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## Does representative volume element exist for quasi-brittle composites?

Thao D.P. Trana, Sze Dai Pangb,\*, Ser Tong Quekc

- a Department of Civil Engineering, National University of Singapore Block E1, #08-20, 1 Engineering Drive 2, Singapore 117576, Singapore
- Department of Civil Engineering, National University of Singapore Block E1A,# 07-03, 1 Engineering Drive 2, Singapore 117576, Singapore
- <sup>c</sup> Department of Civil Engineering, National University of Singapore Block E1A,# 02-15, 1 Engineering Drive 2, Singapore 117576, Singapore

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#### ABSTRACT

The validity on the use of representative volume element (RVE) to predict the mechanical behavior of quasi-brittle composites is addressed based on studies of porous epoxy under tensile action. For the elastic behavior, the more efficient single particle (SP) RVE approach predicts accurately when the volume fraction is less than a critical value of 15–20% depending on the relative stiffness of the matrix and the inclusion. At higher volume fraction, the multiple particle (MP) RVE provides accurate predictions with less than 6% error, for MP-RVE sizes that are at least 6 times larger than the size of the inclusion. In the inelastic softening regime, the RVE does not exist for the homogenized stress–strain behavior due to the high localization of damage. Instead, the fracture energy or toughness should be used as a size-independent measure in the RVE approach to describe the fracture response in quasi-brittle composites. The fracture toughness predicted with the MP-RVE models shows size invariance and compares well with the experiments for volume fractions of up to 20% with deviations of less than 6%, while the SP-RVE models are only recommended for use at volume fractions of less than 10%.

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#### 1. Introduction

The pursuit of advanced materials to build superior machines and structures led to developments in composites. Despite the surge in interest and output of research articles in the field of composites over the last decade, the prediction of effective properties of composite materials continues to be a highly researched problem. Specifically, the knowledge frontier on their mechanical behavior is pushed from the macro, down to the micro, nano, and even to the atomistic level, in an effort to better understand and explain their mechanical behavior at the structural level based on the physical and chemical interactions at the lower length scales. This problem has been tackled on two fronts: a theoretical approach, often with simplifying assumptions to facilitate closed form expressions for the prediction of effective properties, and a numerical approach, which accounts for greater physical details and phenomena at the expense of computational time and effort.

Theoretically, the elastic properties of composite materials were first estimated using Voigt's [1] and Reuss' models [2], in which the constituents are assumed to undergo the same strain and stress respectively. Subsequently, more accurate models have been developed, by relaxing those assumptions and considering compatibility of the stresses and strains, such as the dilute distribution

(DD) model [3], self-consistent (SC) model [4,5], generalized self-consistent (GSC) model [6] and Mori–Tanaka model [7]. All these models are extensions of Eshelby's solution [3] where they approximate the stress and strain fields in the matrix and inclusions by their volume-averaged values. However, such models are limited by the assumptions of linear elastic materials and small deformations imposed in the original Eshelby's equivalent inclusion model. Furthermore, it is difficult to incorporate damage mechanisms such as interface debonding and matrix/reinforcement cracking which occur in composites, thus limiting the application of such models.

With the help of computers, numerical models have been used to develop refined material models for composite materials. This approach offers more flexibility and advantages than theoretical models, namely, (a) inclusions of arbitrary shapes can be modeled, (b) inelastic or time dependent properties can be incorporated into the model easily, (c) imperfect interface between inclusion and matrix can be taken into account, and (d) composites comprising three or more phases can be considered.

The increased complexity of the problem due to refinements in the material and geometrical details would nevertheless escalate the computational cost enormously, especially for heterogenous micro-structure. To overcome this limitation, the representative volume element (RVE) concept is commonly adopted [8–17]. The aim is to construct a super element such that either (i) the micro-structure of the composite can be statistically represented by the structure of the RVE, or (ii) the macroscopic constitutive response of the composite can be predicted from the overall behavior of the RVE with sufficient accuracy. Fig. 1 shows the different types of RVE

<sup>\*</sup> Corresponding author. Tel.: +65 6516 2799; fax: +65 6779 1635.

E-mail addresses: dpttran@nus.edu.sg (T.D.P. Tran), ceepsd@nus.edu.sg (S.D. Pang), st\_quek@nus.edu.sg (S.T. Quek).

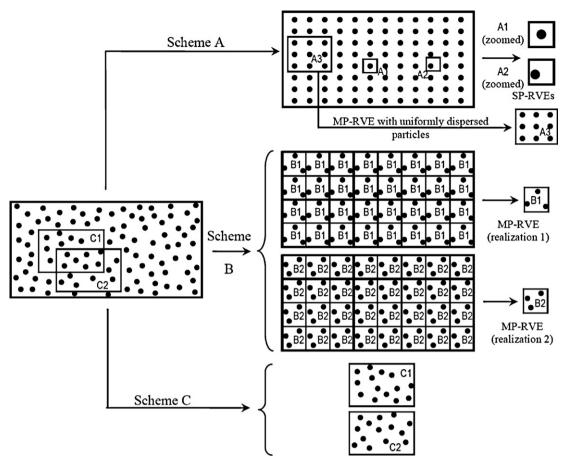


Fig. 1. Schemes to define RVE: SP-RVE with periodic BCs (Scheme A), MP-RVE with periodic BCs (Scheme B), images from real micro-structure without periodic BCs (Scheme C).

models built based on these two requirements in which the former is exhibited by RVEs under Scheme C while the latter is exhibited by RVEs under Schemes A and B.

In Scheme A, the actual micro-structure is assumed to be equivalent, in terms of mean response, to another micro-structure with uniformly distributed particles. The equivalent micro-structure is, in fact, a periodic structure where the smallest "material period" is a square unit cell with a single particle located at the center of the cell and its edge length equals to the distance between the particles. By applying appropriate periodic boundary conditions so that a unit cell is replicable to the entire material domain, the overall behavior of the equivalent micro-structure can be represented by that of the unit cell, also known as the RVE. The position and size of window can be varied by defining the "material period", thus different types of RVEs can be constructed as illustrated by RVEs A1, A2 and A3 in Fig. 1. The construction of a RVE under Scheme B is similar to that under Scheme A, except the smallest "material period" is now a unit cell containing two or more randomly dispersed particles. Due to this randomness, multiple realizations with different arrangements of particles are possible. Each of the realization can be analyzed and the results are averaged over all realizations considered, to obtain the mechanical response of the actual composite. In Scheme C, the RVEs are constructed based on images of the actual micro-structure and periodicity is not considered. It should be noted that the volume fraction of particles in RVEs under Schemes A and B are defined to be the same as that of the real composite, but this is not necessary true for the case of RVEs under Scheme C. The current study adopts the concept of RVE based on the equivalency in the mean mechanical response, which are the RVEs under Schemes A and B. Most numerical models applying the RVE concept are able to predict the linear elastic properties of composites.

Amongst them, some implemented the single-particle RVE (SPRVE) approach, in which there is only one inclusion inside the RVE [9,12,16,18], while others used the multiple-particles RVE (MPRVE) approach, which comprises multiple inclusions within the RVE [10,11,13,19–21]. In many cases, the use of SP-RVE or MPRVE approaches is based on personal judgment of the researchers leading to an unwell-defined criterion for the approach to use. For example, Chen and Mai [18] used SP-RVE approach for rubber reinforced composite with volume fraction of rubber particles varying from a low 0.209% to a high 26.18%; Sun and Vaidya [9] and Xia et al. [12] used SP-RVE approach for fiber composite with very high volume fraction of fiber from 47% to 60%. On the other hand, Kari et al. and Segurado et al. applied the MP-RVE approach in their studies for volume fraction of inclusion ranging from 10% to 60%.

In recent years, the RVE concept has been extended to predict the pre-ultimate non-linear response of composites, as in González et al. [22], Segurado and Llorca [23], Pierard et al. [24,25], Muliana and Kim [26], and Sharma and Socrate [27]. In these studies, the effective properties were predicted either from multiple realizations of a fixed size RVE with random particles placement [15,22,23,27], or from single realization of a fixed size RVE with assumed regular arrangement of the particles [26]. Although the numerical results agree with the experimental data in terms of stress-strain behavior up to the ultimate strength, these studies did not consider the effect of the RVE size on the strain hardening behavior. In addition, the number of realizations may be too few in some cases to provide reliable representation for the results obtained.

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