

GENERATION OF A SHORT FIBRE BIOCOMPOSITE REPRESENTATIVE VOLUME ELEMENT

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ABSTRACT

One of the greatest challenge in working with natural fibre composites is the large variation in mechanical properties that result from the geometric inconsistency amongst fibres. Traditional design tools and models are unable to accurately incorporate this non-homogeneity to predict the resulting local behaviour of biocomposite materials. The following paper presents a methodology to generate a representative volume element (RVE) to simulate the material microstructure of short fibre composites, with the intent of modelling the popular class of short fibre biocomposites materials. The capabilities of a range of particle packing algorithms used in literature are compared in terms of the maximum volume fraction they have been able to achieve and for what fibre length to diameter aspect ratio. The methodology is able to account for the characteristics of fibre geometry samples, according to their probability density functions (PDFs). The RVE generation strategy imposes periodic boundary conditions and fibres are declared invalid if an intersection between fibres is detected. The effect of different PDFs on the resulting RVE are discussed. An RVE populated with data following a Weibull distribution is compared to that from normally distributed data with an equal mean but varied standard deviations. Using a Weibull distribution to simulate the characteristics of an RVE requires a significantly higher number of fibres than any comparable normal distribution, due to the skewness of the data towards large values at low probabilities. The highest volume fraction achieved was 40% for an RVE containing fibres with lengths distributed according to a Weibull distribution and aspect ratios of 15. The future intent of this work is to perform finite element analysis on RVE samples with a range of varied microstructure characteristics to determine the effect on overall composite properties, which will provide new insights on how best to formulate short fibre compounds.

KEYWORDS

Biocomposites, representative volume element, probabilistic design, particle packing, volume fraction.

INTRODUCTION

This study is focused on the analysis of short, or discontinuous, fibre biocomposites. Attributed that influence the microstructure of such a material include the fibre geometry, orientation, packing arrangement and volume fraction (Fowler, Hughes et al. 2006). The geometric properties of the short fibres' geometry are stochastic and are best described by a probability density function (PDF) rather than a discrete value. The most important feature to note from the PDF curves for natural fibre properties is the typically asymmetric shape. An example of the PDF curves for fibre length and diameter of short flax fibres is shown in Figure 1. The source for the PDFs of asymmetric nature stems from the fibre mastication during processing (Biagiotti, Fiori et al. 2004).

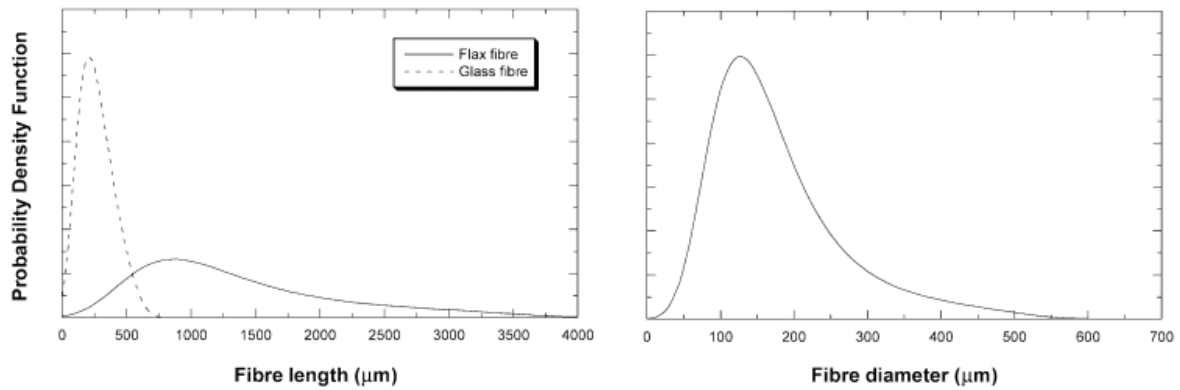


Figure 1: Probability density function (PDF) curves of geometric characteristics of flax fibres: Length (left) and Diameter (right). (Biagiotti, Fiori et al. 2004)

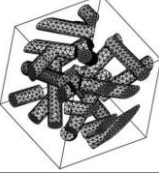
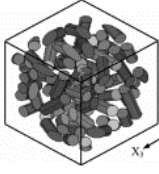
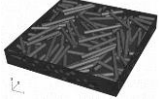



In order to account for the variability in natural fibres, a probabilistic design approach needs to be applied. Traditional structural design analysis does not directly account for the random nature of most input parameters, and thus cannot quantify the inherent risk of design and performance sensitivity to input variables (Long and Narciso 1999). Probabilistic design tools are a well-established concept in civil and structural engineering, despite being somewhat unheard of in the areas of mechanical and composites engineering. The probabilistic modelling approach will focus on the micro-scale. The results from this research can be used to better understand the behaviour of short fibre composites with large property variations. Ultimately this will support the formulation of better performing compounds and industry uptake.

Under the micromechanical classification of material analysis, a heterogeneous composite material is modelled on the level of the individual constituents. Such a model will require the generation of a representative volume element (RVE) containing individual short fibres characterised by their PDFs. The methodology designed and used in this study to generate a computational RVE to simulate biocomposites, will be discussed in terms of their results and implication on future modelling capabilities.


METHODOLOGY

For short fibre composites, fibres may be modelled as cylinders (Pan, Iorga et al. 2008). With this in mind, methods for packing cylindrical particles has been the focus of the research. An extensive literature search was conducted to evaluate different strategies for packing cylindrical particles in a volume element, with the key findings presented in Table 1. The highest volume fraction V_f achieved for a given aspect ratio AR has been tabulated to provide a grounds for comparison between models.

Table 1 Investigation of Cylindrical Particle Packing Algorithms

Source and Packing Algorithm	Description				
<p>(Böhm, Eckschlagler et al. 2002)</p>  <p>Basic RSA</p> <table border="1"> <thead> <tr> <th>Max Vf</th> <th>Max AR</th> </tr> </thead> <tbody> <tr> <td>15%</td> <td>5</td> </tr> </tbody> </table>	Max Vf	Max AR	15%	5	<p>Basic Random Sequential Adsorption (RSA) method. Sequentially add fibre elements to a volume by randomly generating candidate inclusion positions, which are accepted if a reinforcement does not overlap any previously accepted inclusion and are rejected otherwise. Periodic boundary conditions. Maximum volume fraction is limited by fibre aspect ratio observed.</p>
Max Vf	Max AR				
15%	5				
<p>(Kari, Berger et al. 2007)</p>  <p>Modified RSA</p> <table border="1"> <thead> <tr> <th>Max Vf</th> <th>Max AR</th> </tr> </thead> <tbody> <tr> <td>40%</td> <td>Varies</td> </tr> </tbody> </table>	Max Vf	Max AR	40%	Varies	<p>Introduce definition of “jamming limit” i.e. it is not possible to generate higher volume fraction RVE models because of the jamming limit. To overcome the jamming problem and to achieve higher volume fraction, different sizes of fibres used by depositing them inside the RVE in a descending manner using RSA algorithm. They first deposited the largest aspect ratio fibres, and after reaching the jamming limit, deposited the next largest possible aspect ratio fibres in the RVE.</p>
Max Vf	Max AR				
40%	Varies				
<p>(Pan, Iorga et al. 2008)</p>  <p>Modified RSA</p> <table border="1"> <thead> <tr> <th>Max Vf</th> <th>Max AR</th> </tr> </thead> <tbody> <tr> <td>55%</td> <td>10</td> </tr> </tbody> </table>	Max Vf	Max AR	55%	10	<p>RSA algorithm applied for fixed aspect ratio fibres and if no match is found, a new fibre position and orientation is generated until the desired volume fraction is achieved.</p>
Max Vf	Max AR				
55%	10				
<p>(Pan et al, 2008)</p>  <p>Modified RSA</p> <table border="1"> <thead> <tr> <th>Max Vf</th> <th>Max AR</th> </tr> </thead> <tbody> <tr> <td>35-40%</td> <td>20</td> </tr> </tbody> </table>	Max Vf	Max AR	35-40%	20	<p>The representative volume element is divided into sublayers. Fibers are randomly oriented in the xy plane, and in the case of overlap, the newly added fibre changes the sublayer to avoid the existing fibre. The buckled polyhedra do not appear to be very realistic, and the orientation distribution is restricted to the xy plane.</p>
Max Vf	Max AR				
35-40%	20				
<p>(Duschlbauer, Böhm et al. 2006)</p>  <p>Monte Carlo</p> <table border="1"> <thead> <tr> <th>Max Vf</th> <th>Max AR</th> </tr> </thead> <tbody> <tr> <td>21%</td> <td>10</td> </tr> </tbody> </table>	Max Vf	Max AR	21%	10	<p>Monte Carlo method. Procedures starts with a configuration of random fibre locations and orientations in a large box. Fibres are rearranged until a predetermined orientation state is reached. Final step decreases the size of the box towards the desired volume fraction without altering the orientation of the fibres. Intersection of fibres is not allowed at either step during the process. Requires significantly more processing power then RSA with little gain in volume fraction.</p>
Max Vf	Max AR				
21%	10				
<p>(Zhang 2006)</p>  <p>Collective Rearrangement</p> <table border="1"> <thead> <tr> <th>Max Vf</th> <th>Max AR</th> </tr> </thead> <tbody> <tr> <td>35%</td> <td>10</td> </tr> </tbody> </table>	Max Vf	Max AR	35%	10	<p>Collective Rearrangement. Periodic boundary conditions not applied in this research, aim wasn't to generate an RVE but to investigate the limits of the algorithm. A number of cylinders are placed in a domain and a Monte Carlo perturbation process is applied until overlaps between cylinders are removed.</p>
Max Vf	Max AR				
35%	10				

Sequential Deposition algorithm simulates a fall of random particles until they reach a local minimum of their potential energy.

N/A	Sequential Deposition		Methodology is poorly document so replication is not possible in the timeline of this project.
	Max Vf	Max AR	
	59%	10	
(Altendorf and Jeulin 2011)			A force based Random Walk algorithm models fibres as a chain of tangential spheres “like a pearl necklace”. Spheres are modelled as a point with a repelling force. The forces are inspired by the energy-reducing models known from molecular dynamics. Requires significantly more processing power than other models with significant volume fraction improvements.
	Random Walk		
	Max Vf	Max AR	
	72%	9	

Summary of Findings

The following findings have been considered prior to developing the methodology to generate the RVE using Python 2.7 coding language:

- Large fibre aspect ratios inhibit the maximum achievable fibre volume fraction resulting in a “jamming limit”
- The Random Sequential Adsorption (RSA) algorithm should not be used for composites with uniformly sized fibres but may increase in capability if fibre geometry is varied
- Monte Carlo and Random Walk algorithms are very effective in packing fibres, especially for higher aspect ratios at high volume fractions. Trade off performance with significant increase in time and processing power required to generate a valid RVE
- RVE models containing fibres with lengths sampled from a Weibull distribution have not been found in literature
- In all cases for RVE generation, periodic boundary conditions have been applied
- Intersections between cylindrical elements have been tested and rejected in all models by either numerical algorithms or through modelling software capabilities
- Natural fibres may be characterised by a Weibull distribution and these may be contrasted to relatively uniform normally distributed data that is more typical to man-made fibres

Modelling approach

The short fibres will be represented as cylinders of varying length and diameter. The fibre’s centre points will be described by their offset in the X, Y and Z directions from the global origin, constrained within the RVE boundary. Two Euler rotations will be imposed about the X and then the Y axes. The RVE boundary will take the form of a cube with edges of length L_3 , where the term L_3 denotes the maximum fibre length of the sample. The cube is centred symmetrically on the origin of the global coordinate system.

The particle packing strategy follows a modified Random Sequential Adsorption (RSA) algorithm. The RSA algorithm arranges the fibres to be placed in descending order by size then randomly generating a three dimensional coordinate for the centre point of each fibre within the RVE boundary and a rotation about both X and Y axes. If the fibre position and orientation results in an intersection between fibres, then the fibre is rejected and the random values are regenerated until a successful placement is made. The modified RSA algorithm has been chosen as it has proven capable of generating RVEs of significant volume fraction for fixed aspect ratio fibres (maximum of 55% V_f for aspect ratio of 10 by Pan, Iorga et al. 2008). The results offer room for improvement if variable fibre dimensions are introduced, as is the intention of this project.

The RVE is a finite micro-representation of a sample of material. A macro-scale component can be obtained by homogenisation or identically replicating the RVE and extending it periodically in all X, Y, and Z directions (Pan, Iorga et al. 2008). In order to keep the periodicity conditions of the RVE, parts of any fibre that protrude from any surface of the cubic RVE are cut and shifted to the opposite face. In the method developed as part of this study, the fibre returns a true clash if the magnitude of the distance between the fibre's centre point and RVE boundary surface is less than half the fibre's length. The concept of periodic boundary conditions in two- and three-dimensions is visualised in Figure 2.

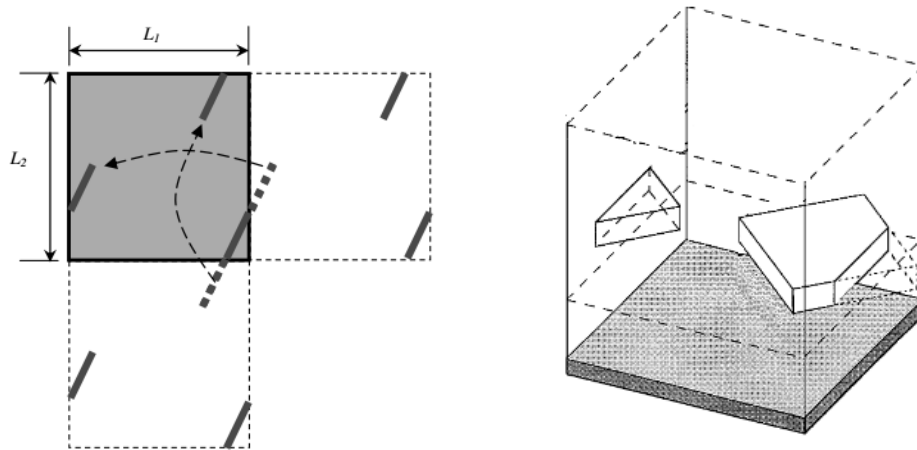


Figure 2 Example of periodic boundary conditions over a volume element in two-dimensions (left) (Pan, Iorga et al. 2008) and three-dimensions (right) (D. Coelho, J.F. Thovert, and P.M. Adler. 1997)

In order to generate a valid RVE that is a true representation of the desired volume fraction, once the periodic state of the fibre is established, the fibre and all its periodic realisations must be checked for any intersection with existing fibres before it may be accepted.

When deciding on the best course of action to take when numerically checking for the intersection between the cylindrical elements, the most obvious choice is to check for the intersection between two cylinders. Literature shows that detecting the intersection of two cylinders is computationally expensive (Eberly 2000). Instead the intersection between capsules has been used to conservatively approximate the volume of a cylinder. This approach is simpler and less computational resource-intensive procedure. A capsule is defined as the surface on which all points on the surface are the same distance from a line segment. Two capsules intersect if the shortest distance between the line segments is less than the sum of their radii (Eberly 2000). The same conditions hold for even arbitrarily rotated capsules, which is why this approach is appealing for the purpose it is intended in this work (Lene 2015). The intersection detection algorithm has been developed from Dan Sunday's Geometry Algorithms originally written in C+ (Sunday 2012). The intersection detection procedure requires the numerical transformation of the local coordinates at the end of the line segment contained within each cylinder to the global reference frame. Rotation matrices have been used to perform this transformation based on the orientations imposed about the local X and Y axes of a fibre.

The overall strategy to generate a short fibre biocomposite RVE based on probabilistic micro-mechanical analysis is outlined in detail in the flow chart shown in Figure 3 over the page.

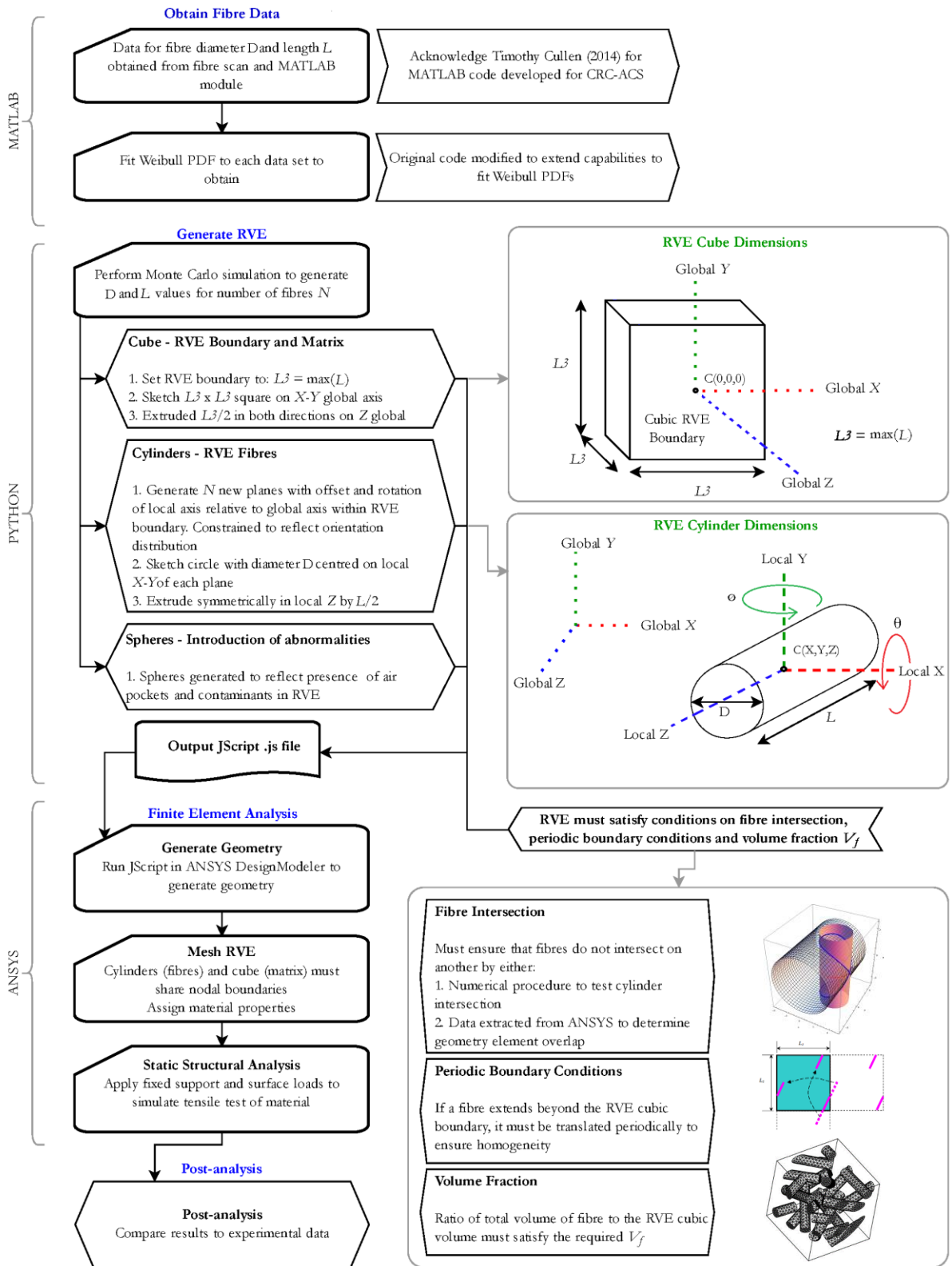


Figure 3 Methodology Flow Diagram

RESULTS AND DISCUSSION

To assess the developed code's capability in generating an RVE for short natural fibre composites in contrast to more geometrically uniform samples, Monte Carlo simulation of normally distributed fibres with varied standard deviations have been generated. The normally distributed fibre data has been generated to have approximately the same mean value as the data generated from a Weibull distribution to allow for a meaningful comparison between the data sets. The probability density function curves of Monte Carlo simulated fibre lengths are seen in Figure 4 below. Natural fibre data has been sourced through The University of Queensland chapter of the CRC-ACS (Cullen 2014).

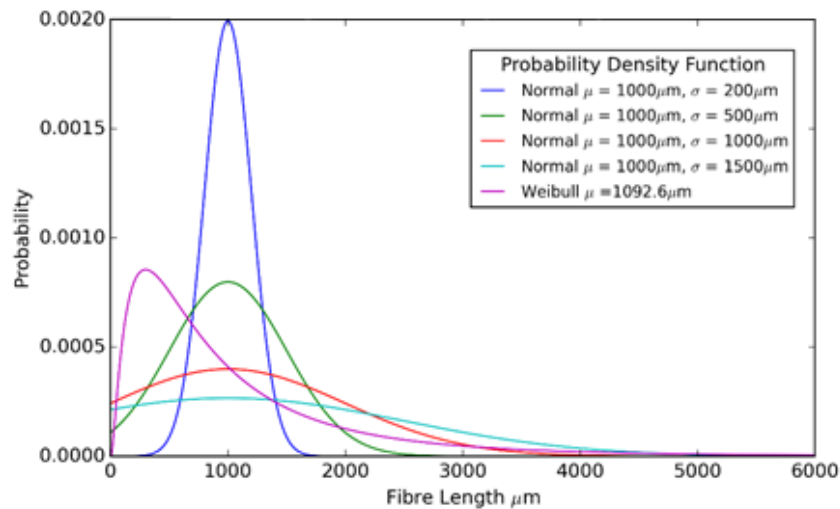


Figure 4 Monte Carlo Simulated Fibre Length Probability Density Functions

It must also be noted that each sample has been truncated at a lower bound value of length equal to $100\mu\text{m}$. The lower bound has been imposed to simulate the sieving out of small, powder like fibres which would occur in the manufacturing of fibre composites.

The number of fibres that the Python code would need to generate and place successfully in the RVE volume in order to meet a user specified volume fraction has been calculated based on the fibre lengths from each PDF using a fixed aspect ratio to calculate their diameter. A summary of each fibre data set estimation for a volume fraction of 30% and aspect ratio of 15 is shown in Table 2.

Table 2 Results of Fibre Sample Prediction for 30% Volume Fraction and Aspect Ratio of 15

Distribution Sample	Number of Fibres N	Smallest Fibre Length [μm]	Largest Fibre Length [μm]	Second Largest Fibre Length [μm]	Percentage Difference Between Largest and Second Largest
Weibull $\mu = 1092.6\mu\text{m}$	7795	100.09	6756.39	6349.65	6.21%
Normal $\mu = 1000\mu\text{m}, \sigma = 200\mu\text{m}$	402	426.03	1544.70	1540.62	0.26%
Normal $\mu = 1000\mu\text{m}, \sigma = 500\mu\text{m}$	1008	120.90	2447.92	2410.57	1.54%
Normal $\mu = 1000\mu\text{m}, \sigma = 1000\mu\text{m}$	1582	100.72	4027.31	4017.20	0.25%
Normal $\mu = 1000\mu\text{m}, \sigma = 1500\mu\text{m}$	3364	100.24	6825.00	6689.08	2.01%

The length of the largest and second largest fibres have been recorded and the percentage difference calculated. The higher percentage difference observed in the Weibull distribution data compared to the normally distributed

data demonstrations the sparseness of long fibres contained in the Weibull distribution sample. The normally distributed data sets contain more large fibres as opposed to the comparatively few found in the Weibull distribution samples. These large fibres which occur with higher probability in normal distributions determine the cubic dimension of the RVE L_3 , recalling that L_3 is equal to the maximum fibre length of the sample. For a Weibull distribution, a large fibre appears and designates a large RVE, but then there are few large fibres to contribute to filling the volume to the specified volume fraction, requiring a significantly higher number or small fibres which occur at higher frequency to occupy the space.

As the volume fraction of an RVE sample is increased a larger sample of fibres is captured. For the data containing fibres with lengths distributed according to the Weibull distributions, as more fibres are included in a sample, the percentage difference between the longest and the second longest fibre decreases. Figure 5 shows the decrease in percentage difference between the longest and second longest fibre found in an RVE sample with Weibull distributed fibre lengths as the volume fraction increases.

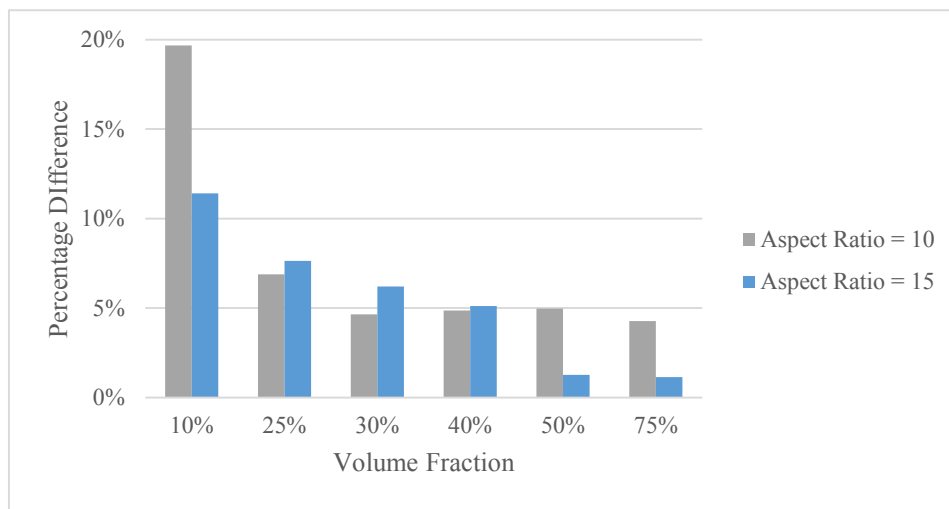


Figure 5 Percentage Difference Between Largest and Second Largest Fibre - Weibull Distribution.

An immediate observation from the fibre sample prediction is that the number of fibres required to generate an RVE for fibre lengths distributed according to a Weibull distribution is much higher than for those of normally distributed data with an equivalent mean. A comparison between the numbers of fibres of an aspect ratio of 15 require to fill an RVE to a range of volume fractions between 10% and 50% may be seen in Figure 6. The results of this figure highlight the obvious spike in the number of fibres required when a Weibull distribution is used to parametise the fibre length input.

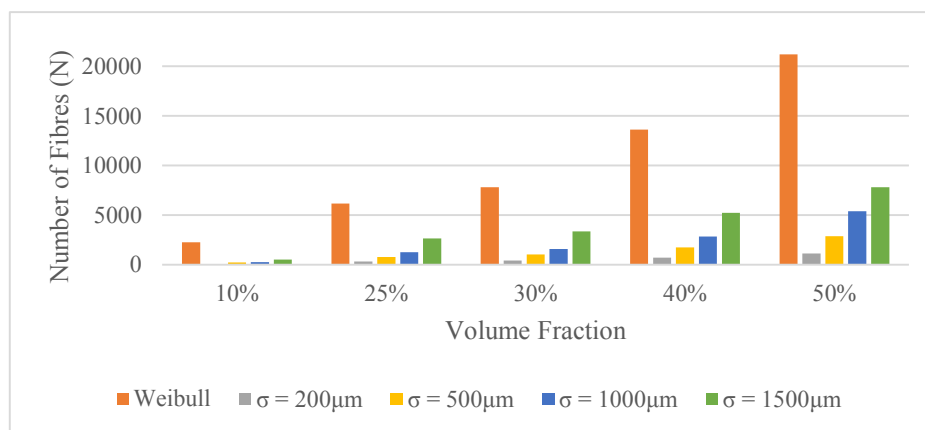


Figure 6 Number of Fibres Required to Fill an RVE to Various Volume Fractions. Fibre Length to Diameter Aspect Ratio of 15.

Comparing the Weibull distribution data to the normally distributed data with a standard deviation of $1500\mu\text{m}$ shows the increase in the number of fibres required to fill the RVE. While the difference in the maximum length

and thus L3 of the two samples is only approximately 1% in the sample with a volume fraction of 30% (resulting in a 3% difference in the cubic RVE volume), the number of fibres required to characterise the Weibull RVE is 2.3 times that of the normally distributed sample.

Results from RVE JScript Generation

To date the RVE generation python script has been successfully able to run the RVE generation code up to a volume fraction of 30% for all distributions, for aspect ratios of both 10 and 15. The results for a volume fraction of 20% and a fibre to length aspect ratio of 15 may be seen in Figure 7. These samples contain fibres that may be oriented about the X and Y axis anywhere between positive and negative 45°.

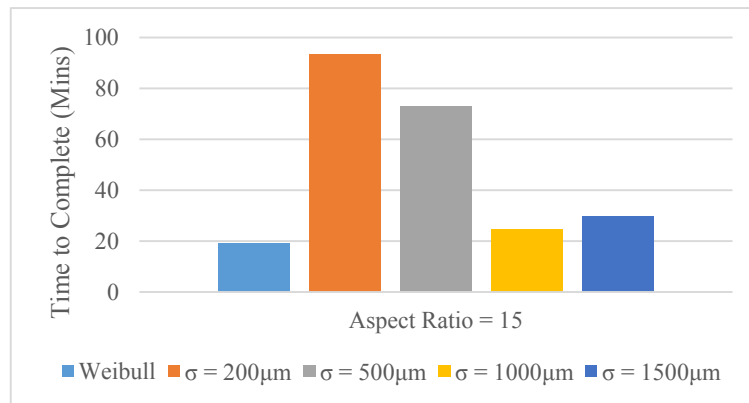


Figure 7 Time to Complete Simulation (mins) for an RVE of 20% Volume Fraction Versus Fibre Aspect Ratios

The Python code is able to reach a solution in approximately 20 minutes for the Weibull distribution containing 3166 fibres. The slowest to reach a solution is the normally distributed sample with a standard deviation of 200 μm containing 227 fibres which takes approximately an hour and a half to complete. The discrepancy between the solution times in contrast to the number of fibres required for the two samples is a result of the difference in the fibre length variance function between the two samples. The Weibull distribution contains few large fibres and many small fibres, which increases the likelihood that a randomly placed fibre will not intersect at low volume fractions, but required more fibres to fill the RVE to the required volume fraction. The normally distributed sample contains fewer fibres than the Weibull distribution sample, but these fibres are of similar proportions, meaning that the chances a new fibre will intersect will increase rapidly with each successive fibre.

The increased chance of detecting a fibre intersection has been measured indirectly by recording the maximum number of attempts taken to place a fibre. For the Weibull distribution, the maximum number of attempts is 557, which is just over one third of the maximum number of attempts required to place a fibre in the normally distributed sample, of roughly 15000. This phenomenon has been observed in literature such as Kari, Berger et al. (2007) who have referred to it as reaching the samples “jamming limit”. An important observation that may be made from the results of this project that extends on the state of current literature on the subject, is that placing fibres whose geometry is generated according to a Weibull distribution can increase the jamming limit threshold of a sample for a given volume fraction.

To reduce the time taken to reach a solution, the orientation of fibres were constrained within positive and negative 30° for samples with an aspect ratio of 10, and 20° for samples with an aspect ratio for 15. The intention is to reduce the likelihood that fibres will intersect and thus reduce the attempts required to place a fibre. Even with the reduced orientation parameter, the samples containing fibres with an aspect ratio of 15 took significantly longer to complete a simulation. A comparison of the times taken to complete a simulation between the fibre length distributions at an aspect ratio of 10 versus 15 may be seen in Figure 8.

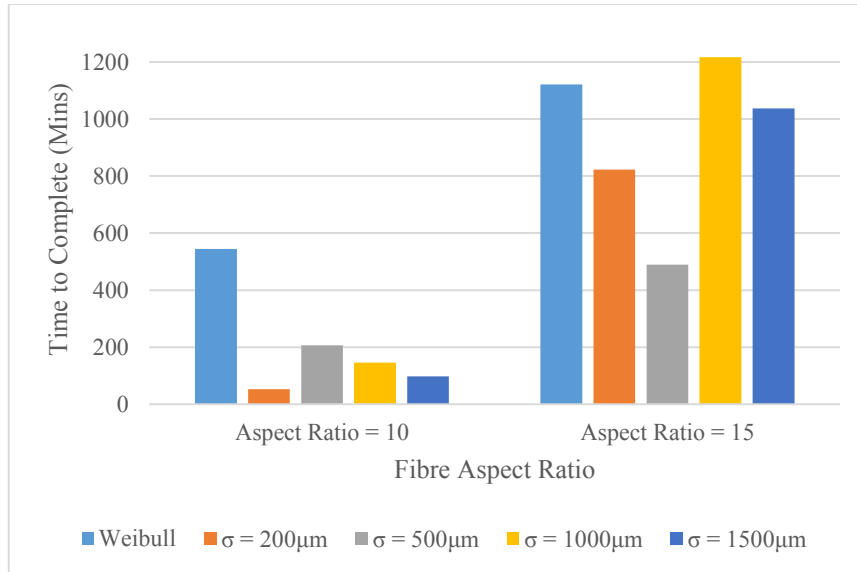


Figure 8 Time to Complete Simulation (mins) for an RVE of 30% Volume Fraction Versus Fibre Aspect Ratios

An attempt to generate an RVE with a volume fraction of 40% was successful when the orientation a fibre may take was reduced to 10° . This scenario was simulated for Weibull distributed data with an aspect ratio of 10 only, and took approximately 20 hours to produce a solution containing 5084 fibres. The maximum number of attempts to place a fibre was less than observed for samples with larger orientation factors at only 4993 attempts. The number of fibres required to generate an RVE of volume fraction of 40% containing fibres with length to diameter aspect ratios of 15 is 1.75 times the number of fibres required for a Weibull distribution of 30% volume fraction, increasing from 7795 to 13618. Attempts to generate an RVE with a volume fraction of 40% and rotations within positive and negative 10° have exceeded reasonable amounts of time that a simulation could be run for, and were cancelled after 72hours of execution.

The maximum number of attempts at placing a fibre may be set prior to initiating the code, however the time taken to reach a solution will unavoidably increase using the modified RSA algorithm. There is potential in future to generate random positions intelligently, as a function of the space already occupied, to cut down on time to generate an RVE wasted on generating coordinates already occupied.

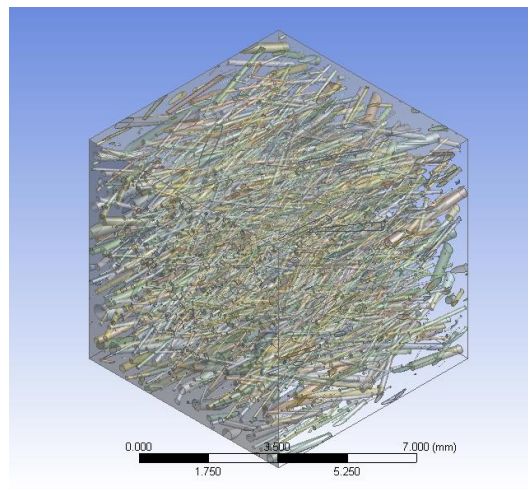


Figure 9 Three-Dimensional RVE with Weibull Distributed Fibres, 10% Volume Fraction and Aspect Ratio of 15. Isometric view.

CONCLUSIONS

Modelling the microstructure of biocomposite materials requires the simulation of a representative volume element (RVE) to capture the inconsistencies in characteristics between fibres. A methodology for the generation of an RVE that enforces periodic boundary conditions and ensures that no fibres occupy the same space has been presented. Short fibres are modelled as cylinders and intersection detection has been performed conservatively by modelling cylinders as capsules. The capabilities of different particle packing algorithms has been evaluated, and the modified random sequential adsorption algorithm has been adopted. RVEs generated from data with a Weibull distribution versus normally distributed data with an equal mean have been compared to evaluate the behaviour of the algorithm. The higher number of fibres required to fill an RVE for a specified volume fraction for a Weibull distribution versus a comparable normal distribution has been attributed to the skewness of the data towards large values at low probabilities. The highest volume fraction that has been achieved to date is 40% for an RVE containing fibres with lengths distributed according to a Weibull distribution and aspect ratios of 15. The future of this work may extend to modelling the RVE samples in finite element software to determine the effects of microstructure characteristics on the macro-scale material properties.

Even at its current stage the developed tool presents a new way of assessing the achievable maximum fibre volume fraction that can be achieved in a short fibre compound as a function of the fibre length and diameter distributions. In contrast to most research where a single discrete fibre length is used the presented tool allows the use of distributions. It was demonstrated in his paper that the fibre size and diameter distribution has a significant impact on the maximum packing density that can be achieved. These findings can be translated directly to practice, by using the metric presented in this paper to specify/assess suitable fibre distributions for compounding and assessing maximum packing density, viz. maximum obtainable fibre volume fraction. Measures such as the number of placement attempts can also be used as a measure to gauge the ease of packing which in the practical sense can be related to the ease of compoundability.

FUTURE OUTLOOK

The purpose of generating a 3D model of an RVE is to then perform finite element analysis to determine the homogenised material properties of the sample. From the results computed by finite element analysis, it is possible to calculate the overall modulus of the sample. Thus the resulting modulus can be compared between samples with different PDF and micro-scale characteristics. It is expected that the tool will also prove its usefulness in other areas where fibrous materials with larger dimensional variability are used. Examples include fibre boards, geo-textiles or filter materials. The developed tool also makes the first step towards the development of RVE to be used in finite element simulations to numerically determine mechanical properties of compounds.

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