SIMULATION OF HEMP FIBRE BUNDLE AND CORES USING DISCRETE ELEMENT METHOD

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ABSTRACT Demands for high-grade hemp fibre are increasing for various industrial applications. To obtain high-grade fibre, it is important to understand the mechanical behaviour of hemp fibre and core. Modelling using discrete element method is a promising approach to simulate mechanical behaviour of any materials, including hemp fibre and core. In this study, a commercial discrete element software, Particle Flow Code – Three Dimension (PFC^{3D}) was used to simulate hemp fibre and core. Because the basic PFC^{3D} particles, named "balls", are spherical. Individual virtual hemp fibres were defined as strings of balls held together by PFC^{3D} parallel bonds. The results showed that the resulting virtual fibre was flexible and could be bended and broken by forces, which appropriately reflect the characteristics of hemp fibre. Using the clump logic of PFC^{3D}, the virtual hemp core was defined as a rigid and unbreakable body, which reflect the characteristics of the core. The virtual fibre and core were defined with several microproperties, some of which were previously calibrated. The five PFC^{3D} bond properties including normal and shear stiffness, *pb_kn* and *pb_ks*; normal and shear strength, σ_c and τ_c and bond disk radius, *R* of the virtual fibre were calibrated in this study. The calibration started with developing a PFC^{3D} model to simulate fibre tensile test. The microproperties of virtual fibre and core were calibrated through running the PFC^{3D} model. The simulations were compared with literature data from fibre tensile tests. The results showed that normal and shear strength of the bond could be considered equal to the external stress applied on the fibre due to axial load during tensile test. Shear stiffness value could be assumed low to make the fibre flexible. The normal stiffness of the bond was determined to be 9e20 N/m by trial and error method.

Keywords: hemp fibre and core, discrete element method, parallel bond, microproperties, tensile strength

INTRODUCTION The stem of hemp (*Cannabis sativa*) plant consists of fibre and core. Fibre (Figure 1a), also called bast fibre, is the surrounding outer layer of bark of the

stems and core (Figure 1b), also called hurd, is the inner layer with hollow pith (Garcia et al., 1998; Mediavilla et al., 2001). The core is responsible for providing stiffness to the hemp stem while the fibre provides tensile and flexural strength. Hemp fibre is extracted from hemp plants through decortication. Decortication is a mechanical process that separates fibre and core. Fibre bundles are the main product of decotication and cores are the by-product.
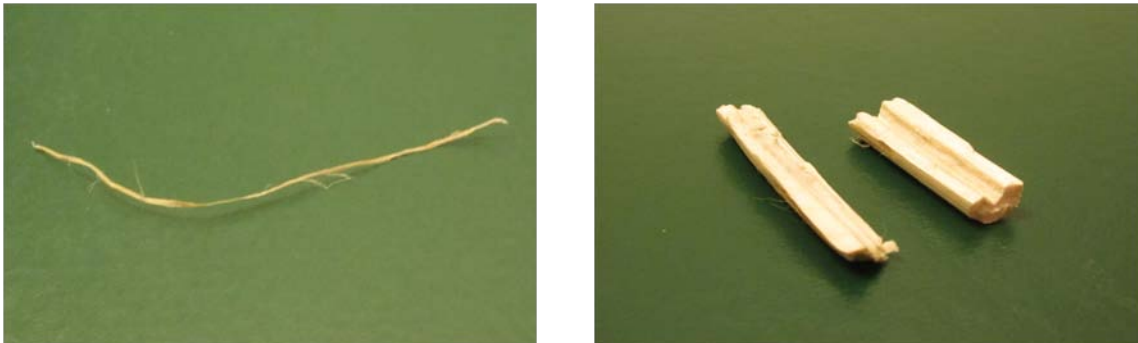
(a)   (b)

Figure 1. Hemp material; (a) single fibre bundle, (b) cores.

Hemp fibre constitutes a valuable source for the manufacturing of environmentally friendly and renewable products. Hemp fibre has been used for textile for a long time. Lately hemp fibres have been used for bio-composites for automobile and many other industrial applications. Cores have also many uses, such as for animal bedding and construction materials. The quality of these materials highly depends on the physical and mechanical properties of the hemp fibre or core. Thus, studying properties of hemp fibre and cores is very important for the quality of these products.

Existing data showed that hemp fibre bundle has a very high strength. Its high value of Young's modulus with a high aspect ratio (length/width) gives an indication of its high strength (Rowell et al., 2000). The tensile strength of hemp fibre bundle is as good as that of high-tensile steel (Munder and Fürll, 2004). Higher tensile strength was also reported by Williams and Wool (2000), Munder and Fürll (2004), Beckermann and Pickering (2008). Limited data could be found in the literature for core properties. To the knowledge of the authors, no research work has been done on the modeling of both fibre and core.

This study used an innovative numerical modeling approach, the discrete element method (DEM), to simulate the properties of fibre bundle and core. DEM is a numerical approach to model a material using discrete assemblages of particles. DEM was first introduced by Cundall and Strack (1979) for analyzing geological materials (rocks and soils). More recently, DEM has been applied to many other materials and it has become a promising tool to simulate the bulk behaviour various materials through their constituent of individual particles.

A widely used commercial DEM software is Particle Flow Code – Three Dimension (PFC^{3D}) developed by Itasca Consulting Group, Inc., Minneapolis, MN (Itasca, 2008). In PFC^{3D}, materials to be simulated are represented by assemblies of individual particles, or "balls". The "surrounding environments" in which the materials are placed, such as

boundaries and machine surfaces, is simulated by "walls". The basic particles in PFC[3D] are spherical (i.e. balls). The recent version of PFC[3D] can be used to model material particles with any arbitrary shape by attaching a group of spherical particles together. The group of spherical particles can be defined either as an autonomous object or a brittle solid. PFC[3D] has been used in simulating not only free-flowing granular materials, such as grains (Lu et al., 1997 and Sakaguchi et al., 2001), but also cohesive materials, such as soil (van der Linde, 2007) and manure (Landry et al., 2006), and solid materials, such as rock (Potyondy and Cundall, 2004 and Pierce, 2004). In a hemp decortication process, hemp plant stems are subjected to external forces, which separate fibre and core. Then the decorticated material goes through a cleaning process in which core materials will be further removed to obtain clean fibre. All these processes encounter flows of fibre buddle and cores around within the decorticator. Thus, PFC[3D] has high potential to be used as a tool to simulate hemp fibres and cores.

PFC[3D] provides users with different contact models among particles and a corresponding set of microscopic parameters of particles at the contact between particles. Regardless of type of material to be simulated, the bottom line is to select the appropriate PFC[3D] contact model and microscopic parameters at the "particle" level, which best describes the macro behaviour at the "material" level.

In summary, understanding the properties of hemp fibre and core is important to industries that use hemp fibre and core. It will also lead to improvement on the design of hemp processing and other handling machines, due to the fact that it will be possible to design these machines according to the material to be handled. No DEM models have been previously developed for hemp fibre and core. The purpose of this study was to use PFC[3D] to simulate fibre bundle and core. The specific objectives were
   a) to examine how hemp fibre bundle and core could be defined with PFC[3D] particles;
   b) to develop a PFC[3D] model to simulate the tensile test of fibre;
   c) to calibrate the microproperties of hemp fibre bundle with existing data from tensile tests.

METHODOLOGY

Virtual fibre bundle and core

<u>PFC[3D] contact model</u> To construct virtual fibre bundle and core with PFC[3D] particles (balls), one needs to determine what kind of interactions should occur between balls. PFC[3D] provides three different models: stiffness model, slip model and contact model. In the stiffness model, there are no bonds between individual balls and the contact force and deflection between balls are governed by the stiffness of the balls. The slip model is similar to stiffness model, but it takes into account friction among balls. The stiffness and slip models are more suitable for simulations of free flow granular materials. Whereas the contact model allows users to add bonds between balls to connect them together. This model is more suitable for the simulation of cohesive materials. Within the contact model, PFC[3D] allows for two different bonding among balls: contact bond and parallel bond. Both bonds are envisioned as a kind of "glue" joining the balls. The glue of the contact bond acts only at the contact point, while the glue of the parallel-bond acts over a

circular cross-section (disk) lying on the contact plane between the balls. The contact bond can transmit only forces, while the parallel bond can transmit both forces and moments.

Definition of virtual core Virtual core was created using the clump logic of PFC^{3D}. A clump consists of a set of balls being rigidly bonded together to behave as a rigid body. PFC^{3D} slip model was used for the contact between balls to simulate the frictional nature of hemp core. Balls within a PFC^{3D} clump may overlap to any extent. A clump will not break apart, regardless of the force acting on it. This means that the virtual core is rigid and unbreakable. Different shapes of core were constructed with different arrangement of balls. Figure 2(a, b) shows two different shapes of core, rectangular and semicircular. Any other arbitrary shapes can be constructed by changing ball arrangement using the PFC^{3D} clump logic.

The wall thickness of core (unbroken hemp stem has a cylindrical and hollow core) varied from 3 to 9 mm (Khan et al., 2009), which is a small dimension. Thus, core was defined to have one layer of balls in the direction of wall thickness, regardless of the shape and the other dimensions of core. Thus, the diameter of the balls was set to be equal to the wall thickness. The number of particles required for a core clump depends on the width and length of the core as follows:
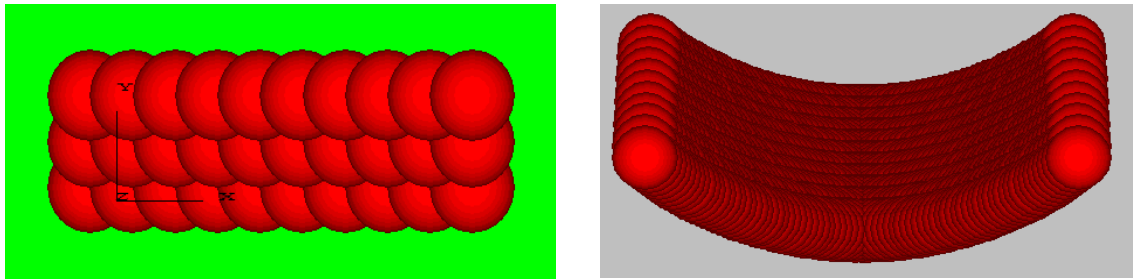
$$n_c = (2b/D_c – 1) (2c/D_c – 1) \qquad (1)$$

where

n_c = number of particles in a virtual core.
D_c = diameter of ball, equal to the wall thickness of the core (mm).
b, c = width and length of core (mm).

(a) (b)

Figure 2. Virtual core; (a) rectangular shape, (b) semi-circular shape

Definition of virtual fibre bundle The **v**irtual fibre bundle was created by the cluster logic of PFC^{3D}. The cluster consisted of a series of balls. Between balls, the radius (R) of the parallel bond was set to be equal to the ball radius, the maximum radius allowed by PFC^{3D}. This maximum value was chosen to increase the bond strength and reduce the roughness of the virtual fibre bundle. Figure 3(a, b) shows two different shapes of virtual fibre: straight and S-shaped. Any other arbitrary shapes of fibre can be constructed by changing the arrangement of the balls.
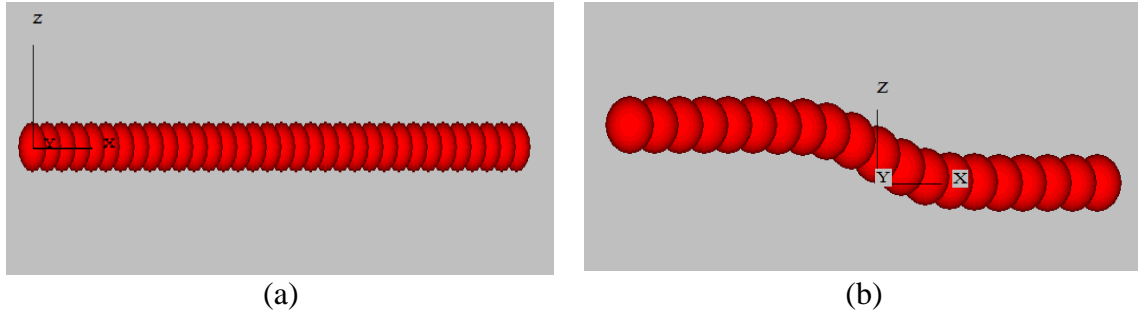
(a)   (b)
Figure 3. Virtual fibre; (a) straight, (b) S-shaped

In the virtual fibre, balls were overlapped by 50% (Figure 4) which is the maximum overlap allowed by PFC^{3D}. This maximum value was used to reduce the surface roughness of the virtual fibre. All balls had a uniform diameter which was equal to the diameter of the real fibre to be simulated. The number of particles required for a virtual fibre bundle depends on the length of the fibre and can be calculated as

$$n_f = 2l/D - 1 \qquad (2)$$

where
   n_f = number of balls in a virtual fibre bundle.
   D = diameter of ball, equal to the diameter of fibre (mm).
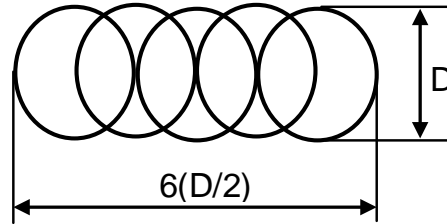 l = length of fibre (mm).

Figure 4. A fibre with five balls overlapped by 50% and the corresponding dimensions

The PFC^{3D} parallel bond model was used to describe the contact between balls in the virtual fibre, with the intention that the balls were held by the bond (the glue), providing both strength and flexibility to the virtual fibre to simulate the real fibre. The parallel bond model is defined by microproperties of both ball and bond. Ball properties include normal and shear stiffness, kn and ks (stress/displacement) and friction coefficient, μ. Bond properties are described by five parameters, including normal and shear stiffness, pb_kn and pb_ks; normal and shear strength, σ_c and τ_c (stress) and bond disk radius, R. Figure 5(a, b) depicts the parallel bond as a cylinder of elastic material and force-displacement behaviours. The bond radius was set to be equal to the particle radius to increase the bonding strength between balls. The maximum tensile (σ_{max}) and shear (τ_{max}) stresses acting on the bond periphery are calculated using the following equations (Itasca, 2008):

$$\sigma_{max} = \frac{-\overline{F}^n}{A} + \frac{\left|\overline{M}_i^s\right|}{I}\overline{R} \qquad (3)$$

$$\tau_{max} = \frac{\left|\overline{F}_i^s\right|}{A} + \frac{\left|\overline{M}^n\right|}{J}\overline{R} \tag{4}$$

where

       A = area of the bond disk,

       J = polar moment of inertia of the disk cross-section and

       I = moment of inertia of the disk cross-section about an axis through the contact point

       $\overline{F}_i^n, \overline{F}_i^s$ = normal and shear component vectors of force

       $\overline{M}_i^n, \overline{M}_i^s$ = normal and shear component vectors of moment

The parallel bond breaks if the maximum tensile stress exceeds the normal strength $\left(\sigma_{max} \geq \overline{\sigma}_c\right)$, or the maximum shear stress exceeds the shear strength $\left(\tau_{max} \geq \overline{\tau}_c\right)$ (Potyondy and Cundall, 2004).
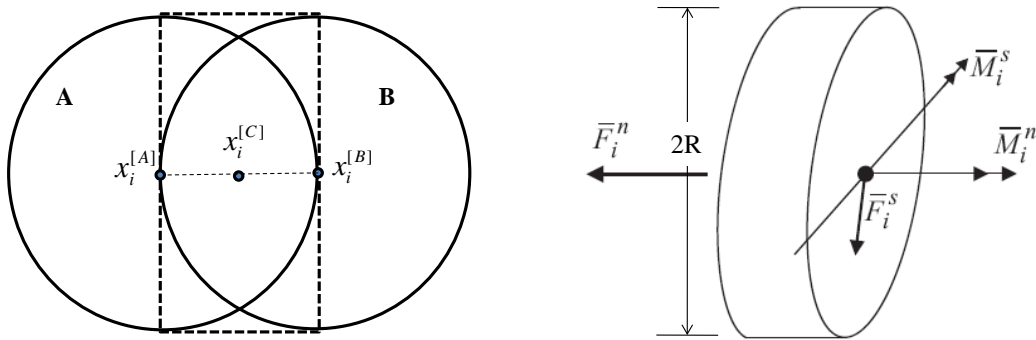

Figure 5. Parallel bond between two balls and force-displacement behavior. n_i = unit normal of the contact plane; $x_i^{[A]}$ and $x_i^{[B]}$ = the position vectors of the centres of Ball A and Ball B; $x_i^{[C]}$ = location of the contact point; $\overline{F}_i^n$, $\overline{M}_i^n$ and $\overline{F}_i^s$, $\overline{M}_i^s$ = normal and shear component vectors of force and moment respectively; $\overline{R}$ = bond disc radius (Itasca, 2008).

Model development for tensile test of fibre bundle The virtual tensile test model was developed using PFC[3D] for a single fibre bundle. One end of the fibre was fixed and the other end was free (Figure 6). The fixed end was at the origin of the coordinate system and the *x*-axis was directed toward the tip and lies along the axis. This setup was similar to a tip-loaded cantilever beam test in PFC[3D]. The fibre was pulled with an axial force, P from the free end of the fibre. The model allows altering magnitudes of fibre diameters and external force.

Z

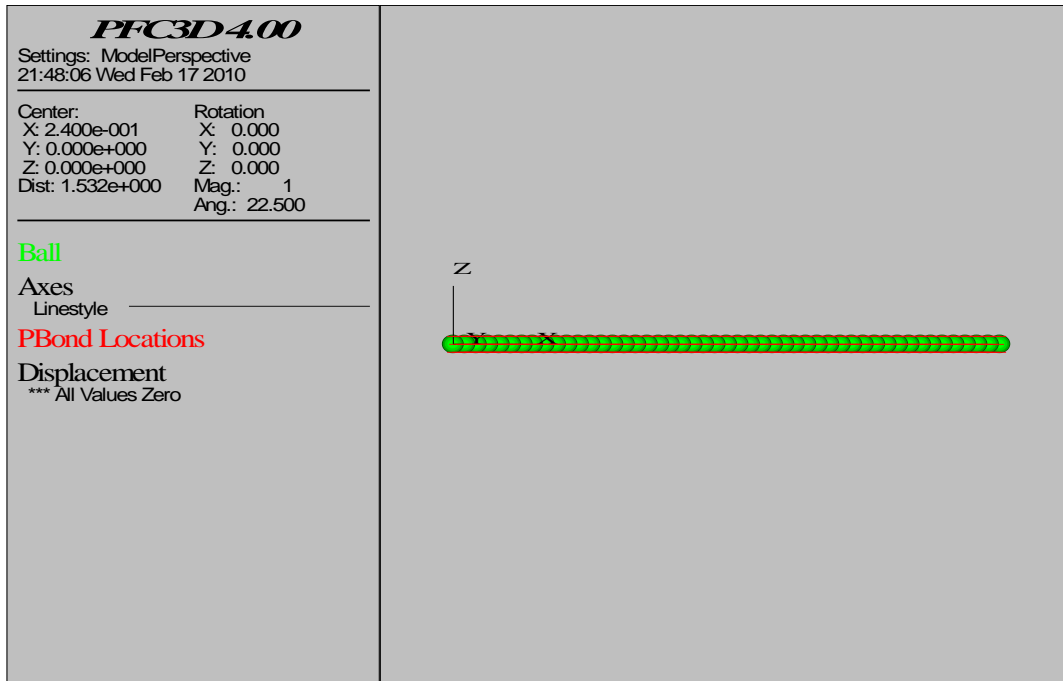D   X   P
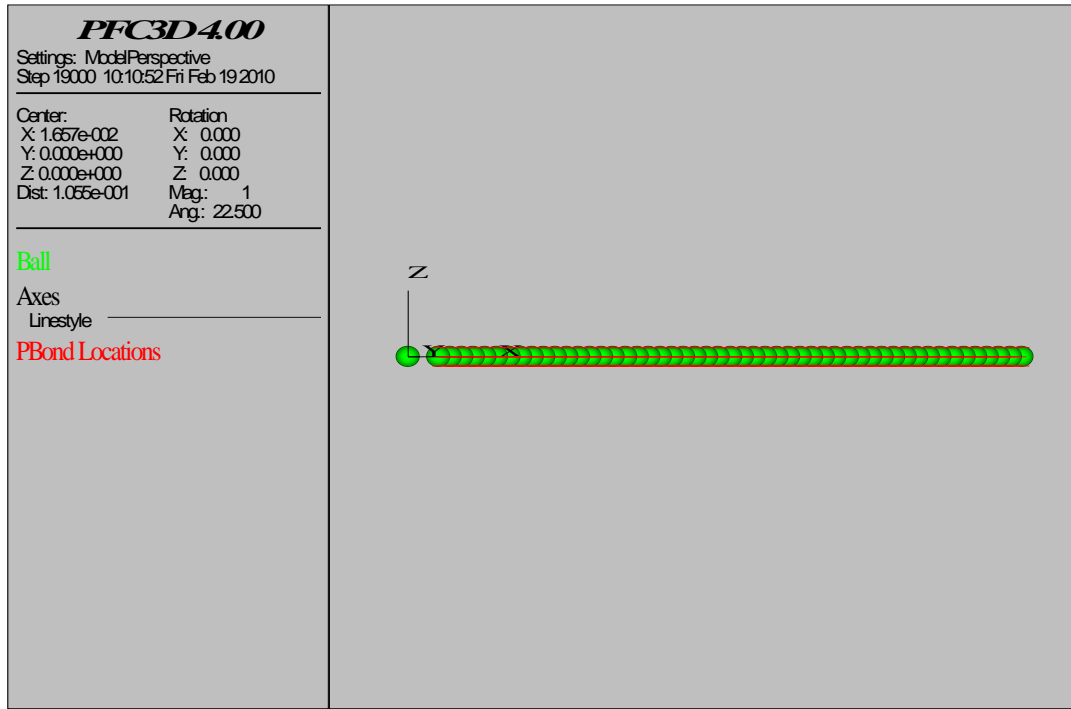
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Figure 6. Fibre for tensile test and for parallel bond

The model was cycled until static equilibrium reached. At the initial condition the displacements of all balls were zero (Figure 7a). Then, *P* was added to the free end of the fibre, causing increasing displacement of fibre. The fibre may break or may not, depending on the magnitude of the tensile force, P, fibre diameter and the strength of the bond, σ_c. Break would occur when the internal stress exceeds the σ_c. The break was physically reflected by the detachment between any of two balls and recorded by fish command in PFC^{3D}. Figure 7 shows initial state (Figure 7a) and final state (Figure 7b) of the virtual tensile test for a single fibre bundle in PFC^{3D}. The break occurred between the first and the second ball. The displacement of the fibre was considered as the displacement of the last ball along the x direction at the time of parallel bond breaks. Thus, the displacement of the last ball at the breaking point can be monitored as the elongation of the fibre.

PFC3D 4.00

Settings: ModelPerspective
21:48:06 Wed Feb 17 2010

Center: Rotation
 X: 2.400e-001   X: 0.000
 Y: 0.000e+000   Y: 0.000
 Z: 0.000e+000   Z: 0.000
 Dist: 1.532e+000   Mag.:   1
                                 Ang.: 22.500

Ball

Axes
  Linestyle

PBond Locations

Displacement
  *** All Values Zero

(a)

(b)

Figure 7. Tensile strength test for calibrating fibre bundle microproperties in PFC^{3D}; (a) Initial state, (b) Final state.

Calibration of bond microproperties of virtual fibre Microproperties (*kn*, *ks* and μ) of ball for both fibre and core have been calibrated by Sadek and Chen (2009). Thus, only the bond properties of virtual fibre were required to calibrate in this study.

Source of data for calibrations To define the PFC^{3D} particles for fibre bundle and to calibrate the microproperties of fibre, existing data from tensile tests of hemp fibre (Belsham, 2000) were used. The setup of the test is briefly summarised here for the information of the readers. In Belsham (2000), test samples of fibre bundle were obtained from manual decortication of unretted hemp. Samples were prepared to have a length of 50 mm, which gave an effective length of 35 mm after being mounted on the tensile machine. An INSTRON machine was used for the tensile tests. Prior to the tests, the diameter of each specimen was measured. The measured diameters varied from 0.03 to 0.33 mm. During the test, the force-elongation curve was recorded with a computerised data acquisition system. The peak force, i.e. the force at the break was read from the curve. This force, together with the fibre diameter, was used to determine the maximum tensile stress, i.e. tensile strength of fibre.

Selection of some microproperties As mentioned above, for the parallel bond model of fibre, there are several microproperties: bond normal and shear strength, σ_c and τ_c (stress), bond normal and shear stiffness, *pb_kn* and *pb_ks* and radius multiplier. Only one microproperty can be calibrated, the others have to be selected based on the logical aspects (Potyondy and Cundall, 2004). As discussed in the previous section, the parallel bond breaks when the external stress exceed the bond normal strength. Thus, it would be logical to let the value of σ_c be equal to the external stress, *P/A*. The shear strength τ_c was considered equal to σ_c. Since the bond radius of the virtual fibre was set to be equal to the

particle radius, the radius multiplier was 1. The shear stiffness was assumed to have a lower value (1e4 N/m, equal to the ball shear stiffness) to make the fibre as flexible as possible and the normal stiffness (*pb_kn)* was calibrated using the tensile test data from (Belsham, 2000).

Calibration of the bond normal stiffness of fibre (*pb_kn*) Virtual tensile tests were performed using the aforementioned model. The values of balls stiffness, *kn* and *ks* were chosen as 1e4 N/m and the friction, and μ was chosen as 0.2, based on the result from Sadek and Chen (2009). As in the real tests, all virtual fibres were 35 mm in length which were the same as those in Belsham (2000). The number of balls for each virtual fibre was determined using equation (2), given the constant length of 35 mm. Data of fibre diameters (D), tensile strengths and elongations at break from Belsham (2000) were used for calibration. The calibration followed the trial and error method, as described below.

The virtual tensile test was run by assigning the measured tensile strength as the bond normal strength, σ_c of the virtual fibre and a set of assumed values of bond normal stiffness; then compared the simulated elongation with the measured one; the calibrated value of the bond normal stiffness was the one which resulted in the best match between the simulated and measured elongations.

The virtual tests were repeated for 11 fibres and it was found that the value of normal stiffness of the fibre, 9e20 N/m, resulted in the best match between the simulated and measured elongations. The results are shown in Figure 8.
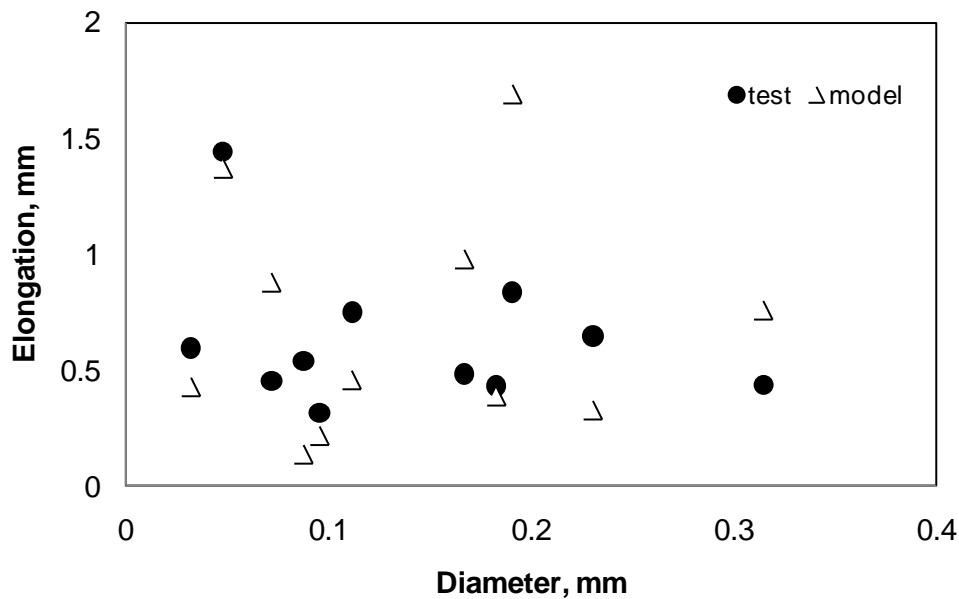

Figure 8. Comparison of test and model results for different fibre.

CONCLUSION In PFC[3D], fibre bundle could be defined using the PFC[3D] cluster logic and core could be defined using the PFC[3D] clump logic. Using these two different logics, differently shaped virtual fibre bundle and core were obtained. The PFC[3D] parallel bond was used for the virtual fibre, so that the virtual fibres were flexible. The virtual cores were rigid and the simple PFC[3D] slip model was used. A virtual tensile test model was

developed for determining the microproperties of fibre bundle. The mocroproperties of the fibre bundle were calibrated through the virtual tensile test using the literature data. In the calibration, the normal strength of the bond was considered equal to the external stress (P/A) applied on the fibre during tensile test. The appropriate normal stiffness of the bond was found to be 9e20 N/m by the calibration. The results from this study were obtained based on limited number of runs of the PFC[3D] model, further tests are required to confirm the results. Also, the calibration was based on the tensile strength and elongation of fibre and whether the virtual fibre reflects the flexibility of a real fibre was not studied.

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