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Micromechanical investigation for the probabilistic behavior of unsaturated concrete

Qing Chen[1,2,3a], Zhiyuan Zhu[3b], Fang Liu[*4], Haoxin Li[2,3c] and Zhengwu Jiang[2,3d]

[1]Jiangsu Key Laboratory of Environmental Impact and Structural Safety in Engineering, University of Mining & Technology, Jiangsu, 221116, China
[2]Key Laboratory of Advanced Civil Engineering Materials, Tongji University, Ministry of Education, 4800 Cao'an Road, Shanghai 201804, China
[3]School of Materials Science and Engineering, Tongji University, Shanghai 201804, China
[4]State Key Laboratory of Disaster Reduction in Civil Engineering, Tongji University, Shanghai, 200092, China

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Abstract. There is an inherent randomness for concrete microstructure even with the same manufacturing process. Meanwhile, the concrete material under the aqueous environment is usually not fully saturated by water. This study aimed to develop a stochastic micromechanical framework to investigate the probabilistic behavior of the unsaturated concrete from microscale level. The material is represented as a multiphase composite composed of the water, the pores and the intrinsic concrete (made up by the mortar, the coarse aggregates and their interfaces). The differential scheme based two-level micromechanical homogenization scheme is presented to quantitatively predict the concrete's effective properties. By modeling the volume fractions and properties of the constituents as stochastic, we extend the deterministic framework to stochastic to incorporate the material's inherent randomness. Monte Carlo simulations are adopted to reach the different order moments of the effective properties. A distribution-free method is employed to get the unbiased probability density function based on the maximum entropy principle. Numerical examples including limited experimental validations, comparisons with existing micromechanical models, commonly used probability density functions and the direct Monte Carlo simulations indicate that the proposed models provide an accurate and computationally efficient framework in characterizing the material's effective properties. Finally, the effects of the saturation degrees and the pore shapes on the concrete macroscopic probabilistic behaviors are investigated based on our proposed stochastic micromechanical framework.

Keywords: unsaturated concrete; probabilistic behaviors; effective properties; deterministic and stochastic micromechanics; distribution-free method; differential scheme; Monte Carlo simulations

1. Introduction

The microstructure demonstrates inherent randomness even using the same manufacturing process, since it is difficult in detailing the exact pre-determined microstructural composites (Ferrante and Graham-Brady 2005, Chen *et al*. 2015, Chen *et al*. 2018a, b, Jiang *et al*. 2019, Zhu *et al*. 2015, Guan *et al*. 2015). Predicting the probabilistic behavior of the material properties for a given microstructure and its spatial distribution plays a significant role in the material design and reliability assessment (Tomar *et al*. 2018, Ostoja-Starzewski 1993, Rahman and Chakraborty 2007, Zhou *et al*. 2017, Huang *et al*. 2019, Yang *et al*. 2019). The stochastic multiscale numerical models are presented with the material's random configurations (Dong *et al*. 2020, Guan *et al*. 2016, Yang *et al*. 2020, Rahman 2009, Banchs *et al*. 2007). Meanwhile, the stochastic multiscale models are proposed for fracture analysis of functionally graded materials (Chakraborty and Rahman 2008, 2009). More stochastic multiscale simulation models can be found from the overview work (Ferrante *et al*.2008). Recently, the stochastic micromechanics-based framework has been employed to quantify the material's probabilistic behavior based on their random microstructures for many areas, such as the composite and the functionally graded material (Ferrante and Graham-Brady 2005, Chen *et al*. 2015, Zhu *et al*. 2015).

As one of the most commonly used materials, the concrete appears fluctuating properties even with the same preparing process. Meanwhile, the concrete material under the aqueous environment (e.g., the dams, ship locks and tunnels) are usually not fully saturated by water (Rossi *et al*. 1992, Ross *et al*. 1996, Yaman *et al*. 2002a, Chen *et al*.2020, Li *et al*. 2020). On one hand, to characterize the fluctuating behavior of concrete material, the commonly used probability density function (PDF) is employed with certain assumptions, which will lead to biased results (Zhu

*Corresponding author, Associate Professor
E-mail: 09146@tongji.edu.cn
[a]Associate Professor
E-mail: chenqing19831014@163.com
[b]Graduate Student
E-mail: 15900737182@163.com
[c]Professor
E-mail: bosomxin@126.com
[d]Professor
E-mail: jzhw@tongji.edu.cn

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et al. 2014, Er 1998). On the other hand, to investigate the effects of the saturation degrees on the concrete macroscopic properties, micromechanical models are proposed for predicting the elastic modulus and Poisson's ratio of unsaturated concrete (Yaman *et al*. 2002b, Wang *et al*. 2007, Zhu *et al*. 2014, Yan *et al*. 2013, Chen *et al*. 2018a, b). It is noted that all these micromechanical models are set up in the deterministic framework and they don't consider the inherent randomness of the unsaturated concrete's microstructures.

In this paper, to overcome the shortcomings mentioned above, a stochastic micromechanics-based framework is proposed to quantify the unbiased probabilistic behavior of the concrete with different saturation degrees. Meanwhile, instead of the Mori-Tanaka method adopted by current micromechanical model for concrete under water conditions, the differential scheme based multilevel homogenization procedures are employed to obtain the effective properties of the concrete with different saturation degrees. Furthermore, a distribution-free method is employed to get the unbiased PDFs of the material's properties based on the maximum entropy principle. Compared with the existing models, the presented framework is computationally efficient and able to predict the unbiased probabilistic behavior of the unsaturated concrete based on the material's random microstructures. The rest of this paper is organized as follows. The differential-scheme for two-phase composite is presented in section 2. Section 3 proposes the deterministic micromechanical framework for the concrete with different saturation degrees. In section 4, the stochastic micromechanical framework is obtained by modeling the properties and volume fractions of the constituents as stochastic. Numerical examples including the validations and discussions are presented in section 5. And some conclusions are reached in the final section.

2. The differential-scheme for two-phase composite

2.1 The effective properties of a composite

To estimate the material effective properties is one of the goals of the continuum micromechanics. The representative volume element (RVE) is usually employed to describe the composite material. The RVE is set up upon a 'mesoscopic' length scale, which is considerably larger than the characteristic length scale of inhomogeneities but smaller than the characteristic length scale of a macroscopic specimen (Ju and Chen 1994a, b). Take a two-phase composite as an example, the effective elastic stiffness tensor of the composite is defined through

$$\bar{\boldsymbol{\sigma}} = \boldsymbol{D} : \bar{\boldsymbol{\varepsilon}} \tag{1}$$

With

$$\bar{\boldsymbol{\sigma}} = \frac{1}{V}\int_V \boldsymbol{\sigma}(x)dx = \frac{1}{V}\left[\int_{V_0} \boldsymbol{\sigma}(x)dx + \int_{V_1} \boldsymbol{\sigma}(x)dx\right] \tag{2}$$

$$\bar{\boldsymbol{\varepsilon}} = \frac{1}{V}\int_V \boldsymbol{\varepsilon}(x)dx = \frac{1}{V}\left[\int_{V_0} \boldsymbol{\varepsilon}(x)dx + \int_{V_1} \boldsymbol{\varepsilon}(x)dx\right] \tag{3}$$

Where V is the volume of an RVE, V_0 is the volume of the matrix, and V_1 is the volume of the inhomogeneity, $\bar{\boldsymbol{\sigma}}$ and $\bar{\boldsymbol{\varepsilon}}$ are volume averaged stress and strain of the RVE, respectively.

2.2 The differential scheme

In terms of the inclusion-based micromechanical theory and the average stress method (Mura 1987), the effective elastic stiffness tensor of the two-phase composite can be rephrased as Eq. (4)

$$\boldsymbol{D} = \boldsymbol{D_0} + \phi(\boldsymbol{D_I} - \boldsymbol{D_0})\boldsymbol{A} \tag{4}$$

where $\boldsymbol{D_0}$ is the elastic stiffness tensor of the matrix phase, $\boldsymbol{D_I}$ is the elastic stiffness tensor of the inhomogeneity, $\boldsymbol{A}$ is the strain concentration tensor for the inhomogeneity, ϕ denotes the volume fraction of the inhomogeneity.

Let us define $\phi = \Omega_1/(\Omega_0 + \Omega_1)$ and $\phi + \Delta\phi = (\Omega_1 + \Delta\Omega)/(\Omega_0 + \Omega_1 + \Delta\Omega)$, where Ω_0 and Ω_1 represent the volume of the matrix phase and the inclusion phase in the current composite, respectively, $\Delta\Omega$ denotes the increment of inclusion volume. For the differential method, a composite with the volume fraction of inclusion equal to $\phi + \Delta\phi$, can be treated as the equivalent composite with the volume fraction of inclusion equal to $\Delta\Omega/(\Omega_0 + \Omega_1 + \Delta\Omega)$. It is noted that the matrix phase in the equivalent composite is the current composite, which includes the current matrix (Ω_0) and current inclusion (Ω_1). According to Eq. (4), the effective properties of the material can be obtained as (Norris 1985, McLaughlin 1977)

$$\boldsymbol{D}(\phi + \Delta\phi) = \boldsymbol{D}(\phi) + \frac{\Delta\Omega}{(\Omega_0 + \Omega_1 + \Delta\Omega)}\big(\boldsymbol{D_I} - \boldsymbol{D}(\phi)\big)\boldsymbol{A}\big(\boldsymbol{D}(\phi)\big) \tag{5}$$

Eq. (5) can be rephrased as below through the simple derivation

$$\frac{\boldsymbol{D}(\phi + \Delta\phi) - D(\phi)}{\Delta\phi} = \frac{1}{1-\phi}\big(\boldsymbol{D_I} - \boldsymbol{D}(\phi)\big)\boldsymbol{A}\big(\boldsymbol{D}(\phi)\big) \tag{6}$$

with

$$\Delta\phi = \frac{\Omega_1 + \Delta\Omega}{\Omega_0 + \Omega_1 + \Delta\Omega} - \frac{\Omega_1}{\Omega_0 + \Omega_1} = \frac{(1-\phi)\Delta\Omega}{(\Omega_0 + \Omega_1 + \Delta\Omega)} \tag{7}$$

When $\Delta\phi \to 0$, Eq. (6) can be expressed as

$$\frac{d\boldsymbol{D}(\phi)}{d\phi} = \frac{1}{1-\phi} \bullet \big(\boldsymbol{D_I} - \boldsymbol{D}(\phi)\big) : \boldsymbol{A}\big(\boldsymbol{D}(\phi)\big) \tag{8}$$

The composite effective properties with no inclusion effects should be the same as those of the matrix phase, which implies

$$\boldsymbol{D}(\phi)|_{\phi=0} = \boldsymbol{D}_0 \tag{9}$$

When the Eshelby method is considered (Mura 1987), we write

$$\boldsymbol{A} = \left[\boldsymbol{I} + \boldsymbol{S}\boldsymbol{D}(\phi)^{-1}(\boldsymbol{D_I} - \boldsymbol{D}(\phi))\right]^{-1} \tag{10}$$

where $\boldsymbol{S}$ is Eshelby's tensor, which depends on $\boldsymbol{D}(\phi)$ and the shape of the inclusions, $\boldsymbol{I}$ defines the fourth-order isotropic identity tensor.

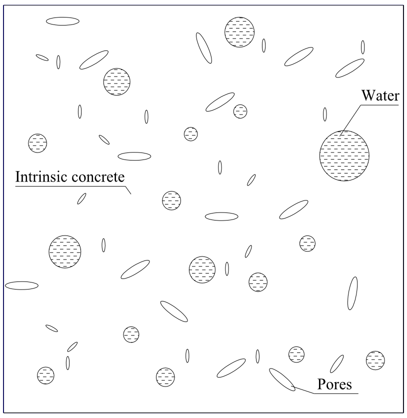


Fig. 1 Multi-phase micromechanical model for unsaturated concrete

3. Differential scheme based deterministic micromechanical framework

3.1 The effective porosity and the effective saturation degree

Given that the porosity of concrete may change due to the effect of further hydration (Delmi *et al.* 2006), the effective porosity concept ϕ_{eff} has been introduced, which can be obtained with $\phi_{eff} = m(k_p, t, v)\phi$, Where ϕ refers to the porosity of dry concrete, $m$is a function of seepage rate (k_p), seepage time (t) and effective viscosity of water (v), and m<1 for wet concrete (Wang and Li 2007).

Generally, saturation degree (SD) is the volume ratio of water to pores. However, this definition is not suitable for the effective property investigation of concrete with different saturation degrees. There are three zones for concrete in the water environment: fully saturated zone, unsaturated zone and dry zone. Saturated zone refers to the outermost zone in which the pores are fully filled with water, dry zone to the innermost zone in which the concrete is dry, and the unsaturated zone to those between. As we know, the compressibility of air in the home state is too high to make the pores stiff. Therefore, only the saturated pores have the effects on the properties of concrete comparing with the dry sample. Therefore, the effective saturation degree refers to the percentage of saturated pores in all pores of unsaturated concrete, which can be defined as $S_{eff} = \frac{V_{P-sat}}{V_P} = h(k_p, t)S_w$, Where V_{P-sat} is the volume of pores which are fully filled with water or the volume of water in saturated zone, V_P is the total volume of pores in concrete (including the pores filled with water), S_w is the general saturation degree h is less than 1 (Wang and Li 2007).

3.2 Micromechanical model for concrete with different saturation degree

At the micro level, the concrete is composed of the pores, the water, the mortar, the coarse aggregates and their interfaces (Yaman *et al.* 2002b, Wang *et al.* 2007). Since this study uses micromechanics to study the influence of the saturation degree, the three traditional solid phases (i.e, mortar, coarse aggregates and their interfaces) are similarly merged into one matrix phase, namely intrinsic concrete, in representative volume element (Yaman *et al.* 2002b, Wang *et al.* 2007). And the inclusions phases are composed of the saturated pores, the unsaturated pores and the dry pores.

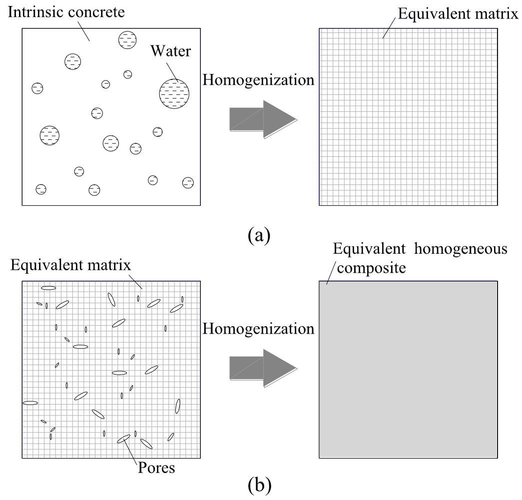


Fig. 2 The multilevel homogenization procedures: (a) the first-level: homogenization of the intrinsic concrete and water, (b) the second-level: homogenization of the pores and equivalent matrix

Because the water pressure inside the pores is symmetric and orientation-independence, the fully saturated zones are assumed to be spheres (Yaman *et al.* 2002b, Wang *et al.* 2007). Conversely, the microcracks and microvoids in the unsaturated/dry zone are presumed to be elliptical thereby incorporating their influences on effective properties (Yaman *et al.* 2002b, Wang *et al.* 2007). Using the aforementioned assumptions, a multi-phase micromechanical model for concrete with different saturation degrees is proposed, as displayed in Fig. 1. It is noted that the connected pores in the concrete is not considered as the previous works (Yaman *et al.* 2002b, Wang *et al.* 2007).

Multilevel homogenization scheme has been proved to be effective to obtain the properties of the multiphase composite, such as the fiber reinforced concrete (Ju and Zhang 1998, Sun and Ju 2004, Chen *et al.* 2016a), shale rocks (Mousavi *et al.* 2016, Chen *et al.* 2016b) and repaired concrete (Chen *et al.* 2015a, b, 2016c, 2017a). A new differential scheme based multi-level homogenization is utilized to attain the effective properties of the concrete material with different saturation degrees, as shown in Fig. 2. Firstly, the equivalent matrix is reached by homogenization of the two-phase composite consisting of the water phase and intrinsic concrete, Secondly, the concrete material's properties are calculated by homogenization of the two-phase composite made up of the equivalent matrix and different pores. For the fully saturated (S_{eff}=100%) or dry concrete (S_{eff}=0), only the first or second level homogenization is performed to obtain the material's properties.

3.3 Differential scheme based homogenization for the equivalent matrix

In this section, the equivalent matrix made up of the saturated pores and intrinsic concrete is obtained by the differential scheme based homogenization process.

Suppose $\boldsymbol{D}_1$, $\boldsymbol{D}_3$ and $\boldsymbol{D}_{em}$ signify the stiffness tensor of the water phase, the intrinsic concrete and the equivalent matrix obtained by the differential scheme based homogenization process. For the isotropic matrix and spherical inclusions, the tensorial components of $\boldsymbol{I}$, $\boldsymbol{D}_1$, $\boldsymbol{D}_3$, and $\boldsymbol{D}_{em}$ are as follows

$$I_{ijkl} = \frac{1}{3}\delta_{ij}\delta_{kl} + \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \frac{2}{3}\delta_{ij}\delta_{kl}) \tag{11}$$

$$\boldsymbol{D}_{3ijkl} = K_3\delta_{ij}\delta_{kl} + \mu_3(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \frac{2}{3}\delta_{ij}\delta_{kl}) \tag{12}$$

$$\boldsymbol{D}_{1ijkl} = K_1\delta_{ij}\delta_{kl} + \mu_1(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \frac{2}{3}\delta_{ij}\delta_{kl}) \tag{13}$$

$$\boldsymbol{D}_{em_{ijkl}} = K_{em}\delta_{ij}\delta_{kl} + \mu_{em}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \frac{2}{3}\delta_{ij}\delta_{kl}) \tag{14}$$

where δ_{ij} is the Kronecker delta. K_3 , μ_3 (K_1 , μ_1 and K_{em} , μ_{em}) are respectively the bulk modulus and shear modulus of the intrinsic concrete (the water and the equivalent matrix).

By substituting Eqs. (11)-(14) into Eqs. (8)-(10), the effective bulk modulus and the shear modulus of the equivalent matrix are obtained by solving the following nonlinear ordinary differential equations after some derivations

$$\frac{dK_{em}}{d\phi_F} + \frac{(K_{em} - K_1)(3K_{em} + 4\mu_{em})}{(1-\phi_F)(3K_1 + 4\mu_{em})} = 0 \tag{15}$$

$$\frac{d\mu_{em}}{d\phi_F} + \frac{5\mu_{em}(\mu_{em} - \mu_1)(3K_{em} + 4\mu_{em})}{(1-\phi_F)[3K_{em}(3\mu_{em} + 2\mu_1) + 4\mu_{em}(2\mu_{em} + 3\mu_1)]} = 0 \tag{16}$$

with the initial conditions as below

$$K_{em}(0) = K_3 \tag{17}$$

$$\mu_{em}(0) = \mu_3 \tag{18}$$

Where $\phi_F = S_{eff}\phi_{eff}/\big(1-(1-S_{eff})\phi_{eff}\big)$ denotes the volume fraction of the water in the equivalent matrix composed of the water phase and the intrinsic concrete. See details for Yan *et al.* (2013).

3.4 The homogenization for the equivalent homogenous composite

Let K_2 , μ_2 and K_{ec} , μ_{ec} be the effective bulk modulus and shear modulus of the air and equivalent homogenous composite (i.e., the unsaturated concrete). For simplicity, the properties of the air can be assumed to be zero. K_{ec} and μ_{ec} can be obtained by replacing the matrix phase in Berryman's work with the equivalent matrix obtained by the first level homogenization herein (Berryman 1980). The resulting iteration schemes are described by the expressions below

$$(K^*)_{n+1} = \frac{(1-\phi_k)K_{em}(P^{*2})_n}{(\phi_k)(P^{*1})_n + (1-\phi_k)(P^{*2})_n} \tag{19}$$

$$(\mu^*)_{n+1} = \frac{(1-\phi_k)\mu_{em}(Q^{*2})_n}{(\phi_k)(Q^{*1})_n + (1-\phi_k)(Q^{*2})_n} \tag{20}$$

$$\phi_k = (1-S_{eff})\phi_{eff} \tag{21}$$

$$(P^{*1})_n = \frac{(K^*)_n}{\pi\alpha(\beta^*)_n} \tag{22}$$

$$(P^{*2})_n = \frac{(K^*)_n + \frac{4}{3}\mu_S}{K_{em} + \frac{4}{3}\mu_{em} + \pi\alpha(\beta^*)_n} \tag{23}$$

$$(Q^{*1})_n = \frac{1}{5}(1 + \frac{8(\mu^*)_n}{\pi\alpha((\mu^*)_n + 2(\beta^*)_n)} + \frac{4(\mu^*)_n}{3\pi\alpha(\beta^*)_n}) \tag{24}$$

$$(Q^{*2})_n = \frac{1}{5}(1 + \frac{8(\mu^*)_n}{4\mu_{em} + \pi\alpha((\mu^*)_n + 2(\beta^*)_n)} + 2\frac{K_{em} + \frac{2}{3}\mu_{em} + \frac{2}{3}(\mu^*)_n}{K_{em} + \frac{4}{3}\mu_{em} + \pi\alpha(\beta^*)_n}) \tag{25}$$

with

$$(\beta^*)_n = (\mu^*)_n\frac{(3(K^*)_n + (\mu^*)_n)}{(3(K^*)_n + 4(\mu^*)_n)} \tag{26}$$

$$\alpha = \frac{1}{N}\sum_{i=1}^{N}\frac{a_i}{b_i} \tag{27}$$

where $(K^*)_{n+1}$, $(\mu^*)_{n+1}$ and $(K^*)_n$, $(\mu^*)_n$ are the (n+1)th and nth approximations of K^* and μ^* , respectively; $(P^{*1})_n$, $(P^{*2})_n$, $(Q^{*1})_n$, $(Q^{*2})_n$ are coefficients defined by the nth approximations to K^* and μ^*, i.e., $(K^*)_n$and $(\mu^*)_n$. α is the equivalent aspect ratio of the pores, a_i and b_i are the lengths of the pores' minor and major axes, respectively, and N is the number of the different pores in the unsaturated and dry zones of the concrete.

When the difference between these two successive approximations is small enough (in the present case, this value is 0.0001), the effective properties of the unsaturated concrete can be expressed as follows

$$K_{ec} = (K^*)_n, \mu_{ec} = (\mu^*)_n \tag{28}$$

Furthermore, the Young's modulus of unsaturated concrete can be obtained based on the theorem of the elastic mechanics, provided that the bulk modulus and shear modulus are known

$$E_{ec} = \frac{9K_{ec}\mu_{ec}}{3K_{ec} + \mu_{ec}} \tag{29}$$

where E_{ec} is the Young's modulus of the equivalent homogenous composite.

In the proposed homogenization framework, we assume that the initial flaws (like the (micro-) pores) are evenly distributed. The localized flaws are not considered herein.

4. Stochastic micromechanical framework for the unsaturated concrete

4.1 Stochastic descriptions for the microstructures of the unsaturated concrete

There is an inherent randomness of the unsaturated concrete and the saturation degrees fluctuate when different specimens are considered. To consider these uncertainties, the input of the micromechanical predicting model should be random. Therefore, in this section, the volume fraction and the material properties of the constituents in the unsaturated concrete are described by the appropriate random variables. Accordingly, our proposed micromechanical model is readily extended to a stochastic framework.

Let $(\boldsymbol{\Omega}, \boldsymbol{\xi}, P)$ be a probability space, where $\boldsymbol{\Omega}$ is the sample space, $\boldsymbol{\xi}$ is the σ-algebra of subsets of $\boldsymbol{\Omega}$, and P is the probability measure, and $\boldsymbol{R}^N$ be an N-dimensional real vector space. The constituents of unsaturated concrete include the intrinsic concrete, water and air. Their properties should be random according to the stochastic micromechanical framework. Further, the sum of the volume fractions of the different constituents should equal to one, which means that the volume fractions of all the components are not independent. Meanwhile, the volume fraction of saturated and unsaturated pores can be represented by the effective saturation degree and effective porosity as $S_{eff}\phi_{eff}$ and $\left(1-S_{eff}\right)\phi_{eff}$. Furthermore, the equivalent aspect ratio should also be described as random variable which characterizes the shape fluctuations of the different pores. Therefore, the random vector $\left\{E_1, v_1, E_2, v_2, E_3, v_3, S_{eff}, \phi_{eff}, \alpha\right\}^T \in \boldsymbol{R}^9$ characterizes uncertainties from all sources for unsaturated concrete based on our proposed micromechanical model. The characterization of the effective properties of the unsaturated concrete becomes a problem of characterization of a random function with multivariate. In the next section, the maximum entropy principle is employed to get the unbiased PDFs of the effective properties based on our latest work.

4.2 Maximum entropy based probability density function for the effective properties

4.2.1 Maximum entropy principle based probability density function

According to the maximum entropy principle (Jaynes 1957), the unbiased PDF for a random variable can be represented as the following expression (Zhu *et al.* 2015)

$$f(x)=\exp[a_0+\sum_{i=1}^{N} a_i x^i] \tag{30}$$

where $a_i, i=0,1,2\ldots n$ are the Lagrangian multipliers. And these parameters can be obtained by solving the following equations

$$\begin{bmatrix} 1 & m_1 & \cdots & m_{n-1} \\ m_1 & m_2 & \cdots & m_n \\ \vdots & \vdots & \ddots & \vdots \\ m_{n-1} & m_n & \cdots & m_{2n-2} \end{bmatrix} \begin{bmatrix} a_1 \\ 2a_2 \\ \vdots \\ na_n \end{bmatrix} = \begin{bmatrix} 0 \\ -1 \\ -2m_1 \\ \vdots \\ -(n-1)m_{n-2} \end{bmatrix} \tag{31}$$

$$a_0 = ln\left(\frac{1}{\int_{-\infty}^{+\infty} e^{a_1x+a_2x^2+\cdots a_nx^n}dx}\right) \tag{32}$$

where m_i ($i=1,2\ldots 2n-2$) are the different order moments for x. It is noted that the moment matrix in Eq. (31) usually becomes singular, when the number of parameters becomes large (Zhu *et al.* 2015). To obtain the more stable results, the normalization procedures are adopted. Specifically, Let $\bar{f}(\bar{x})$ be the PDF of the normalized variable $\bar{x}=\frac{x-\mu_x}{\sigma_x}$, with μ_x and σ_x representing the mean and standard deviation. $\bar{f}(\bar{x})$ can be reached by solving the following equations according to the maximum entropy principle

$$\begin{bmatrix} 1 & 0 & \cdots & \bar{m}_{n-1} \\ 0 & 1 & \cdots & \bar{m}_n \\ \vdots & \vdots & \ddots & \vdots \\ \bar{m}_{n-1} & \bar{m}_n & \cdots & \bar{m}_{2(n-1)} \end{bmatrix} \begin{Bmatrix} \bar{a}_1 \\ 2\bar{a}_2 \\ \vdots \\ n\bar{a}_n \end{Bmatrix} = \begin{Bmatrix} 0 \\ -1 \\ \vdots \\ -(n-1)\bar{m}_{n-2} \end{Bmatrix} \tag{33}$$

$$\bar{a}_0 = ln\left(\frac{1}{\int_{-\infty}^{+\infty} e^{\bar{a}_1x+\bar{a}_2x^2+\cdots \bar{a}_nx^n}dx}\right) \tag{34}$$

where $\bar{a}_i$ ($i=0,1,2\ldots n$) are the Lagrangian multipliers for the normalized variable $\bar{x}$, $\bar{m}_i$ ($i=1,2\ldots n$) are the different order moments for $\bar{x}$. With the PDF $\bar{f}(\bar{x})$ of normalized variable $\bar{x}$, the PDF $f(x)$ of the variable x can be obtained as follows

$$f(x)=\frac{1}{\sigma_x}\bar{f}\left(\frac{x-\mu_x}{\sigma_x}\right) \tag{35}$$

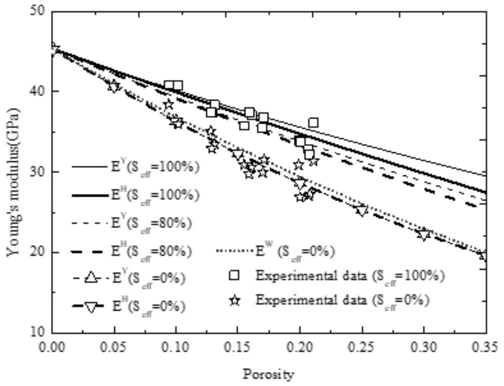
4.2.2 The moments and PDFs of the effective properties

Through the stochastic descriptions of the microstructures, the effective properties of the unsaturated concrete turn to a random function with multivariate random variables based on our proposed deterministic micromechanical model. Hence, the effective modulus, such as K^*, μ^* or E^*, can be regarded as a random variable, which can be represented by x.

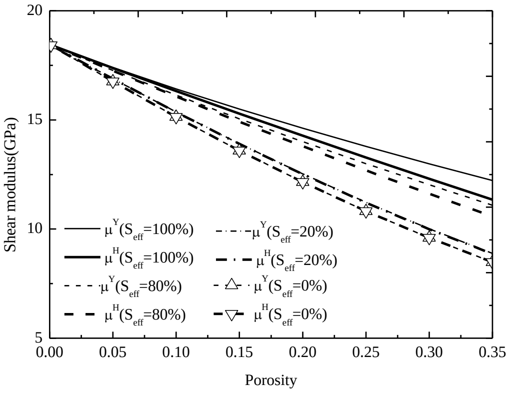
Take the effective bulk modulus as an example. The ith moment of the effective properties after the normalization procedures can be reached using the following formulas.

$$\bar{m}_i^{K^*} = \frac{1}{M}\sum_{m=1}^{M}\left[\frac{K_m^*-mean(K^*)}{sd(K^*)}\right]^i \tag{36}$$

with



(a) Young's modulus



(b) Shear modulus

Fig. 3 Comparisons among our predictions, the existing micromechanical results and the experimental data (Yaman *et al.* 2003a) for the properties of concrete with different saturation degrees, where superscripts Y, W, H represent results of Yan *et al.* (2013), Wang and Li (2007) and our presented framework

$$mean(K^*) = \frac{1}{M}\sum_{m=1}^{M}(K_m^*),$$

$$sd(K^*) = \sqrt{\left(\frac{1}{M}\sum_{m=1}^{M}\left(K_m^* - mean(K^*)\right)^2\right)^{1/2}} \tag{37}$$

where $\bar{m}_i^{K^*}$ stands for the ith moments of the normalized effective bulk modulus, M is the sample size, $mean(\ )$ and $sd(\ )$ denote the mean and standard deviation, respectively, K_m^* is the mth sample of the effective bulk modulus.

By replacing $\bar{m}_i$ in Eq. (33) with $\bar{m}_i^{K^*}$ obtained by Eqs. (36)-(37), the coefficients for the PDFs of the normalized effective bulk modulus can be obtained, with which the PDFs of the non-normalized properties can be calculated with Eqs. (35). Similarly, through the Monte Carlo simulations, the different moments of effective shear modulus and Young's modulus can be obtained based on our proposed model, with which the maximum entropy based PDFs for these properties can be reached. It is noted that the uncertainties over the measurement equipment are not taken into considerations.

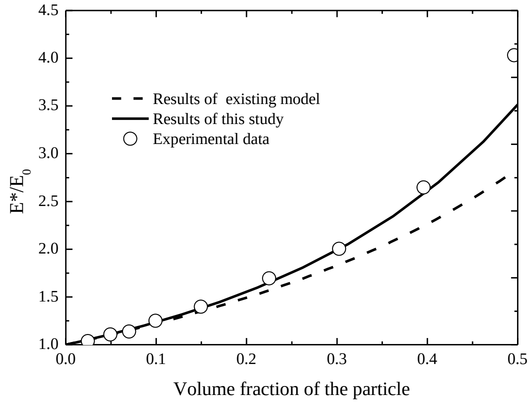


Fig. 4 Comparisons among our predictions, the existing micromechanical results (Yan *et al.* 2013) and the experimental data (Smith 1976) for particle reinforced composite

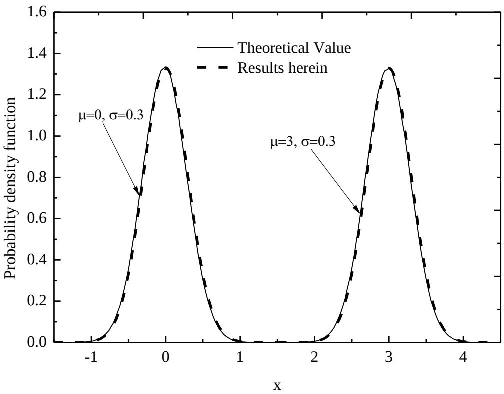
5. Verifications and discussions

5.1 Verifications

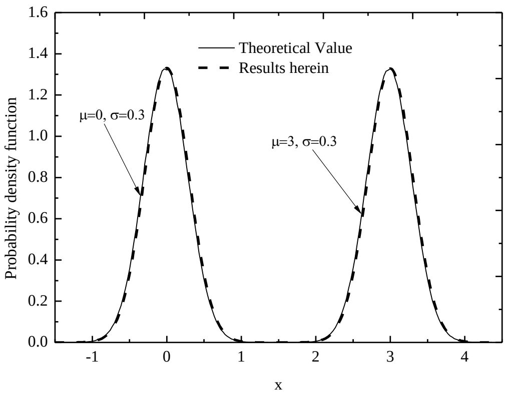
Numerical examples including limited experimental validations, comparisons with existing micromechanical models, commonly used PDFs and the direct Monte Carlo simulations are utilized to verify the proposed micromechanical framework.

Firstly, the experimental data of Yaman *et al.* (2003a) and two estimated results of existing models (Yan *et al.* 2013, Wang and Li 2007) are compared to our predicted results to test the accuracy of our deterministic model, as presented in Fig. 3. In the numerical case, the equivalent aspect ratio equals 0.2 (Wang and Li 2007). Fig. 3(a) shows that results of the model developed in this paper fits well with the experimental results. Meanwhile, our results are the same as those of Yan *et al.* (2013) and close to those of Wang and Li (2007) at the dry state. Given that water in saturated pores limits the concrete deformation and increases the concrete stiffness, it can also be observed that the Young's modulus of the wet concrete improves with the increasing saturation degree. As demonstrated by Fig. 3(b), a similar trend can be obtained as to the effective shear modulus. If the unsaturated pores are ignored, the proposed deterministic micromechanical model is capable of predicting the effective properties of particle-reinforced composite by changing the water phase into the particle phase. Fig. 4 shows the comparisons among our results, those of Yan *et al.* (2013) and the experimental data (Smith 1976). It can be found that our results correspond better with the experimental data than those of Yan *et al.* (2013), when the volume fraction of the particle increases.

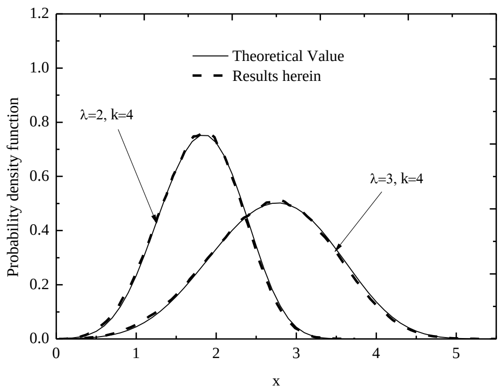
Secondly, three commonly used PDFs, including the normal distribution, lognormal distribution and Weibull distribution, are employed to verify our proposed distribution-free method. The PDF and statistical parameters are listed in Table 1. The sample size M=1000 and n=3 in this numerical example. As to the normal distribution, our proposed distribution-free method is capable of representing these distributions without any



(a) Normal distribution

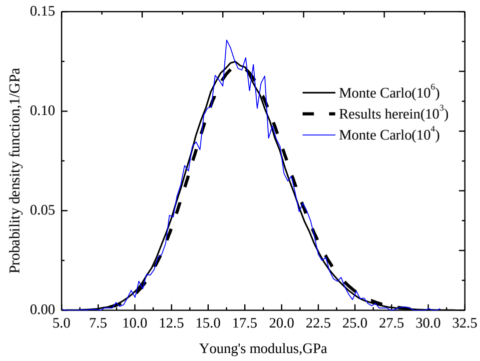


(b) Lognormal distribution

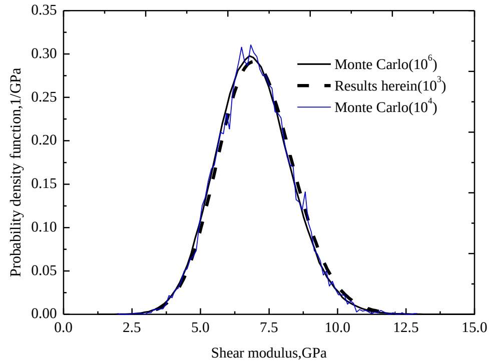


(c) Weibull distribution

Fig. 5 Comparisons among our predictions and the commonly used PDFs



(a) Young's modulus



(b) Shear modulus

Fig. 6 Comparisons among our predictions and those of the direct Monte Carlo simulations

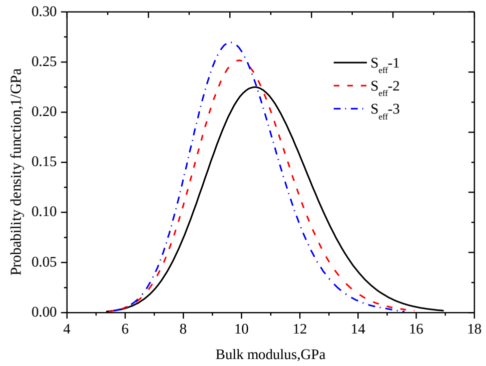
premise. When the means or standard deviations change, the results herein are still closed to the theoretical results, which is displayed by Fig. 5(a). Similarly, the proposed maximum entropy based PDFs corresponds well with the theoretical solutions of the lognormal distribution and Weibull distribution when different statistical parameters are considered, as shown in Fig. 5(b) and Fig. 5(c).

Thirdly, PDFs obtained by our proposed stochastic micromechanical framework are compared with the direct Monte Carlo simulations. The properties of intrinsic concrete are independent lognormal random variables. According to the previous works (Chen 2014), the mean for the Young's modulus and Poisson's ratio are 45.36 GPa and 0.229, the coefficients of variation of these two parameters are 0.1. Since the range of effective saturation degree, the effective porosity and equivalent aspect ratio is between 0 and 1, their distribution types are considered to be a Beta distribution. With the moments of the effective properties obtained by Monte Carlo simulation, the PDFs of effective properties of the unsaturated concrete can be obtained by the maximum entropy principle. Two sample sizes are adopted for the direct Monte Carlo simulaitons. Fig. 6(a) exhibits the PDF of the Young's modulus calculated by direct Monte carlo method and our proposed simulation framework. It can be found that our predictions, with sample size M=10^3, are better than or close to those using direct Monte Carlo simulaitons with sample size M=10^4 or M=10^6. It means that to get the PDF with acceptable accuracy the iterative times in solving the micromechanical equations by direct Monte carlo method is 10^6. However, the iterative times can be dramatically reduced to 10^3 when our proposed simulation framework is used. Similar conclusions can be reached for the PDF of the shear modulus, which are exhibited in Fig. 6(b).

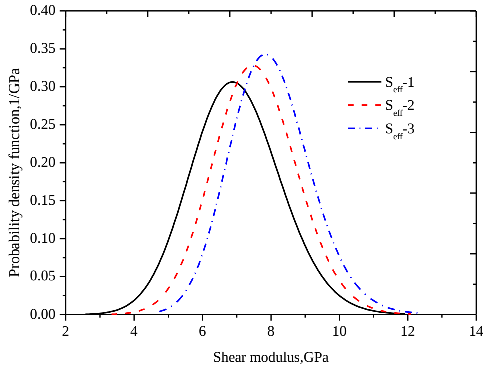
5.2 Discussions

The saturation degree and the shape of pores in unsaturated zones have significant effects on the effective properties of the unsaturated concrete.

Three types of saturation degrees are employed as examples to investigate the influence of the randomness of saturation degrees on the probabilistic characters of the concrete. The mean values for the effective saturation



(a) Bulk modulus



(b) Shear modulus

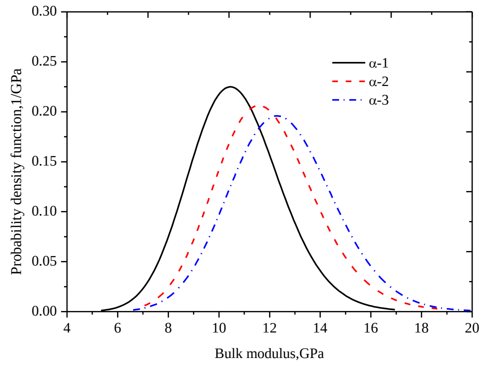
Fig. 7 Influence of saturation degrees on the probabilistic behavior of unsaturated concrete

degrees are 0.8, 0.6 and 0.4 with coefficients of variation being 0.1 in this example. It can be found that with the increase of the mean value for the effective saturation degree, the unsaturated concrete demonstrates greater bulk modulus statistically from Fig. 7(a). Meanwhile, due to the randomness of the microstructures, some samples obtained using the greater mean values are still lower than those reached with smaller mean values of the effective saturation degrees. For the effective shear modulus, similar conclusions can be reached, as shown in Fig. 7(b).

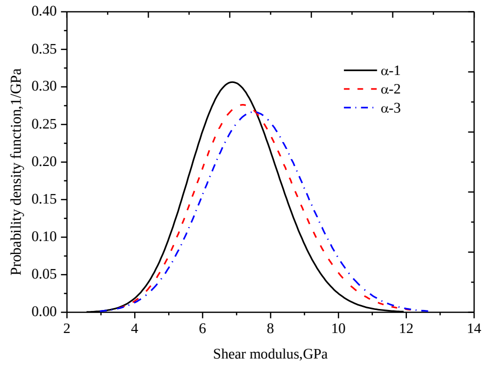
To investigate the effects of different shapes of pores in the unsaturated zone, three types of equivalent aspect ratios are employed to obtain the PDFs of the concrete properties. The distribution parameters for the aspect ratios also include the mean values (which are 0.6, 0.4 and 0.2, respectively) and coefficients of variation (which is 0.1). Fig. 8 (a) and (b) display the comparisons among PDFs of the effective bulk modulus and shear modulus of unsaturated concrete with different mean values for the equivalent aspect ratios. It can be concluded that with the increase of the mean values for the equivalent aspect ratio, the predicted properties become greater statistically for unsaturated concrete.

6. Conclusions

The concrete under water are usually not fully saturated by water. Meanwhile, there is an inherent randomness in material's microstructure, which will lead to the fluctuations



(a) Bulk modulus



(b) Shear modulus

Fig. 8 Influence of pore shapes on the probabilistic behavior of unsaturated concrete

of the concrete properties. A stochastic micromechanical framework is proposed to obtain the unbiased probabilistic behavior of the concrete with different saturation degrees. Two-level homogenization procedures based on the differential scheme are proposed to quantitatively predict the effective properties of the saturated, unsaturated and dry concrete. The deterministic framework was extended to stochastic by modeling the volume fractions and properties of constituents as random variables. Maximum entropy based simulation framework is employed to get the unbiased PDFs. The predicting results are compared with limited experimental validations, those obtained by existing micromechanical models, commonly used PDFs and the direct Monte Carlo simulations. Finally, the effects of the effective saturation degrees and pore shapes are investigated based on our proposed stochastic micromechanical framework. From this study, the following main conclusions can be drawn:

(1) The proposed stochastic micromechanical framework is capable of predicting the probabilistic behavior of the concrete with different saturation degree. The differential scheme based deterministic micromechanical model estimate the material's effective properties better than the previous models when the volume fraction of the inclusions is higher.

(2) The presented maximum entropy based simulation framework can approximate the commonly used PDFs without primer assumptions. Meanwhile, the proposed simulation framework is accurate and computationally efficient compared with the direct Monte Carlo

simulation.

(3) Based on the proposed framework, the saturation degree and pore shape play important role in determining the unsaturated concrete's properties. With the increase of the mean value for the effective saturation degree or the equivalent aspect ratio, the unsaturated concrete demonstrates greater properties statistically.

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