

Multi-Scale Modelling of Particulate Composite [†]

Abdalla Elbana ^{1,*} , Amar Khennane ¹, Safat Al-Deen ¹ and Muhammad Talha Junaid ²

¹ School of Engineering & IT, The University of New South Wales, Canberra 2600, Australia; a.khennane@adfa.edu.au (A.K.); s.al-deen@adfa.edu.au (S.A.-D.)

² Department of Civil & Environmental Engineering, University of Sharjah, Sharjah, United Arab Emirates; mjunaid@sharjah.ac.ae

* Correspondence: a.elbana@adfa.edu.au

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Abstract: The proposed study aims to investigate the micromechanical behavior of a reinforced polymer matrix with fly ash cenospheres. This study involves utilizing random sequential adsorption (RSA) theory to describe the distribution of the cenosphere particles in the polymer matrix at the microscale level, and to develop a finite element (FE) model based on volume representative element (RVE) theory that represents the microstructure of the composite. The FE model is then to be validated by conducting laboratory experiments. The validated FE model will be used for virtual testing to explore and develop cenosphere composites.

Keywords: multi-scale modelling; fly ash cenospheres; RVE; nanoparticles



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1. Introduction

Particulate composites are characterized as being composed of particles randomly distributed within an inorganic or organic medium. The medium could be a polymer matrix or a cementitious material. The particles can have virtually any shape, size, or configuration. Particulate composites offer a great opportunity to recycle waste materials as the particles can be sourced from different waste materials: plastic, timber, rubber, tires, fly ash, etc. Particulate composites often have superior properties such as a lightweight and high durability. These attractive properties promote particulate composites in many applications from construction to the aircraft and marine industries. Herein, the particulate composite of interest is a fly ash cenosphere composite.

2. Background

2.1. Cenospheres

Fly ash is a manufacturing waste product resulting from burning coal in a coal-fired power plant. Fly ash particles have a great disparity of sizes, where most of them are spherical [1]. Among these spheres are iron-rich (Fe_3O_4 , MgFe_2O_4) magnetic spheres that are mostly crystal with a low glass content, and glass-rich spheres (cenospheres). The volume fraction of cenospheres in fly ash is often much higher than that of iron-rich spheres. The particles of interest in this work are cenospheres.

2.1.1. Morphology

Cenospheres are thin-walled glass microspheres filled with air or gases. Their diameters range between 8 and 1000 μm [2]. In a bulk sample, it was found that 90% of the particles ranges between 45 to 250 μm in diameter, and about 70% are between 45 and 150 μm in diameter [3]. Particles that have a lower density than water and float to the surface in water are considered cenospheres. [4]. The denser, vesicular spheres and irregular particles usually do not float due to the absence of trapped gases or air [5]. Therefore, cenospheres are mostly well-rounded shells. Their thickness varies even if they have similar

diameters. Nonetheless, the wall thickness-to-diameter ratio is usually between 2.5% and 10.3% [6].

2.1.2. Chemical Composition

Cenospheres are mostly composed of silica (SiO_2) and alumina (Al_2O_3); the silica content is usually between 52% and 74% of the total weight, while the alumina content ranges between 16% and 32.07% [7]. Minor amounts of calcium oxide (CaO), iron oxide (Fe_2O_3), and sodium oxide (Na_2O) are also present in cenospheres. The insides of these spheres are filled with gas due to the burning and decomposition of the organic and inorganic substances in coal. These gases are condensed and retained inside the spheroid.

2.1.3. Properties and Applications

Cenospheres are utilized to reinforce a matrix to form what is known as a particulate composite. The addition of cenospheres into a cementitious medium offers a great reduction in density without necessarily compromising its mechanical strength. The density of these composites was found to range between 760 and 2001 kg/m^3 [8–10], which is considerably lower than traditional concrete (2400 kg/m^3). Meanwhile, the compressive strength and flexural strength could be as high as 69.4 MPa and 7.3 Mpa, respectively [11].

Cenosphere composites can be utilized in many applications. They can be used as a core in an FRP sandwich panel for flooring in the construction field. They are also suitable for bridge decks, pavements, and highways [12,13], and as a part of aircraft or ships. Moreover, they are an interesting alternative to recycled industrial waste.

2.2. Random Sequential Adsorption (RSA)

RSA [14,15] is a process of randomly distributing particles in a given volume without the particles overlapping. The process starts with introducing particles to the inclusion in a sequential manner. The particles are then adsorbed and remain fixed in their original spot. If an attempt to introduce a new particle within the inclusion results in overlapping with another particle, this attempt is rejected, and a new random spatial position is sought. This process comes to an end when no more particles can be packed within the inclusion or at a specified volume fraction. Because the process is monotonous, RSA is usually processed by an algorithm carried out by a computer simulation set to identify the coordinates of the particles (Figure 1).

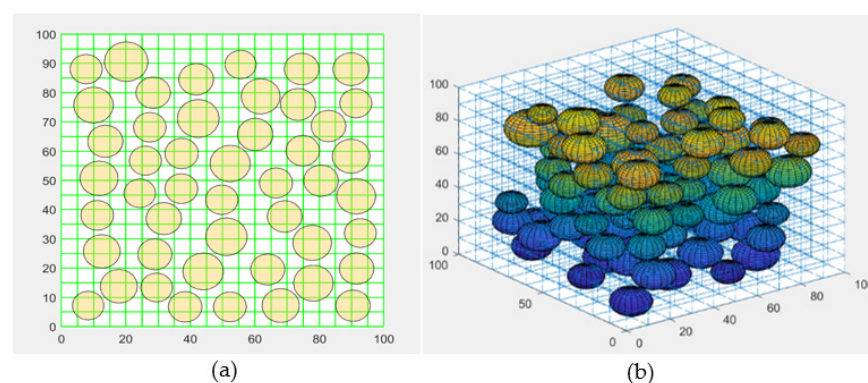


Figure 1. RSA generated by a MATLAB code of: (a) 2D disks and (b) 3D spheres (dimensions are in μm).

In this work, the particles of interest are cenospheres (spheroids), and the inclusion is a cube in a 3D Cartesian coordinate. This inclusion represents the elementary volume element (RVE), where the medium is a polymeric/or cementitious composite, and the spheres are fly ash cenosphere particles.

2.3. Representative Volume Element (RVE)

One of the issues in materials mechanics is to assess the elastic properties of a particulate composite due to its heterogeneous macro/microstructure. The concept of the RVE is often essential for analyzing the micromechanical properties of a heterogeneous material because its performance is chiefly dependent on its microstructure.

The RVE [16] is the fractional volume of a material at the lower length scale that qualifies as representing the material properties as a whole in the upper length scale. The RVE volume should be sufficiently large at the lower length scale in which any larger volume would have equal properties. The effective properties of the RVE can be obtained by imposing periodic boundary conditions by applying a uniform displacement or uniform traction force (surface force) over the RVE faces.

While analytical models offer a practical approximation, alternatively, numerical methods offer more accurate solutions and allow for a deeper microstructural analysis. The current work focuses on carrying out a finite element simulation of the RVE with periodic boundary conditions that aim at characterizing the microstructure of a polymer matrix reinforced with cenospheres.

3. Research Gap

The incorporation of fly ash cenospheres into a polymer matrix is a relatively new technique to develop a composite material that offers attractive and suitable properties for several applications. Based on the current literature, it has been noticed that many aspects of this topic have not yet been explored or are rather scarce. A research gap is observed in these areas:

- The microstructural characteristic of such composites is not well understood. Multi-scale modelling that allows for exploring and developing this heterogeneous material is not found in the literature.
- An FE model to investigate the cenospheres interaction with the surrounding medium, the particle fracture and the damage evolution of the composite.
- The lightweight properties of these composites could be exploited in an application where dynamic loading is present, such as structures built on active seismic zones, wind loads on aeroplanes, dynamic loads due to waves on ships and ship motions, or impact loads if ships or a marine structure are hit by obstacles. Nevertheless, research on cenosphere composites under any form of dynamic loading is very scarce.

4. Objectives

1. To develop an algorithm in MATLAB to simulate the random sequential adsorption (RSA) of cenospheres in a 2D and 3D representative volume element (RVE).
2. To develop a finite element model to simulate the RVE with periodic boundary conditions using ABAQUS and Python scripting.
3. To validate the FE model by implementing a laboratory test on a cenosphere composite material within an acceptable margin of error. The laboratory tests include uniaxial tests and compressive strength tests to find the two elastic parameters: young's modulus E and Poisson's ratio ν .
4. To use the validated FE model for research applications that help in understanding and developing this composite material.
5. To investigate the interaction between the cenosphere particles and the surrounding medium, and the damage evolution of the composite.
6. To study the effect of cenosphere composites under dynamic and impact loading.
7. To optimize the proportion of cenospheres in the matrix for maximum property performance.

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