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Paper No. CSBE11- 503

Stochastic Modelling of Hemp Fibre-Core Interface

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Written for presentation at the
CSBE/SCGAB 2011 Annual Conference
Inn at the Forks, Winnipeg, Manitoba
10-13 July 2011

ABSTRACT The use of natural fibres is becoming more popular as environmental awareness and the search for new renewable materials increases. Hemp fibres are attached to other constituents of the hemp stalk by pectic substances, which form an interface layer between the fibre and the core. This study incorporates three important components involved during debonding process: the tensile strength of the fibre, the strength of the core and the strength of the fibre-core interface. In industry, decortication is responsible for this debonding process and it is applied to mechanically break the interface layer to obtain fibre. Therefore, understanding the properties of the fibre-core interface is required to further develop effective decorticators for industrial applications. Peeling forces were measured by using a modified peeling test in two hemp varieties under different retting conditions. Average peeling force ranged from 0.37 to 0.51 N and average work-to-peel ranged from 183 to 433 J/m^2. A stochastic model was described and implemented to simulate the mechanical behaviour of the hemp fibre-core interface during a fibre peeling test. This approach was chosen because of its capability to represent the stochastic behaviour of fibre observed during debonding.

Keywords: Stochastic model, Hemp, Peel test, Debonding, Fibre-core interface

INTRODUCTION Current technologies for processing hemp are relatively inefficient due to lack of interest in the hemp plant until recently. However, the development of new markets and the varied uses of the plant is an indication of technology overcoming the challenges of processing hemp. It is expected that as technologies for hemp-processing become more commercialized and mature that there will be increased market penetration by hemp-based products (Brook et al. 2008). Hemp fibres are among the strongest natural fibres due to their high tensile strength and wet strength, which are desirable characteristics in applications such as biocomposites and textiles. The hemp core is composed of cellulose-rich, short fibres which are ideal for applications such as animal bedding and paper products (Brook et al. 2008). Ideally, separation of the fibres from the core would allow for a better overall use of the plant, and is most efficient with minimal waste remaining on the hemp core. This process of fibre separation from the core is known as decortication. The

quality of the fibre will be largely affected by the decortication process. Therefore, studying the behaviour of fibre during the debonding process is a fundamental step towards the design of more efficient decorticators. The decortication process should not adversely influence the mechanical properties of the fibre (Xu 2010).

In order to investigate the behaviour of the fibre-core interface during peeling, it is important to understand the fundamental structure of a hemp stalk. Hemp produces phloem fibres which are cemented into place by a complex mixture of pectins, hemi-celluloses and lignin (Booth et al 2004). The basic arrangement of layers within a typical hemp plant cross-section is illustrated in Figure 1, albeit the proportions of space that the layers take up are not to scale. The outer layer is known as the cortex, which is a thin protective layer containing chlorophyll. The phloem layer consists of chlorophyll-containing short cells as well as long cells known as the bast fibres. These two layers combine to form the fibre component of the hemp stalk. The cambium layer is also known as the interface layer, where fibre and core separate during the peeling procedure. This layer will be referred to as the fibre-core interface of the hemp stalk. The pith layer provides structural support and can be identified as the core of the plant. The hemp stalk possesses a hollow core through its length, with the exception of the joints between internodes.

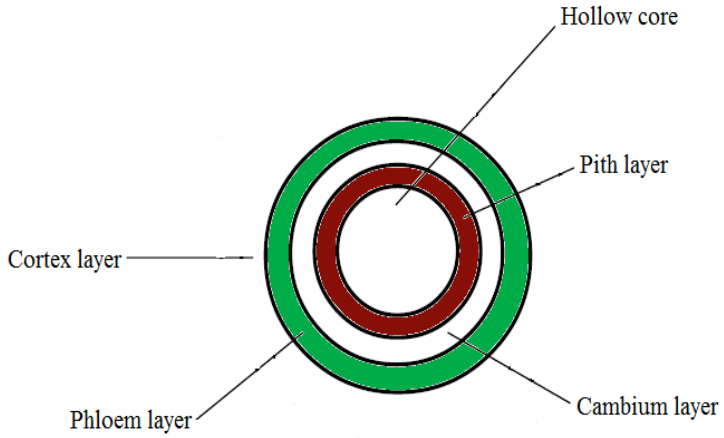

Figure1. Hemp stalk cross-section.

The use of energy based models can describe stable debonding of long embedded fibres (Zhong et al. 2003), which is comparable to the removal of hemp fibre during decortication. The Ising model is a useful tool for the study of fibre behaviour, having been applied previously to studies regarding different processes of a stochastic nature. The processes were simplified as systems consisting of the interaction of subsystems with two interchangeable states (Lukas et al. 1996, Zhong et al. 2001, Zhong et al. 2003 and Zhong et al. 2004). Of particular interest is the work of Zhong et al. (2003), who discusses the simulation of the single-fibre-peel process. One of the advantages of the present method is its simplicity in application (Lukas et al. 1996) and also its applicability to such phenomena as partial debonding, fibre breaking, and matrix failure; these phenomena are difficult to be dealt with by other existing methods (Zhong et al. 2003).

It is important to study the peeling forces required to separate the fibre-core interface of hemp in order to identify forces that will cause minimal damage to the fibre. This would enhance the understanding of current hemp-processing methods as well as help design and select suitable decorticators. Hence, the objectives of this study were to (1) implement 90-degree resistance to peel test, evaluating the strength of the hemp stalk fibre-core interface and (2) employ the Ising

model combined with Monte Carlo simulation to generate a stochastic simulation which will describe the behaviour observed in the resistance to peel test.

MATERIALS AND METHODS

Sample Preparation Currently, there are several varieties of the hemp plant being grown in Canada. For the purposes of this study, the peel test was performed on two hemp varieties, USO 14 and Alyssa. Forty stalks from each variety were randomly selected to perform the peel test. Each variety was exposed to two different treatments; for each variety, half of the stalks were retted and the other half remained unretted. Retting was achieved by laying the samples in the field, which is also known as dew retting. Dew retting was chosen since it seems to be the most commonly used method in Canadian agricultural practice. After three weeks, the samples were brought back to the laboratory in order to start preparations for the peel test.

Having two varieties and two retting treatments resulted in a total of four different scenarios, which produced a number of 20 samples per scenario. The samples were cut into appropriate lengths using a method that will ensure minimum damage to the hemp fibre-core interface. The cut was done as a two-step process. The first step was to use an exacto knife to cut around the outer layers of the stalk and the second step involved using a small metal saw to cut the inner core of the stalk. Using the exacto knife to cut the outer layer prevented damage to the fibre-core interface before performing the peel test. This method was applied to obtain samples that were between 10 cm and 15 cm in length. The sample length was chosen in accordance to the distance between internodes in the hemp stalks.

Properties of materials, including natural fibres, are known to vary at different environmental conditions. Temperature and humidity are crucial in determining the mechanical properties of fibres. The relative humidity of the environment has an effect in the amount of moisture in the sample as well as its moisture content. Temperature is also an important factor because of its direct relationship to humidity. In an effort to maintain the condition of the samples constant, they were conditioned for seven days at 21ºC and 40 % RH.

Sample Characterization Hemp stalks were characterised based on their most important physical properties, including diameter, linear density, and moisture content. The diameter of the hemp stalk varies along its length, hindering the accuracy of measuring the diameter of the stalks. The average diameter was measured to be the mean value of three measurements at different locations of the hemp stalk; one measurement at each one of the edges and also one at the middle of the hemp stalk. Measurements of the linear density provide additional information about the sample, which will be helpful for preparing the computer model implemented in this investigation. The linear density is the measurement of the weight per unit length of hemp stalk. As mentioned in the previous section, moisture content is an important factor in determining the mechanical properties of materials. The work of Booth et al. (2004) clearly shows how moisture content can have a large influence in the resistance to peel of hemp stalks, especially at lower moisture contents. Therefore, the moisture content was measured as designated by ASTM standard D4442-07, which helped provide better means of evaluating the comparison between both, retted and unretted, sample treatments.

Mechanical Test The peeling of the fibre-core interface was initiated manually for each hemp stalk. Each peel was prepared to have the same thickness, which allowed for effective comparison between samples. Two parallel blades, 2 mm apart, were used to make a cut along the major axis, ensuring constant thickness of each peel as the test was performed. The cutting tool was composed of two blade tips extracted from an exacto knife. The blades were separated by a metal that provided the 2 mm distance between the blades. This 2-mm distance will later be used as

means of converting the peeling force to work required to peel. Figure 2 shows the assembly of the cutting tool components. After the cutting tool was used to prepare the sample for peeling, a transverse cut was made to manually initiate separation of the fibre from the core. Peeling is considered initiated if the fibre starts to cleanly peel away from the core. This process usually took 30 – 40 mm of manual peeling. In order to ensure that the peeling distances between each peeling were all the same, the fibres were consistently clamped at a distance of 20 mm away from the stalk.

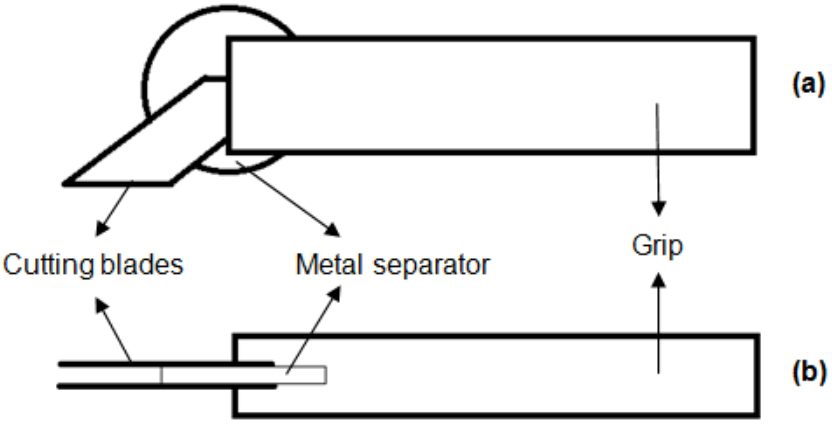

Figure 2. Assembly of cutting tool components: (a) Side view. (b) Top view

A universal test frame was employed as a mean to measure the strength of the fibre-core interface of each hemp stalk. The test performed in this experiment is normally used for testing the bonding strength of adhesives attached to a rigid surface. This test is commonly known as a 90-degree resistance to peel. The methodology implemented followed a combination of methods introduced by ASTM standard D6862 – 04 and the work described by Booth et al. (2004). The test frame used was an Instron 5965, which was equipped with a 5-N load cell. Figure 3 shows a simplified diagram of the assembly as well as the geometry of the test during both initial (X_o, Y_o) and final (X_f, Y_f) steps. A 300-mm extension piece was used to maintain relatively constant geometry as the peeling action is extended during the test. The expected change in the peeling angle is approximately three degrees. A bulldog clip was attached to the extension piece to allow the fibre to be peeled as the upper fixture moved up at a rate of 40 mm/min. The effective peeling distance was 20 mm for each sample. Using this assembly resulted in minimizing the change in peeling angle while allowing the use of a simple clamp to attach the samples to the test frame. The lower fixture managed to keep the stalks in a fixed horizontal position with the help of rubber attached to its surface. The top clamping position was coloured with ink to ensure that any slippage would be detected and discarded if necessary.

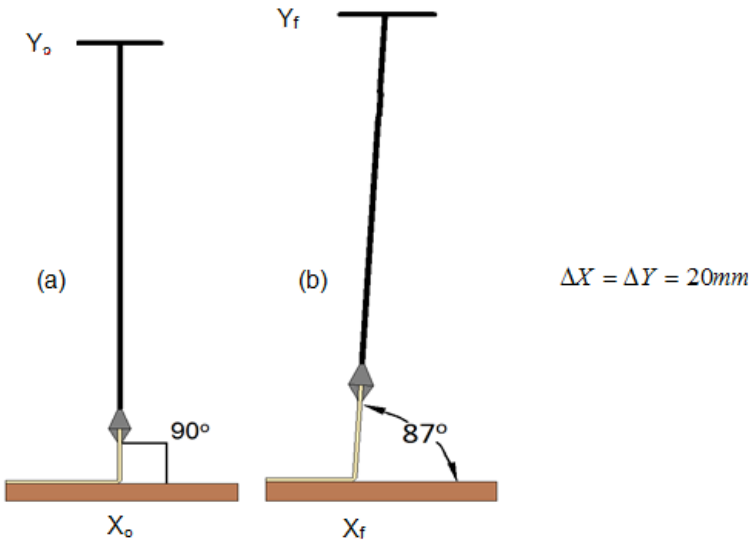

Figure 3. Assembly of peel test geometry: (a) Initial geometry before test
(b) Final geometry after test

STOCHASTIC SIMULATION

Ising Model The working principle of the computer model incorporates three important components involved during the peeling process: the tensile strength of the fibre, the strength of the core and the strength of the fibre-core interface. These three components describe a complex system, which can be described by the Ising model in a simplified fashion, as subsystems bearing two interchangeable configurations. The macro characteristics of the system are represented as the interactions and resulting balances among the micro characteristics of each cell within the system. The change in the internal energy (*dE*) of the system can then be described as:

$$dE = \sum e_i \, dm_i + \sum m_i \, de_i = dH + W \qquad (1)$$

where m_i is the number of subsystems having the internal energy e_i, which can be altered by either the change of state of e_i or the rearrangement of m_i during the peeling process. The first term on the right-hand side of equation (1) represents the change in the internal energy of the system, described as the Hamiltonian (*dH)*. This represents the summation of the interactions between each cell and its nearest neighbours. The second term on the right-hand side represents the change in energy due to extrinsic work (*W*) done to the system. In this model, the extrinsic work is representing the peeling force responsible for the change in state of the fibre-core interface.

The system was discretized into a two-dimensional structural framework composed of square cells. The cells can be filled with three possible states; empty, filled by fibre or filled by core. However, fibre and matrix shall not simultaneously occupy any individual cell at any given time. This configuration resulted in a total of four variables capable of describing the state of each cell.

(i) F_i = Cell *i* is occupied by fibre (F_i = 1) or not (F_i = 0)

(ii) f_i = Fibre cell *i* is bonded to the core (f_i = 1) or not (f_i = 0)

(iii) C_i = Cell *i* is occupied by core (C_i = 1) or not (C_i = 0)

(iv) c_i = Core cell *i* is bonded to adjacent core (c_i = 1) or not (c_i = 0)

(cell *i* is above or below cell *j*)

(cell *i* is directly connected to cell *j*)

The energy of the system (*H*) can be expressed for each single cell as:

$$H = -T\sum_{j}^{cn} F_i F_j S_{ij} - U\sum_{j}^{cn} c_i c_j S_{ij} - G\sum_{j}^{ct} (f_i c_j + C_i f_i) S_{ij} \quad (2)$$

The first term in the right hand side of Equation (2) represents the tensile strength of the hemp fibre, where: *T* is representative of the cohesive energy between each connecting fibre cell, *cn* denotes the sum of the *F* value over all the fibre cells connected to cell *i*, and S_{ij} accounts for the interaction area between cell *i* and cell *j*. The second term represents the strength of the core, where *U* is representative of the cohesive energy between each connecting core cell. In this term, *cn* denotes the sum of the *c* values over all of the core cells in connection to cell *i*. Similarly to the first term, S_{ij} accounts for the interaction area between cell *i* and cell *j*. The last term in the equation represents the fibre-core interface, where *G* reflects the adhesive energy between the fibre and the core and *ct* denotes the sum of *c* or *f* values of the cells in contact with cell *i*. It is important to note that if a given cell *i* is occupied by fibre, which is bonded to the core, only the first term inside the brackets has nonzero values. Similarly, if the given cell *i* is occupied by core, only the second term inside the brackets has nonzero values. Another feature shown in Equation (2) is the fact that *G* is no longer in effect after debonding of the fibre cell occurs (f = 0).

The expression for the interaction area, S_{ij}, is determined under the assumption that fibres are shaped as cylinders. Therefore, the interaction area at the fibre-core interface was modelled as half a cylinder with both diameter and height equal to the fibre diameter *d*. Interaction areas at connecting fibre-fibre or core-core cells were modelled as circles of diameter *d*.

$$S_{ij} = \begin{cases} \frac{\pi d^2}{2} \\ \frac{\pi d^2}{4} \end{cases} \quad (3)$$

Monte Carlo Simulation Based on the energy difference, the model needs to determine the behaviour of the fibre as it is being peeled. The Monte Carlo simulation has the capacity of appropriately determining which scenario will manifest itself during the peeling process. The scenarios are based in the energy difference between each change in state and include fibre breaking, fibre debonding and core pull-out. The most common change in state for this particular simulation is likely to be dictated by the energy difference before and after fibre debonding. A debonding fibre cell *i* is represented by a fibre cell which has changed from a bonded state (f_i=1) to a debonded state (f_i=0). The expression for the energy difference can be expressed as:

$$\Delta E = H_2 - H_1 - W_t \quad (4)$$

where H_1 and H_2 are terms representing the internal energy of the system at different states and W_t is the work done to the system by tensile load. The magnitude of W_t is given by the product of the tensile force *R* and the elongation of the fibre, which is equivalent to the diameter *d*. From taking into account these assumptions, a new expression can be derived from Equation (4) in the form:

$$\Delta E = H_2 - H_1 - Rd \quad (5)$$

It is important to note that energy equations involving fibre breaking and core pull-out are also included in the model. The energy difference expression for the breaking scenario is the same as Equation (5) and the expression for matrix pull-out is similar as well. The main difference being that the last term *Rd* is excluded because pull-out occurs in combination with the debonding scenario, which already includes *Rd*.

Each step in the calculation of energy difference, for a given cell *i*, involves the use of a probability distribution. The probability *P* for a change of the system from one state to another is calculated by using the Metropolis function (Yeomans 1992) given by:

$$P(E_2|E_1) = \min\left[1, e^{\left(\frac{-\Delta E}{\beta}\right)}\right], \qquad (0 < P \leq 1) \qquad (6)$$

where *P* is given a value of 1 when $\Delta E = E_2 - E_1 \leq 0, or\ E_2 \leq E_1$. This means that changes from higher energy states to lower energy states are have a definite probability of occurring. In the opposite situation, whenever $E_2 > E_1$, *P* falls somewhere within $0 < P < 1$. A random number *r*, which is uniformly distributed and falls between zero and one, is selected and the state change occurs only if $r < P$. The previously described arrangement implies that the internal energy difference ΔE at any possible state change scenario is always positive and therefore, quite unlikely to occur spontaneously. As a consequence of this, a sufficient amount of extrinsic work is required to counteract the positive internal energy difference and produce a probability *P* which is large enough to produce a state change. The effect of thermal perturbation is reflected by the thermodynamic constant β. For the purposes of the Monte Carlo simulation, β is given a constant value of 0.008 at room temperature. This value could be adjusted to account for thermal fluctuations, but the contribution of thermal energy to the current simulation is insignificant. Figure 4 illustrates the flow chart of the implemented simulation program.

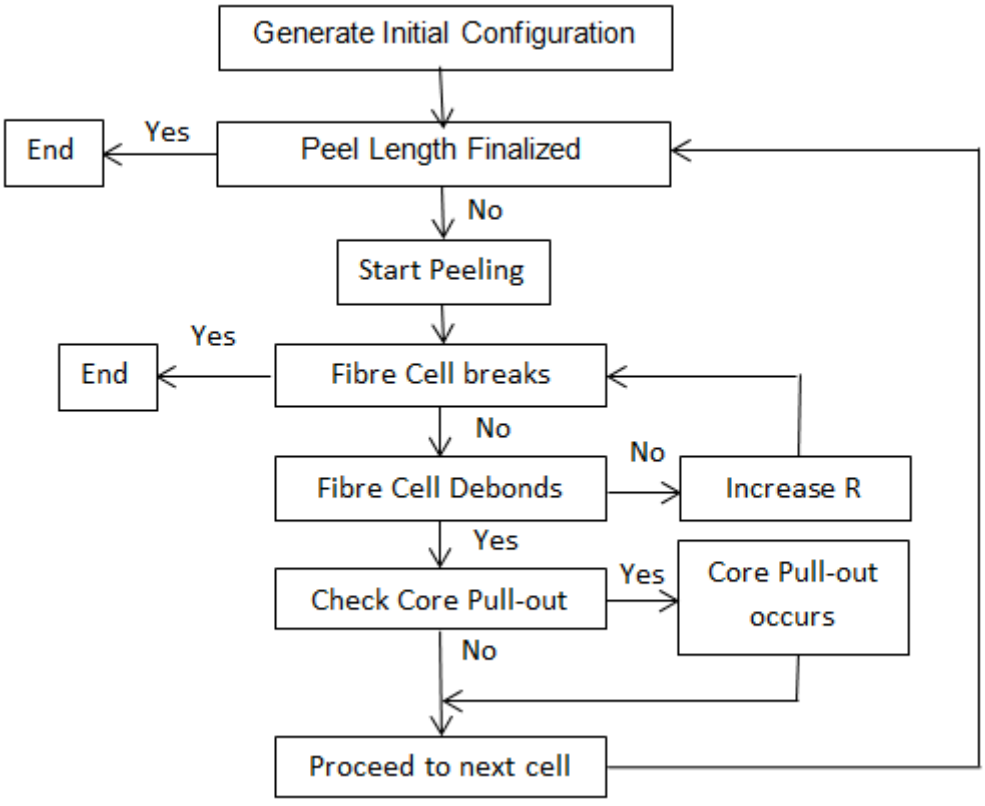

Figure 4. Flow chart of Monte Carlo simulation

RESULTS AND DISCUSSION

Sample Characterization The moisture content for both hemp varieties was determined to be approximately 7% and 8% for unretted and retted samples, respectively. Average linear density was highly variable and ranged between 8 and 35 g/m. The average diameter for the Alyssa variety was determined to be 86 ± 15 mm for the unretted samples and 84 ± 11 mm for the retted samples. The USO 14 variety possessed a larger average diameter with measurements of 129 ± 25 mm for the unretted samples and 122 ± 30 mm for the retted samples.

Mechanical Test The amount of force required to peel the hemp fibres was measured for each variety and treatment. The average peeling force for the Alyssa variety was 0.37 ± 0.25 N for unretted samples and 0.41 ± 0.23 N for retted samples. The USO 14 variety was found to have larger average peeling forces, with values of 0.86 ± 0.51 N for unretted samples and 0.87 ± 0.59 N for retted samples. As mentioned previously, this could be a consequence of the difference in average diameter. Figure 6 indicates a typical force-elongation curve observed during the resistance-to-peel tests. The peeling force reached a peak value at approximately 5 mm of displacement, followed by a load diversion approximate to an average value until the test was completed.

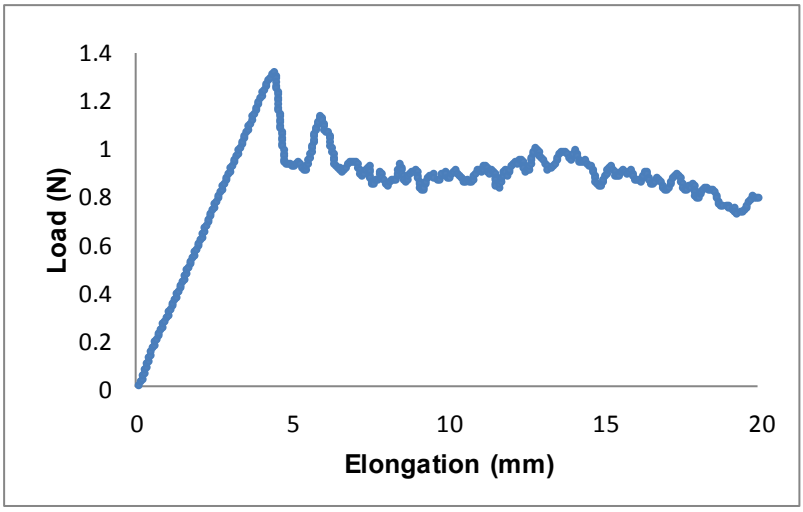

Figure 6. Typical load Vs elongation curve

Within the Alyssa variety, the work required to peel the fibre from the core was 183 ± 126 J/m^2 for unretted samples and 203 ± 117 J/m^2 for retted samples. The work required to peel fibres of the USO 14 variety had minimal differentiation between treatments, resulting in 428 ± 256 J/m^2 and 433 ± 292 J/m^2 for unretted and retted samples, respectively. Figure (7) shows a summary of these results for each variety and treatment, indicating that retting for a period of three weeks did not decrease the required work to peel for the given sample conditions.

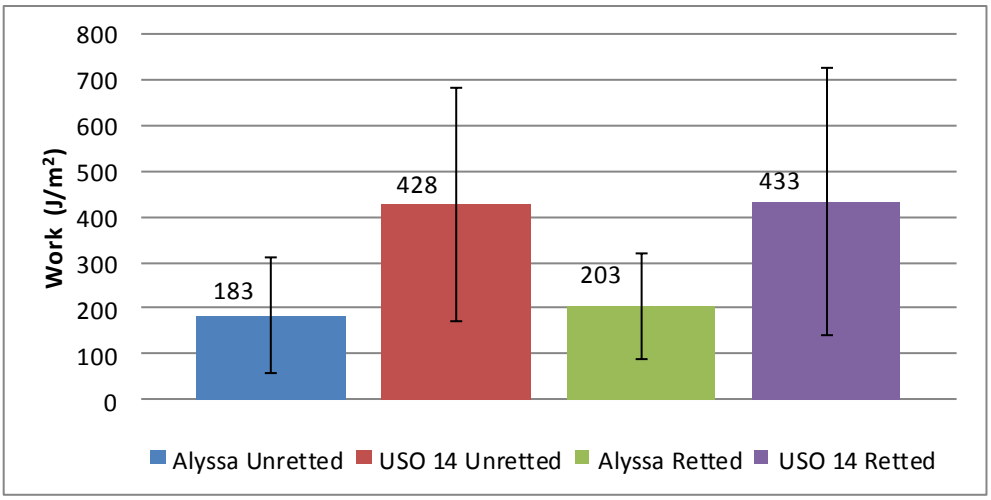

Figure 7. Average work to peel

Monte Carlo Simulation The computer simulation is still in need of further calibration to be able to reflect the results which are representative of the real system. Figure 8 shows the raw output of a section of the program, arbitrary values where given for the initial configuration. Horizontal axis represent displacement in mm and vertical axis represent peeling force in N. Future work will involve refining this output. However, preliminary raw data shows the potential to achieve a proper calibration of the model. In order to achieve this, cohesive and adhesive energy terms of equation (2) should be modified as required.

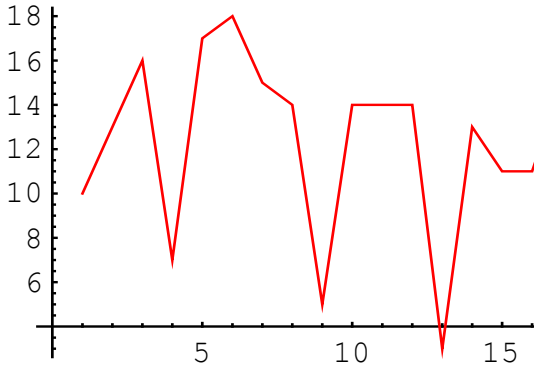

Figure 8. Raw program output

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