

$$\text{Misfit} = \left[\text{Fiber radius} \right] - \left[\text{Hole radius after shrinkage} \right]$$

Figure 5.18 Fiber/matrix misfit (after Naaman et al [88])

Figure 5.19 Correlation between autogenous shrinkage and W/C [89]

The frictional bond of PVA fiber is more complicated than that of PE fiber due to the existence of chemical bond which would lead to two types of debonding as described above. Moreover, for some cases, the debonding of PVA fiber occurs in part of ITZ and part of the fiber surface which is a tortuous paths to pass. Therefore, the frictional bond is firstly dependent on the chemical bond to control the debonding location. For PVA fiber without coating, it is identified as debonding at the ITZ from the above analysis of the chemical bond. Thus, it is the friction between two surfaces inside ITZ. As Fig. 5.20 (a), the general profile of the fractional bond τ_0 shows decreasing trend due to the decreasing clamping stress, but the coefficient of friction may vary with different W/C. For PVA fiber with 1.2% coating, the frictional bond decreases as Fig. 5.20 (b) due to the decreasing clamping stress and the constant coefficient of friction, which is because the fiber debonding occurs at fiber surface. The clamping stress which is related to the autogenous shrinkage can be reflected in Fig. 5.20 which shows the decreasing trend.

Figure 5.20 τ_0 vs. W/C for PVA (a) without, and (b) 1.2% coating

4) Slip hardening coefficient β

The frictional force of fiber pullout from matrix is not constant, it may decrease, constant or increase dependent on the fiber type. The slip hardening coefficient is to quantify the increase of the frictional bond for PVA fiber as mentioned in Section 5.4.1. As reported in the Reference [73], the slip hardening phenomenon is due to the scrapping of fiber by surrounding matrix and the jamming effect of the matrix debris as can be seen from Fig. 5.21, in which the tip of the fiber has been scrapped to quite smaller diameter after being pullout. So far, no research on the variation of slip hardening coefficient along with W/C.

Figure 5.21 The fiber after pullout from matrix

From the above statement, the slip hardening coefficient may be linked to the relative hardness of the fiber and matrix. As Fig. 5.22 (a), β decreases with W/C, while the hardness of matrix decreases along with W/C [90]. But the slip-hardening coefficient β does not change along with W/C ratio for PVA fiber with 1.2% coating as shown in Fig. 5.22 (b). According to the discussion on the chemical bond, it debonds at fiber/matrix interface, which may have negligible relation with the relative hardness of fiber/matrix.

Figure 5.22 β vs. W/C for PVA without coating

5.4.3 Effect of sand-to-cement (S/C) ratio

1) Matrix toughness K_m

Fig. 5.23 shows the matrix properties of composite with the addition of the sand. With increasing sand-to-cement (S/C) ratio, there is a parabolic trend of matrix toughness, attaining the highest value with S/C of 0.8. The increase magnitude of toughness is not quite large with different addition of sand, however, it augments greatly compared with cement paste with the same W/C as can be seen from the solid symbols in Fig. 5.23. It is because the matrix with the addition of the silica sand requires more energy to break the crack because the sand may act as stress concentrator during the fracture process. And the crack propagates as tortuous paths along the sand surface in cement mortar system sketched in Fig. 5.24. But an excess of sands also causes poor workability of the composite and high porosity [91], thereby leading to lower matrix toughness.

Figure 5.23 Matrix toughness vs. S/C ratio

Figure 5.24 Schematic illustration of crack propagation

2) Interfacial Properties

The addition of sand is generally regarded as an important influencing factor on the matrix [45], while its effects on the interfacial properties have not been discussed. Thereof, the frictional bond is affected most because the enhancement of the matrix toughness [92].

In this study, PVA fiber with 1.2% coating is used to illustrate the interfacial properties with S/C. As Fig. 5.25 (a), the chemical bond G_d is kept below 1 J/m² lower than the result of the same coating PVA fiber in cement paste. It indicates that the overall binder content reduces mainly CH and CSH and therefore chemical

adhesion between fiber and matrix reduces as well. Excess of sand like S/C up to 1.0, a quite low chemical bond is also derived, again reflecting the effective CH and CSH reduces because of higher porosity. And it implies that PVA fiber with 1.2% coating in cement mortar system is inclined to occur debonding at the fiber surface. But the low chemical bond is good for achieving strain hardening behavior of the composite.

The frictional bond τ_0 as Fig. 5.25 (b) has distinct upward trend along with S/C ratio. However, the autogenous shrinkage decreases with the addition of the sand, Igarashi et al. [93] has been shown that adding aggregate to a mixture can decrease the amount of autogenous shrinkage. It is because cement paste is the portion of the mixture responsible for the shrinkage, and the overall cement paste decreases with increasing content of sand. This can be seen from the comparison of the frictional bond τ_0 in cement paste (red dot) and the result with S/C of 0.2, it decreases with the addition of the sand due to the decrease of the autogenous shrinkage. Thus, the increase of the frictional bond would attribute to the coefficient of friction, which may increase along with the increasing sand content. No literature has discussed about the coefficient of friction, but the same trend of increasing frictional bond was observed in strain hardening cementitious composites with incorporation of recycled concrete fines [92].

From Fig. 5.25 (c), the slip-hardening coefficient β increases when adding the sand compared with the result in cement paste, since the enhancement of the hardness in the cement mortar. Along with the increasing sand content, it shows slight descending trend with increasing S/C, but within a small range of variation. Excessive sand content also affects the slip hardening behavior as can be seen from

S/C of 1.0 and 1.2.

Figure 5.25 Interfacial properties vs. S/C ratio

5.5 Summary

In this chapter, the methodology of building up the relation between

micromechanical parameters and the factors of mix design is proposed, comprising of experimental and numerical methods. Using this method, the relationship of mix composition involving fiber type, W/C and S/C with matrix properties and interfacial properties are investigated. It mainly presents that:

- 1) Different fiber types have different interfacial properties, e.g. for PE fiber, there only exists the frictional bond, while PVA fiber exhibits the chemical bond, the frictional bond and the slip hardening behavior.
- 2) By virtue of the relation between the micromechanical parameters and W/C in cement paste, the mechanism of the chemical bond and the frictional bond are discussed. Once the fiber debonding occur at the surface, the chemical bond is related to the volume fraction of CH+CSH; and the debonding occur at the ITZ, it is dependent on the properties of ITZ, like porosity. While the frictional bond is expressed by

$$\tau_0 = f(G_d, T, \gamma)$$

where T denotes the clamping stress related to the autogenous shrinkage; γ is the coefficient of friction which is simply evaluated as constant value along with W/C, but a variable along with S/C when debonding occurs at the fiber surface.

- 3) Slip hardening behavior is observed for PVA fibers, which may attribute to the relative hardness of the matrix and the fiber.

6 Mix Design Method for SHCC

6.1 Introduction

The material ingredients which make up strain hardening cementitious composites (SHCC) are similar to FRC that contain cement, sand, water, and admixtures. A large body of SHCC versions has been developed using local material ingredients in various countries, including USA [86, 94], Japan [95, 96], Europe [97], and South Africa [98]. But each version of SHCC is hard to repeat due to the variability of all the raw materials according to the reported mix design in literatures. Thus, researchers have to go through trial-and-error approaches to get one sound mix with unknown strain capacity. If the tested strain capacity is not as expected or satisfactory, to change the mix proportion in correct directions becomes a critical issue. As of today only "reference recipes" were presented, there exists no generally accepted mix design method for SHCC.

Concrete mix design is defined as the appropriate selection and proportioning of constituents to produce a concrete with pre-defined characteristics in the fresh and hardened states. In general, concrete mixes are designed in order to achieve workability, strength and durability. However, for general purpose of SHCC, the mechanical properties involving compressive strength and tensile properties are the sole design consideration at the current stage. The fresh state is required to ensure good dispersion of fibers using admixtures, and supplementary cementitious materials (SCM) are incorporated to mitigate the durability issue. As far as we know, very often requirements of concrete design are more stringent than those demanded

by the strength requirements. Different from concrete, the paramount requirement of SHCC design is the tensile ductility, and workability also take significant effects on the mechanical property. With addition of fibers in SHCC, three phases of fiber, fiber/matrix interface and matrix are needed to deliberately control the material constituents for achieving desired properties of SHCC, which is more complicated than normal concrete. Therefore, it is reasonable to view the mechanical property of SHCC as the target at present development stage.

In this chapter, the linkage between the factors of mix design and composite tensile properties has been connected through micromechanical parameters as shown in Fig. 6.1. Chapter 5 can relate the factors of mix design to the micromechanical parameters, and Chapter 4 can be used to modeling the composite tensile properties by micromechanical parameters. Due to the multivariate nature of mix composition and the micromechanical parameters, an appropriate methodology is needed to link the mix composition with the ultimate composite performance. This chapter focuses on the systematic design methodology for producing SHCC as input for structural design.

Figure 6.1 The objective of Chapter 6

All the variability of the composite no matter of the mix processing or batching can be considered by the distribution of the parameters as in Chapter 3, so the design method of SHCC can conduct pre-assessment of failure possibility in advance. So the mix design on the basis of recommended method is expected to be a reliable mix proportion, other than an initial guess at the optimum combination of ingredients like normal concrete.

6.2 The principle of proposed mix design method

6.2.1 Basic considerations

As described in Section 2.1, the compressive strength of concrete is directly related to the factors of mix design based on a large pool of experimental database. And it assumes the compressive strength of concrete is governed by its water-to-cement ratio, and the workability is governed by its water content. Unlike the design of concrete, the mechanical property of SHCC is the only consideration at present stage. So the selection and proportioning of material constituents merely depend on the mechanical performance requirement of the material.

There is a bridge between the factors of mix design and composite tensile at micro level of SHCC, resulting in a complex many-to-many relation between factors of mix design and micromechanical parameters as Chapter 5. For example, varying water-to-cement (W/C) ratio would not only change the properties of matrix (K_m), but also affect the interface properties (G_d , τ_0 , β). All of these micromechanical properties are not linear relationship with the ultimate composite performance, they must be compatible to achieve the desired mechanical requirement. Obviously, best

combinations of micromechanical parameters can relate to several classes of SHCC mixes.

6.2.2 Outline of mix design method

The various factors for determining the concrete mix proportions and the step by step procedure for SHCC mix design can be schematically represented in Fig. 6.2. The procedure includes two phases, the first phase will provide a first approximation of the proportions and the second phase is to optimize the mix proportion to achieve the targeted composite performance including compressive and tensile behavior.

Figure 6.2 The flow chart of the mix design methodology for SHCC

First phase (selection of first mix):

The first phase is to select the type of ingredients involving cement, sand, fiber, and other SCM, as well as the ingredients proportioning for the first mix. For example, high early strength cement should be chosen if the application requires short construction time. The proportions like W/C and S/C are determined based on the compressive strength f_c . For fiber type and proportion, the aim of the designer should always be to get SHCC mixtures of optimum behavior with available type of fiber and minimum fiber volume. The consideration of fiber type and fiber volume

is discussed in detail as follows.

a. Fiber type

There are numerous fiber types available for commercial and experimental use for making SHCC. Generally, the basic fiber categories used are polymeric or metallic fibers. Specific descriptions of these fiber types are included in ACI 544.1R-96 [99]. Table 6.1 describes the geometry and mechanical properties of various types of fibers that can be used as randomly dispersed filaments in a cementitious matrix. Because of the wide range of properties for each type of fiber, the designer should be guided by the manufacturer's data on each particular product and experience with it before a fiber type is selected. Additionally mentioned, polyvinyl alcohol (PVA) is a water-soluble synthetic polymer with high tensile strength and flexibility, which is well-suited to be used in making SHCC and has been applied more and more. The PVA fiber can be easily tailored via the control of the surface coating. For this hydrophilic fiber, the untreated fiber has a too high chemical and frictional bond with cementitious material. A surface coating content between 0.8 and 1.2% by weight of fibers tends to lower the interface chemical and frictional bond properties to a level that causes the critical fiber volume fraction to drop to a minimum of about 2% [5].

Table 6.1 Typical properties of fibers

Type of fiber	Diameter (mm)	Density (g/cm ³)	Tensile strength (GPa)	Young's modulus (GPa)	Elongation (%)
Steel	0.2	7.8	2.2	210	3 ~ 4
PE	0.04	0.97	2.7	120	5
PVA	0.04	1.3	0.88 ~ 1.8	25 ~ 42	6 ~ 10
PP	0.02	0.91	400	5 ~ 12	25

The principle behind the design of SHCC as discussed in Section 6.2 does not depend on a particular fiber. Fibers with certain properties, however, may meet the criteria for tensile strain hardening behavior. Decisions on what fibers to use will depend on their natural characteristics, including mechanical, diameter ranges, and surface characteristics, on resulting SHCC mechanical, durability, and sustainability performances and on economics.

b. Fiber volume

The additional cost of SHCC over normal concrete derives mostly from the use of fibers and higher cement content. This is the reason why optimization of the composite to minimize the fiber content is so important. In comparison to steel fibers used in many FRC, polymer fibers such as PVA may be more expensive on a unit weight basis. However, it should be noted that polymer fibers have density six to seven times lower than that of steel, and it is the volume content of fibers and not the weight content which governs the performance of the cementitious composite.

Fiber length, denier and configuration are additional factors that will affect workability and consolidation of the SHCC. These factors should also be taken into consideration when adjusting SHCC mixes with elevated dosage levels of fibers. The use of a water reducer is a definite consideration when higher fiber dosage levels are required. Workability of SHCC is directly related to providing sufficient mortar to coat the fibers in a given mix. If there is sufficient mortar present to accommodate the fibers the loss of workability, if any, will be minimized.

Second phase (optimization of mix proportions):

The second phase is to optimize the first trial mix if the ultimate performance cannot meet with the expectation. Following the information from Table 4.2, which

points out critical parameters to affect different design factors, a simple guidance on optimizing mix proportions is proposed based on Chapter 5 as illustrated in Table 6.2. For example, high J_b' is typical index to achieve strain hardening behavior of SHCC, corresponding lower τ_0 is needed, thereby high W/C and low S/C are desirable. Fiber types also can be tailored according to the guidance. However, low τ_0 may result in low σ_0 , so the second phase may undergo several iterations to get an optimal mix design.

Table 6.2 A simple guidance on optimizing mix proportions based on Chapter 5

Design factors	Micromechanical parameters	Mix proportions			
		Fiber		W/C	S/C
Crack opening $\delta \downarrow$	$\tau_0 \uparrow$	$\sigma_{fu} \downarrow$	$d_f \downarrow$	$\downarrow$	$\uparrow$
Fiber bridging strength $\sigma_0 \uparrow$	$\tau_0 \uparrow$	$\sigma_{fu} \uparrow$	$V_f \uparrow$	$\downarrow$	$\uparrow$
Complementary energy $J_b' \uparrow$	$\tau_0 \downarrow$	$\sigma_{fu} \uparrow$	$E_f \downarrow$	$\uparrow$	$\downarrow$
Matrix toughness $K_m \downarrow$	---	---		$\uparrow$	$\downarrow$

In the second phase, except the requirement of mechanical performance, other considerations also can add into the optimization, e.g. lowering the cement content with high SCM for sustainability.

6.2.3 Detailed procedure of mix design

Each step of the mix design procedure according to the flow chart in Fig. 6.2 are narrated in this part.

To select the basic mix proportions according to the compressive strength

The relationship of the compressive strength and basic proportions involving water-to-cement ratio (W/C), sand-to-cement ratio (S/C) and SCMs can be achieved

using the experimental results database of concrete like design of experiment (DOE) method. In addition, some cement hydration model like VCCTL software can be used to estimate compressive strength, which inputs all the mixtures and easily output viewable calculations of concrete elastic moduli and compressive strength. So basic proportions can be obtained for the targeted compressive strength. For simplicity, fiber contribution for the compressive strength is ignored here because either increase [100] or decrease [101] is very slight.

To determine the μ -parameters

Chapter 5 provides an approach to relate the factors of mix design and micromechanical parameters with experimental and numerical methods. And three factors involving fiber type, W/C and S/C are investigated. However, there are many others factors in SHCC mixes needed to build up the relationship with micromechanical parameters. The same method as Chapter 5 can be used to fill up the database in the future, or some factors can be found in the literatures, such as the relation of fly ash as supplementary cementitious materials (SCM) in SHCC with the micromechanical parameters [86], and the relation of PVA fiber coating with the micromechanical parameters [73]. The Example 2 in Section 6.3 will demonstrate the determination of the micromechanical parameters using the information from the literature.

To calculate the tensile properties

There are two judgements before and after this step. Before it, first assessment of the basic mix proportions can be conducted using PMM in Chapter 3 to rough estimate the strain softening behavior or the strain hardening behavior of the composite, accordingly the level of strain capacity can be roughly known. If the

strain capacity can achieve the target, the tensile properties can be calculated using the model in Chapter 4. Otherwise, the mixture has to be tailored through the same procedure until satisfied tensile behavior. This assessment can be save much computational energy and time.

The second assessment after the calculation of the tensile properties is to exactly know whether the basic mix proportions are met with the targeted performance with the specific application. When the tensile and compressive behavior of the mixture is satisfied, the tensile behavior can be output using the model in Chapter 4 and the compressive behavior can be known during the process. This step is not only to know the strain capacity, but also the ultimate tensile strength, crack opening, and crack interval which are also important information for the application. If any of the information is not met with the requirement of the specific application, the tailoring of the mixture still needs to be conducted.

6.3 Demonstration of SHCC mix design

In the following, two SHCC mix design examples are demonstrated mainly to present the applicability of the holistic mix design method. Example 1 is mainly to demonstrate the procedure of the first phase in order to emphasize the importance of the first trial selection of mixture. In reality, reference recipes can be used to assist in the first phase of SHCC mix design. Example 2 is to show the tailoring of the mix design with the aim of lowering the cement content.

6.3.1 Example 1

Following the mix design procedure as Fig. 6.2, Example 1 is realized step by

step as follows with the specified characteristic compressive strength and the tensile strain capacity of 40 MPa and 1%, respectively. In this example, PVA fiber with 1.2% oil coating is selected in this mix according to the availability of the fibers. Its properties are in Table 6.3, namely, E_f , L_f , d_f , σ_{fu} which are also micromechanical parameters as inputs in the following model. Due to the low density of PVA fiber, fiber volume would be used in the mix design. Considering the ease of fiber dispersion, low fiber volume of 2% is tried first.

Table 6.3 Micromechanical parameters

Fiber						Interface					Matrix			
E_f	L_f	d_f	σ_{fu}	V_f		G_d	τ_0	β	f	f'	E_m	σ_{mu}	K_m	
(GPa)	(mm)	(μm)	(MPa)	(%vol.)		(J/m ²)	(MPa)				(GPa)	(MPa)	(MPa·m ^{1/2})	
				μ	σ							λ	k	
42.8	8	39	1070	2	0.3	1.5	1.9	0.35	0.5	0.3	24	1.1	2.4	0.5

To select W/C and S/C according to the compressive strength

In the mix, only ordinary Portland cement (OPC) of ASTM Type I and water are used in the matrix. The consistency of this pure mixture is highly dependent on the quality of cement and admixtures, so the probability factor k is chosen as 3 which assure the compressive strength with maximum probability. According to the specified characteristic compressive strength f_c of 40 MPa, the targeted mean compressive strength f_m is

$$f_m = f_c + k \times s = 40 + 3 \times 8 = 64 \text{ MPa}$$

s is simply determined using the values of the normal concrete design in Fig. 6.3 [6].

Figure 6.3 Minimum standard deviation as a function of strength (DOE method)

[6]

Next, based on the relation of compressive strength and W/C as Fig. 6.4, the water-to-cement ratio is selected as 0.35. In addition, the compressive strength can be verified using VCCTL software. Hence, the mix proportions are in Table 6.4.

Figure 6.4 The relation of compressive strength (f_c) with W/C

Table 6.4 Designed mixture

Cement	Water	HRWRA (%)	Fiber (% vol.)
1.0	0.35	0.1	2

To determine the μ -parameters

For this mixture, the micromechanical parameters can be acquired based on the database in Chapter 5 as illustrated in Fig. 6.5. Thus, all relevant micromechanical parameters are shown in Table 6.2. According to the discussion in Section 3.4.2, f and f' are assumed as constant values. The variation of fiber volume V_f is assumed as a normal distribution with standard deviation of 0.2. σ_{mu} is assumed as two-parameter Weibull distribution based on literature with scale parameter and shape parameter of 1.1 and 2.4, respectively.

Figure 6.5 Relations of micromechanical parameters (G_d , τ_0 , β , E_m , K_m) with W/C

To calculate the tensile properties

Using the probabilistic-based micromechanics model in Chapter 3, the failure probability and reliability index are indicated in Table 6.5. Based on the conclusions from Chapter 3, the targeted tensile strain capacity of 1% can be achieved. Thus, no further tailoring is needed for this mixture.

Table 6.5 Probabilistic assessment of the mixture

Failure probability $P_f(\%)$		Reliability index α	
P_{f1}	P_{f2}	α_1	α_2
0	10.35	57.8	1.26

Based on derived micromechanical parameters, the tensile behavior of the mixture is calculated and compared with experimental results as Table 6.6 and Fig. 6.6. The minimum cracking strength is needed in order to get the distribution of σ_{fc} . The determination of this value is needed to be further discussed, in this example, the value of 3.5 MPa is used from the experimental result.

As can be seen from the simulation results, the targeted compressive strength and tensile strain capacity can be acquired using this mix design. Compared with experimental results, the simulated results are good enough which indicates that the mix design methodology for SHCC is valid. In addition, the simulated results can give the information of ultimate tensile strength, crack number, crack opening and crack interval. If the engineering designer is not satisfied with any one of the information, the same procedure can be applied to tailor the mixture.

Figure 6.6 Stress-strain curve of the mixture

Table 6.6 Ultimate performance

Minimum cracking strength (MPa)	Ultimate tensile strength (MPa)		Tensile strain capacity (%)		Compressive strength (MPa)	
	Exp.	Cal.	Exp.	Cal.	Exp.	Target
3.5	4.6	4.62	1.15	1.02	62.9	64

6.3.2 Example 2 [86]

This example is mainly to demonstrate the optimization procedure of SHCC mix design, the optimized factor is the usage of fly ash so as to reduce the cement content. For this example, the specified characteristic compressive strength and the tensile strain capacity of 30 MPa and 2%, respectively. The targeted mean compressive strength f_m is

$$f_m = f_c + k \times s = 30 + 3 \times 8 = 54 \text{ MPa}$$

PVA REC15 fiber with surface oiling coating 1.2% is selected and the fiber volume of 2% is selected here.

To select basic mix proportions according to the compressive strength

In the mix, ordinary Portland cement (OPC) of ASTM Type I is selected to use and it is tried to incorporate Class F coal fly ash in the mixture to lower the cement content. According to the targeted mean compressive strength of 54 MPa, there are many groups of mixtures with different W/C ratio and sand content. In reality, the maximum required W/C ratio and the maximum S/C ratio would be selected as the basic mix for achieving the minimum cement content. But for demonstration in this study, M41 is used as the basic mix design in Table 6.7. The compressive strength of M41 is 77 MPa, which is calculated using VCCTL.

Table 6.7 The designed mixture proportions

Mix		Cement	FA/C	S/cm	W/C	W/cm	HRWRA (%)	Fiber (%vol.)
Basic	M41	1.0	0.1	0.4	0.27	0.24	3.0	2
Optimized	M45	1.0	1.2	0.4	0.53	0.24	3.0	2

To determine the μ -parameters

The relationship of mix proportions with micromechanical parameters is from experiments as Fig. 6.7 [86]. Consequently, all relevant micromechanical parameters are shown as Table 6.8. The assumption of f, f', V_f and σ_{mu} are the same as **Example 1**, except that the standard deviation of V_f is assumed as 0.5 and 0.1 because fly ash is good for the fiber dispersion.

Figure 6.7 Relations of micromechanical parameters (G_d , τ_0 , β , K_m) with FA/C [86]

Table 6.8 Micromechanical parameters of ECC M45 [86]

Mix	Fiber						Interface					Matrix			
	E_f (GPa)	L_f (mm)	d_f (μm)	σ_{fu} (MPa)	V_f (%vol.)		G_d (J/m ²)	τ_0 (MPa)	β	f	f'	E_m (GPa)	σ_{mu} (MPa)	K_m (MPa·m ^{1/2})	
					μ	σ							λ	k	
M41	25.8	12	39	900	2	0.5	3.5	3.5	0.4	0.5	0.3	20	1.1	2.4	0.79
M45	25.8	12	39	900	2	0.1	1.0	3.5	0.55	0.5	0.3	20	1.1	2.4	0.68

To calculate the tensile properties

The failure probability and reliability index are calculated using PMM, results are shown in Table 6.9. Based on the conclusions from Chapter 3, it indicates that no strain hardening behavior is assessed for M41.

Table 6.9 Probabilistic assessment of the mixture

Mixture	Failure probability $P_f(\%)$		Reliability index α	
	P_{f1}	P_{f2}	α_1	α_2
M41	50	9.56	0	1.31
M45	0.02	7.99	3.52	1.41

To tailoring the basic mix proportions

Here, the aim is to increase the usage of fly ash for lowering the cement amount, M45 with FA/C of 1.2 is used for demonstration as Table 6.7. And all the micromechanical parameters are shown in Fig. 6.7 and Table 6.8. Using PMM, the failure probability and reliability index are listed in Table 6.8, showing the targeted tensile strain capacity of 2% may be achieved by mixture M45.

Based on derived micromechanical parameters, the tensile behavior of M45 is calculated as Table 6.10, presenting that strain capacity of 2.49% can be achieved. By comparing the calculated results and the experimental results of M41 and M45, it indicates that the mix design methodology is applicable, but the accuracy is closely dependent on the assumption of the distribution of micromechanical parameters.

Table 6.10 Ultimate performance of M41 and M45

Mixture	Minimum cracking strength (MPa)	Ultimate tensile strength (MPa)		Tensile strain capacity (%)		Compressive strength (MPa)	
		Exp.	Cal.	Exp.	Cal.	Exp.	Target
ECC M41	4.64	5.48	4.64	0.37	0	75.2	77
ECC M45	4.11	4.86	4.94	2.49	2.02	52.6	54

6.4 Summary

In this study, unlike the mix design of normal concrete, the mix design of SHCC is to achieve required mechanical properties without considering the workability and durability. The linkage between the factors of mix design and composite tensile properties has been connected through micromechanical parameters by integration of Chapter 5 and Chapter 4. And during the mix design procedure of SHCC, Chapter 3 contributes to the advanced estimate of strain softening or strain hardening behavior thereby saving computational time and energy. The design procedure of SHCC is the most important achievement in this research and simply demonstrated using two examples. The demonstration shows that the procedure is applicable and can be extended into more complex cases given the large enough database about the relations of micromechanical parameters and mix compositions.

7 Conclusions and Future Work

7.1 Conclusions

In this research, all the work is based on the micromechanical model of strain hardening cementitious composites (SHCC) [2]. The final goal of this study is to relate the mix composition of SHCC with the ultimate properties involving the compressive strength and more importantly, the tensile stress-strain behavior. The significance of this study is apparent to facilitate the users of SHCC to do mix design according to various applications, without onerous trial-and-error experiments which is the only option currently. Main conclusions can be drawn from this study as follows.

In order to achieve the goal of this research, two relations are needed to build up, one is the tensile stress-strain relation as Chapter 3 and Chapter 4 with considering the heterogeneity of SHCC, the other relation is between the mix composition and micromechanical parameters as Chapter 5.

In Chapter 3, a novel probabilistic-based micromechanical model (PMM) is proposed by introducing the probability concept, instead of the deterministic safety factors of energy performance index J_b'/J_{tip} and stress performance index σ_0/σ_{fc} . The critical process is to explicitly express the performance indices J_b' and σ_0 using the MARS method. It provides an insight and understanding of underlying micromechanical parameters which can deliver the information to guide mix design of ECC. Based on the built MARS model, reliability analysis can be conducted by minimizing the reliability index subject to the constraint of the performance function.

Lower probability of failure or higher reliability index is expected to attain high strain hardening behavior of ECC.

In Chapter 4, a novel model for calculating the tensile stress-strain relation is proposed based on the strain hardening criteria of SHCC. This model is not perfect, but aiming to show the feasibility of simulating the multiple cracking sequence and tensile stress-strain properties of SHCC with considering the variation of both fiber distribution and matrix. In this model, different opening of each crack can be captured taking into account of the variation of fiber distribution by virtue of the fiber bridging model starting from single fiber pullout properties. In addition, the mechanism of multiple cracking sequence and saturation of SHCC is clarified, which presents that they are jointly determined by the cracking strength of the composite and the stress transfer distance x_d . The new model of x_d is also achieved based on this fiber bridging model, which can consider the stochastic nature of the composite.

In Chapter 5, the relations of mix composition involving fiber type, W/C and S/C with matrix properties and interfacial properties were investigated and discussed. It claimed that different fiber types have different interfacial properties, e.g. for PE fiber, there is only frictional bond, while PVA fiber, it presents chemical bond, frictional bond and slip hardening behavior. The mechanism of the chemical bond and the frictional bond are discussed. Once the fiber debonding occur at the surface, the chemical bond is related to the volume fraction of CH+CSH; and the debonding occur at the ITZ, it is dependent on the physical and chemical properties of ITZ such as porosity. While the frictional bond is expressed by

$$\tau_0 = f(G_d, T, \gamma)$$

where T denotes the clamping stress related to the autogenous shrinkage; γ is the coefficient of friction.

In Chapter 6, the principle and procedure of mix design methodology for SHCCs is proposed and simply demonstrated using two examples. It shows that this methodology is applicable to predict the compressive and tensile behavior from mix proportions. The design procedure of SHCC is the most important achievement in this thesis, which is expected to provide a useful method to conduct SHCC mix design.

7.2 Future work

In Chapter 3, although the framework of PMM of SHCC is firstly proposed here, many aspects of this model still can be modified and improved as follows.

- 1) The database can be enriched by more combinations of micromechanical parameters or selecting other types of fibers. Using the created database, it may be feasible to build up MARS model for each type of fibers through the same procedure of PMM.
- 2) From the theory of probabilistics, there are other alternatives with the same aim of MARS and FORM. For example, the artificial neural networks (ANN) is also successfully applied to a number of civil engineering problems. Comparative work could be carried out to come up with more approximate substitution model with the true model.

- 3) For the reliability analysis, FORM is adopted here for simplicity with certain accuracy, while Monte Carlo simulation (MCS) is more accurate than FORM to assess the failure of probability due to fewer assumptions of the distributions of input variables.

In Chapter 4, the model to simulate the cracking sequence and tensile ductility is feasible with full account of all the variability of micromechanical parameters. However, four things should be mentioned,

- 1) The precision of the model is directly dependent on the distribution of the parameters. In this study, the distribution of parameters is acquired from fitting the experimental results or reasonable assumptions. Only a few of researchers have done some work on the fiber distribution and flaw size distribution using fluorescence microscopy, therefore, a big database of the distribution of micromechanical parameters has to be created and new techniques should be developed in order to investigate the heterogeneity of the composite like computed Tomography.
- 2) The prediction of the first cracking strength is not perfect in this research. Many assumptions are adopted for simplicity, like the penny shape crack, the parabolic crack profile and the fraction of fiber contribution.
- 3) In modeling the cracking process, crack interaction is not considered. When two cracks occur within small distance saying a half of the fiber length, the potential crack section may be affected by both of the two existing cracks. In addition, intersected cracks are observed in real experiments, the mechanism of this phenomenon is not clear yet.

- 4) After the first crack is formed, the elastic modulus of the uncracked composite is replaced by the fiber bridging relation, i.e. $\sigma_B(\delta)$. Accordingly, the load drops suddenly due to force equilibrium between the cracked section and the adjacent uncracked composite section. The load will again increase gradually with an increase of deformation until the induced stress reaches a sufficient level to cause the formation of another crack in the composite. This phenomenon reflected in the stress-strain relation is zig-zag curve, but this study treats it instead of smooth line which can be further investigated.

In Chapter 5, the experimental method combining with cement hydration model is a good way to do further studies, several aspects can be conducted in the future work.

- 1) The relations of other mix compositions are also necessary to know, like aggregate type, supplementary cementitious materials (SCM), maturity of the composite, and so forth.
- 2) The mechanism of the chemical bond, the frictional bond and the slip hardening coefficient should be quantitatively investigated related to the chemical or physical properties of the interface transition zone (ITZ).
- 3) Other micromechanical parameters may also have relation with the mix composition, such as the snubbing coefficient f and the strength reduction coefficient f' .

In Chapter 6, only simple examples are used to demonstrate the applicability of the mix design procedure of SHCC. Further studies can be conducted to use the methodology to extend into the large scale field of application.

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Appendix I

Program	Notes
<pre> a=load('Training.txt'); X2=a(:,2); X3=a(:,3); X4=a(:,4); X5=a(:,5); X6=a(:,6); X7=a(:,7); X8=a(:,8); X9=a(:,9); X10=a(:,10); X11=a(:,11); X=[X1, X2,X3,X4,X5,X6,X7,X8,X9,X10,X11]; Y=a(:,12); </pre>	Input training data
<pre> params = aresparams(150, 0, false, [], [], 2); model = aresbuild(X, Y, params) </pre>	Build MARS model
<pre> aresanova(model, X, Y) </pre>	ANOVA decomposition analysis
<pre> Yq=arespredict(model,X); J=Yq-Y; J1=sum(J.^2); S1=sum((Y-mu).^2); K1=1-J1/S1 S=mean(J); tmse=sum((J-S).^2); mse=tmse/length(Y); mae=sum(abs(J))/length(Y); rmse=sqrt(mse); K=(J-S)/rmse; </pre>	Residual analysis to remove outliers with $K \in [-1, 1]$

<pre> b=load('Testing.txt'); Xt(:,1)=b(:, 1); Xt(:,2)=b(:, 2); Xt(:,3)=b(:, 3); Xt(:,4)=b(:, 4); Xt(:,5)=b(:, 5); Xt(:,6)=b(:, 6); Xt(:,7)=b(:, 7); Xt(:,8)=b(:, 8); Xt(:,9)=b(:, 9); Xt(:,10)=b(:, 10); Xt(:,11)=b(:, 11); Yt=b(:, 12); </pre>	Input testing data
<pre> [MSE, RMSE, RRMSE, R2] = arestest(model, Xt, Yt) </pre>	Assess MARS model with test data
<pre> aresplot(model) areseq(model,5) </pre>	Output MARS model in an mathematical form