Application of stochastic modelling for simulating hemp fibre peeling behaviour

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http://dx.doi.org/10.7451/CBE.2013.55.2.1

Guzman, L., Y. Chen, S. Potter, W. Zhong and M. Rahman. 2013. **Application of stochastic modelling for simulating hemp fibre peeling behaviour.** Canadian Biosystems Engineering/Le génie des biosystèmes au Canada **55**: 2.1-2.8. The separation of fibre and core components of hemp stem is a fundamental step in hemp decortication, mechanical separation of fibre and core. This research aimed to enhance the understanding of fibre-peeling behaviour of hemp to improve the current decortication technologies. Peel tests were performed on retted and unretted hemp samples for each of two hemp varieties, USO 14 and Alyssa. Results showed that force and work required to peel did not vary with the retting condition, but with the hemp variety. The average peeling force for the Alyssa variety was 0.39 N and that for the USO 14 variety was 0.87 N. Within the Alyssa variety, the work required to peel the fibre from the core was 193 J m^{-2}, and the work required to peel the fibres of the USO 14 variety was 431 J m^{-2}. The Ising model was implemented to produce a stochastic model which simulated the peeling force obtained from the peel tests. The behaviour of the simulated peel test was similar to that observed during the peel test and the process of fibre peeling was successfully simulated through the use of a stochastic algorithm. The stochastic model simulated the average peel force to be 0.86 N for the USO 14 variety and 0.39 N for the Alyssa variety. **Keywords:** stochastic model, hemp, peel, debonding, fibre, core, force, work

La séparation des composantes fibreuses et du cœur de la tige de chanvre est une étape fondamentale dans la décortication du chanvre par la séparation mécanique de la fibre et du cœur. Ce projet de recherche avait pour objectif d'améliorer les connaissances en ce qui à trait au comportement de séparation des fibres de chanvre pour améliorer les technologies actuelles de décortication. Des tests de séparation étaient faits sur des échantillons de chanvre roui et non roui pour chacune des deux variétés, USO 14 et Alyssa. Les résultats ont montré que la force et le travail requis pour la séparation ne variaient pas avec les conditions de rouissage mais avec la variété de chanvre. La force moyenne de séparation pour la variété Alyssa était de 0,39N et de 0,87N pour la variété USO 14. Pour la variété Alyssa, le travail requis pour séparer les fibres du cœur était de 193 J m^{-2} et le travail requis pour les fibres de la variété USO 14 était 431 J m^{-2}. Le modèle Ising était utilisé pour produire un modèle stochastique qui simulait les forces de séparation obtenues par les essais de séparation. Le comportement des tests de simulation de séparation était similaire à celui observé durant le test de séparation et le processus de séparation de la fibre était représenté efficacement avec l'utilisation de l'algorithme stochastique. Le modèle stochastique représentait la force moyenne de séparation à 0,86 N pour la variété USO 14 et à 0,39 N pour la variété Alyssa. **Mots clés:** modèle stochastique, chanvre, séparation, décollement, fibre, coeur, force, travail.

INTRODUCTION

There is increasing interest from many potential end-users of hemp-based products, especially hemp fibre (Brook et al. 2008). Hemp (*Cannabis sativa* Linnaeus) fibres are among the strongest natural fibres, which is a desirable characteristic in applications such as bio-composites and textiles. The cross-section of hemp stem is illustrated in Fig. 1. The outer layer is known as the cortex, which is the thin protective layer containing chlorophyll. The phloem layer consists of chlorophyll-containing short cells and long cells known as the bast fibres. These two layers combine to form the fibre component of the hemp stem. Hemp produces phloem fibres, which are cemented into place by a complex mixture of pectins, hemi-celluloses and lignin (Booth et al. 2004). The cambium layer is also known as the fibre-core interface layer. The pith layer provides structural support and can be identified as the core of the plant. The hemp stem possesses a hollow centre through its length, with the exception of the joints between internodes. In modeling of mechanical properties of hemp in this study, the hollow structure of hemp stem is considered to have only two distinct components: fibre and core.

The process of mechanically separating fibre and core is commonly known as decortication. Decortication requires the use of machinery such as hammer mills and roll crushers. Fibre and core debond during decortication. Current decortication machines are not energy efficient and

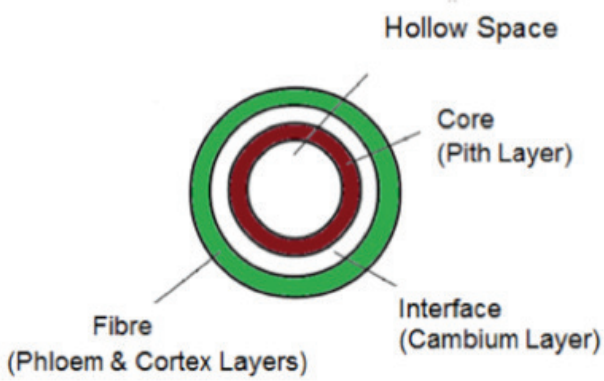


Fig. 1. Hemp stem cross-section (the proportions of the layers are not to scale).

yield low purity product due to lack of knowledge about the mechanical properties of hemp (Baker 2009). Energy requirement and effectiveness of the decortication process depend on the adhesive energy bonding fibre and core together. Therefore, understanding the bonding strength between fibre and core is essential for the design and improvement of decortication processes.

Mechanical peel tests are generally used by engineers to study adhesives (Hadavinia et al. 2006; Bundy et al. 2000) and are implemented to investigate the separation of plant tissues (Goodman et al. 2002; Booth et al. 2004). Mechanical decortication processes, for example, using hammer mills and roll crushers, may not directly involve a fibre peeling process. However, peeling would be one of the phenomena among others, such as impacting, shearing, and compression, which occur in decortication. Therefore, studying of fibre peeling is highly relevant to hemp decortication. The results will have implications to the energy consumption in mechanical processing of hemp. However, this study was not associated with any fibre decortication method; rather it was a fundamental study aiming to understand the bonding strength between bast fibre and core, independent of any decortication applications.

The mechanical peel test consists of two adherents, one being rigid and one being flexible, which are fixed together with an adhesive. Once the elements are combined, the force required to separate the adherents is measured to determine the adhesive energy, which is bonding them together. Booth et al. (2004) used a mechanical peel test in hemp stems to investigate factors that affect the work to peel, including peeling angles and moisture content; the results provided insight on the comparability of peel tests performed under combinations of the previously mentioned factors.

The process of peeling hemp fibre from the core is subjected to oscillations in the peeling force (Booth et al. 2004), as observed during peel tests of other materials (Inoue and Suganuma 2009; Von Maubeuge and Ehrenberg 2000; Xie and Karbhari 1997). The oscillations of the peel force are a product of the adhesive's properties, which can be described as stochastic in nature. The Ising model is a useful tool for the study of stochastic behaviour in multiple interactive subsystems (Yeomans 1992). The macro characteristics of the system are represented as interactions and resulting balances among the micro characteristics of subsystems present in the model. Energy based models, such as the Ising model, serve as a tool to describe stable debonding of long embedded fibres (Zhong and Pan 2003), which is comparable to the removal of hemp fibre from the core. The processes were simplified as systems consisting of the interaction of subsystems with two interchangeable states (Zhong et al. 2001; Zhong and Pan 2003; Zhong et al. 2004). Of particular interest is the work of Zhong and Pan (2003), which discusses the simulation of a hypothetical single-fibre-peel process of a polymer with half of its volume embedded lengthwise in a block of cured matrix. One of the advantages of the presented method is its applicability to describe such phenomena as partial debonding, fibre breaking, and matrix failure; these phenomena are difficult to be dealt with by other existing methods.

The objectives of this study were to (1) conduct peel tests to evaluate the strength required to separate the hemp fibre-core interface and (2) to develop a stochastic model to predict the peeling strength of hemp fibre using the Ising model.

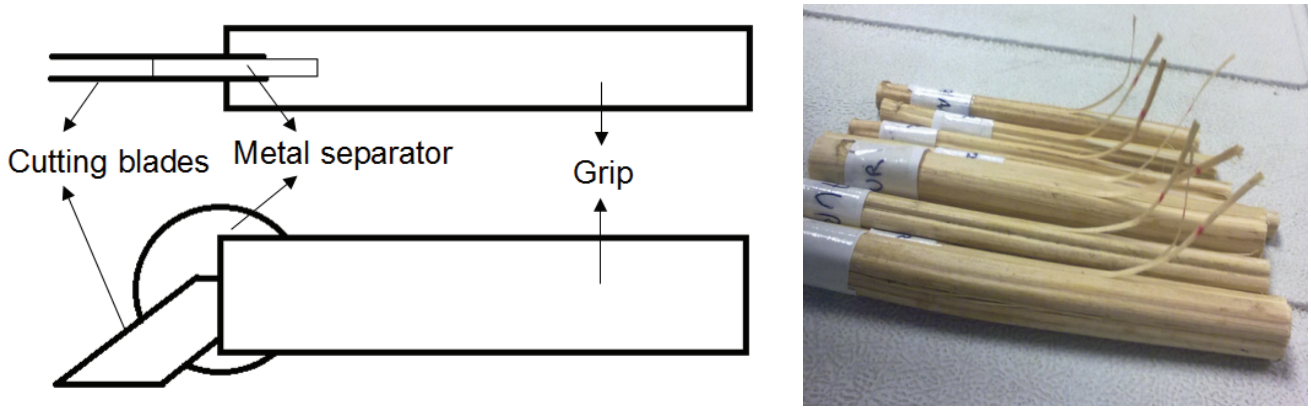
MATERIALS AND METHODS

Peel test

Experimental design The peel test was performed on two hemp varieties, USO 14 and Alyssa, from crops grown in Manitoba, Canada. Hemp was harvested while pollen was being shed. Hemp plants were manually harvested at different random locations of the field. Retting may affect the energy required for fibre peeling. Retting is a biological process that removes the pectic substances that bind the fibre to the core, and can be achieved by the combined action of dew and showers of rain (Franck 2005). For each hemp variety, half of the plants were retted and the other half remained unretted. Retting was achieved by leaving hemp plants in the field for a period of three weeks. Having two varieties and two retting conditions resulted in a total of four different treatments. Ten samples were tested for each treatment, giving a total of 40 peel tests.

Sample preparation Hemp samples were air-dried, and the average moisture content of unretted and retted samples was 7.5%. The first step was to cut hemp stems into segments of 100 and 150 mm in length (. 2). Cutting was done using an X-Acto knife to cut around the outer layers of the stem and using a small metal saw to cut the inner core of the stem. This prevented damage to the fibre-core interface prior to the peel test. The sample length was chosen in accordance to the distance between internodes within the hemp stems. The segments were taken from different regions along the hemp stem. The average diameter of the segments was 8.5±1.3 mm for Alyssa

Fig. 2. Hemp stems used for peeling test.



(a) (b)

Fig. 3. Sample preparation: a) Assembly of cutting tool components and b) Prepared hemp stems prior to peeling test.

variety and 12.6±2.8 mm for USO14. Hemp properties are strongly influenced by the conditioning humidity, and consequently by the moisture content in the fibres (Hoffmeyer et al. 2007). Therefore, the second step was to condition the samples in an environmental chamber for seven days at 21ºC and 65 % relative humidity prior to the peel test (ASTM 1998).

The final step was making a cut along the major axis of each sample, ensuring a constant width of 2 mm for each peel as the test was performed. The cutting tool was composed of two blade tips extracted from an X-Acto knife and a grip (Fig. 3a). The blades were separated by a piece of metal that provided the 2-mm distance between the blades. The 2-mm distance in combination with the peel force was also used as a means to determine the work required to peel. Then, a transverse cut was made to manually initiate separation of the fibre from the core (Fig. 3b). The peeled fibre was consistently clamped to the upper grip at a distance of 20 mm away from the stem.

Testing procedure The implemented procedure followed a combination of methods introduced by ASTM standards (ASTM 2004) and the work described by Booth et al. (2004). The test frame (Fig. 4a) was an Instron 5965 equipped with a 5-N load cell. A long (300-mm) non-extensible string was used to maintain relatively constant peeling angle, 90º ± 3º, as the peeling action was extended during the test (Fig. 4b). Booth et al. (2004) reported that peeling angles of 90º ± 15º would not significantly affect the work to peel hemp fibre from the core. A bulldog clip was added to the extension piece to facilitate the attachment of the fibre to the upper fixture. The rate of extension of the upper fixture was 40 mm min^{-1}. The effective peeling distance was 20 mm for each sample. The use of this assembly resulted in minimum change in peeling angle, while allowing the use of simple screw side-action grips to attach the samples to the test frame. The lower fixture kept the stem in a fixed horizontal position with the aid of rubber attached to its surface. The contact point between the bulldog clip and the fibre was coloured with ink to ensure that any slippage would be detected and the test was discarded if necessary.

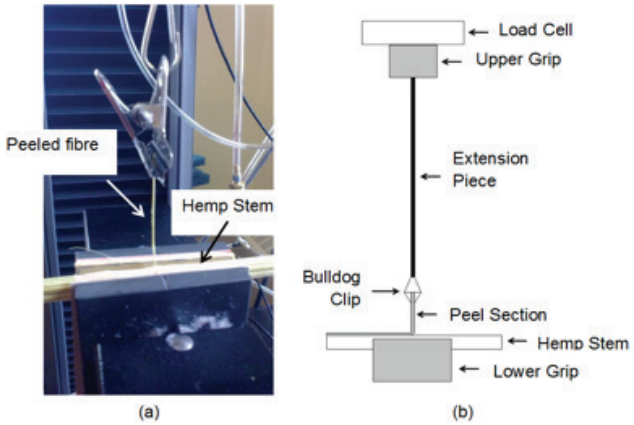


Fig. 4. Peel test assembly: a) Actual peel test assembly and b) Simplified diagram.

Measurements and data analysis The force against displacement data from the peel test were recorded with an interfaced computer. The average peeling force was determined as the average of the peel force between 5 and 15 mm of displacement expressed in N, which ensured that the peeling force had stabilized after the characteristic initial peak in force. The work required to peel the fibre from the core, W_p, was calculated, in J m^{-2}, from the experimental data as:

$$w_p = \frac{R_e x_e}{A} \quad (1)$$

where R_e is the average force required to peel the fibre from the core, x_e is the experimental peeling distance, and A is the surface area of the peeled section of fibre. The data was examined using an analysis of variance fitted to a generalized linear model (GLM) of the Statistical Analysis System (SAS 9.1) computer package.

Stochastic model of fibre peeling

The application of two mathematical principles, the Ising model and a Monte Carlo simulation, dictated the overall behavior of the stochastic model. The Ising model defined the distribution of the internal energy of the

modeled hemp stem. The proposed model scenarios – including fibre breaking, fibre debonding, and core pull-out – were based on the energy difference between each change in state. The Monte Carlo simulation had the capacity of appropriately determining which scenario will manifest itself during the peeling process.

Energy determination The fibre and core components were represented by the Ising model as subsystems bearing two interchangeable configurations, bonded or debonded, between adjacent components. The components of the system were discretised as cells representing individual subsystem regions. The position of the subsystem regions was arranged in a two-dimensional structural framework. Figure 5 represents the cross-section of a hemp stem along the axial direction, where the state of individual cells was stored in an *nxn* matrix in which *n* was equal to 20. The arrangement of the actual system was assigned an *n* value equal to 400 to increase the resolution of the model as well as to provide enough peeling length later on the model. The cells within the proposed system could be filled with three possible states: empty, filled by fibre or filled by core. Fibre and core shall not simultaneously occupy any individual cell at any given time. Hence, allowing the assignment of only one state per cell (i.e core, fibre, or empty).

The model incorporates three important properties involved during the peeling process: the tensile strength of the fibre, the strength of the core and the strength of the fibre-core interface. The change in the internal energy (dE) of the system was described as:

$$dE = \sum e_i \, dm_i + \sum m_i \, de_i = dH + W \quad (2)$$

where e_i is the internal energy of given cell i, m_i is the number of subsystem having internal energy e_i, dH is the change in the Hamiltonian, and W is the extrinsic work done to the system. The internal energy of the system can be altered by either the change of state of e_i or the rearrangement of m_i during the peeling process. The Hamiltonian, dH, represents the summation of the interactions between each cell and its nearest neighbours. The change in energy due to extrinsic work (W) done to the system is representative of the applied peeling force.

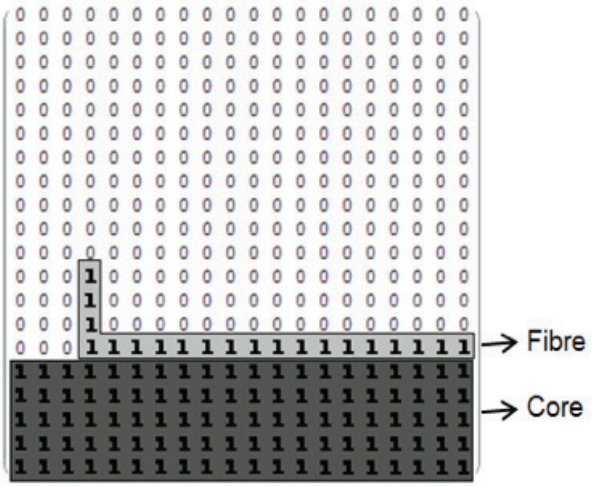


Fig. 3 Sample discretization of fibre and core components (n=20).

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 ($C_i = 0$); and (iv) c_i = Core cell i is bonded to adjacent core ($c_i = 1$) or not ($c_i = 0$). The energy of the system (H) can be expressed for each single cell i as:

$$H = -T \sum_{j}^{cn} F_i F_j S_{ij} - U \sum_{j}^{cn} C_i C_j S_{ij} - G \sum_{j}^{ct} (f_i c_j + c_i f_j) S_{ij} \quad (3)$$

where the first term in the right hand side of Eq. 3 represents the tensile strength of the hemp fibre, where: T denotes 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 cells i and j. The second term denotes 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. The last term denotes 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, which is bonded to the fibre, only the second term inside the brackets has nonzero values. Another feature shown in Eq. 3 is the fact that G is no longer in effect after debonding occurs from the fibre cell ($f = 0$).

The expression for the interaction area, S_{ij}, is determined under the assumption that fibres are shaped as cylinders (Eichhorn et al. 2001). The diameter of each fibre bundle is approximated to be 0.15 mm (Khan et al. 2011). The interaction area at the fibre-core interface was modelled as half the surface area of a cylinder with both diameter and length equal to the fibre diameter d. Interaction areas at connecting fibre-fibre or core-core cells were modelled as circles of diameter d. These interaction areas were then multiplied by the number of fibre bundles to account for the peel thickness. The number of fibre bundles per peel, b, is a unitless constant determined by both the approximate diameter of the bundles and the peel. The width of the peeled fibre is 2 mm. Therefore, the value of b was equal to 13.3 fibre bundles per peel.

$$S_{ij} = \begin{cases} b\frac{\pi d^2}{2} & (\text{cell } i \text{ is above or below cell } j) \\ b\frac{\pi d^2}{4} & (\text{cell } i \text{ is directly connected to cell } j) \end{cases} \quad (4)$$

Fibre peeling simulation 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

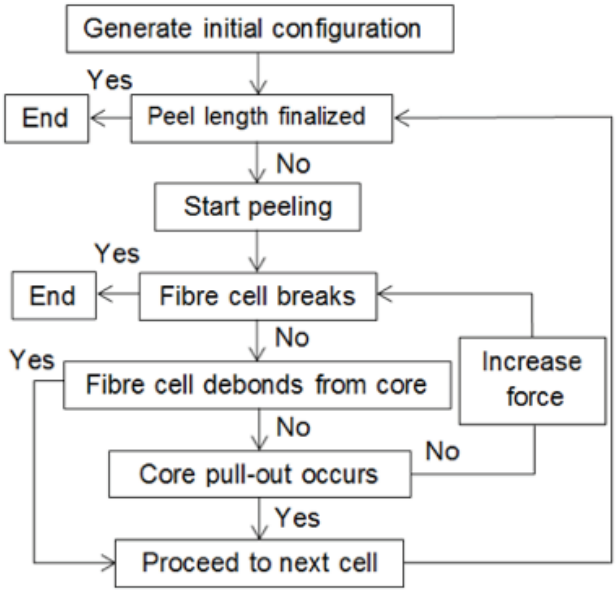


Fig. 6. Computer model flow chart.

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 written as:

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

where H_1 and H_2 represent the internal energy of the system at different states, R is the peeling force, and x_s is the peeling distance for each step. The peeling distance for each step was assigned the same value as d (i.e x_s=d=0.15mm). The product of R and x_s is the work done to the system by peeling force.

Using the Monte Carlo method requires calculations to rely on repeated random samplings to determine the outcome of the model. Each step in the calculation of energy difference, for a given cell *i*, involves the use of a probability distribution. The probability, P, of change in the system from one state, E_1 to another, E_2, is calculated by using the Metropolis function (Yeomans 1992) given by:

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

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 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 $r < P\mathrm{r} < \mathrm{P}$. 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. In the case of fibre debonding, the energy of the bonded state (E_1) will always have a larger magnitude than the energy of the debonded state (E_2); the energy of the bonds in E_1 is no longer present in E_2. Other changes in state, such as fibre breaking and core pull-out, behave in a similar fashion. 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 that is large enough to generate a state change. The effect of thermal perturbation is reflected through the thermodynamic constant, β, and is assigned a constant value of 0.008 at room temperature as prescribed by Zhong et al. (2004). This value could be adjusted to account for thermal fluctuations, but the contribution of thermal energy to the current simulation is insignificant. Figure 6 summarizes flow of the main modules of the implemented simulation program.

RESULTS AND DISCUSSION

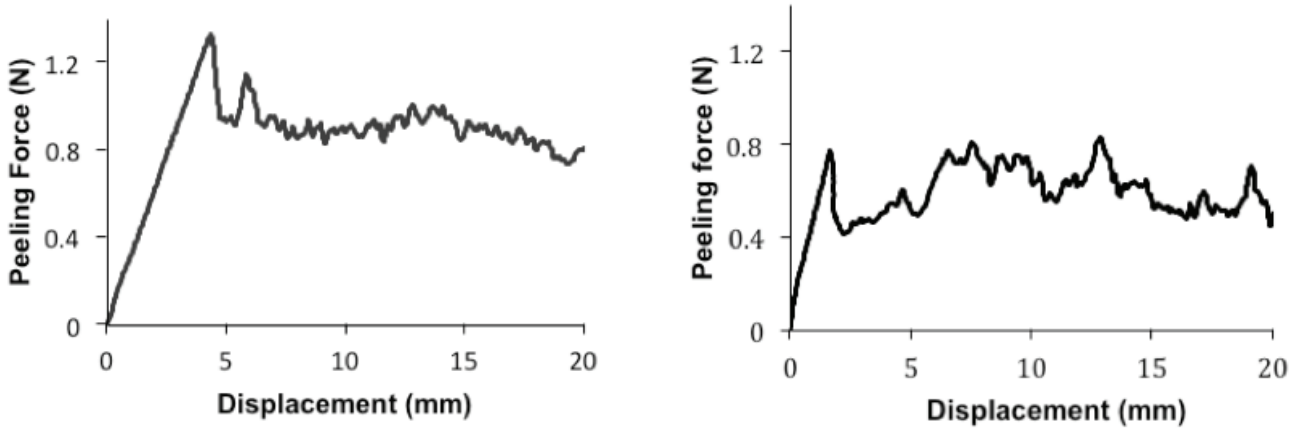
Peeling test

Force-displacement curves The oscillation patterns of the peel force versus displacement curves varied for all samples independently of hemp variety and retting conditions. Most samples of both varieties behaved in a similar pattern but varied in the magnitude of the average peeling force. The peeling force reached a peak value approximately between 0 and 5 mm of displacement. Subsequently, the load oscillated about an average value until the test was completed. The load oscillations varied in their range for the different samples; some samples produced curves with fairly small oscillations about the average value of the peel force (Fig. 7a), while others observed an oscillation behaviour consisting of larger oscillations about the average value of the peel force (Fig. 7b).

Peeling force and work Results for each hemp variety showed that the peeling force was significantly different from one another (Fig. 8a). However, retting for a period of three weeks did not yield significantly different peeling force when compared to the samples that were unretted. The average peeling force for the Alyssa variety was 0.37 ± 0.25 N and 0.41 ± 0.23 N for unretted and retted samples, respectively. The USO 14 variety had larger average peeling forces, with values of 0.86 ± 0.51 N for unretted samples and 0.87 ± 0.59 N for retted samples. Similarly, the peeling work was significantly different between the hemp varieties, but not between the retting conditions (Fig. 8b). 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 two retting conditions, resulting in 428 ± 256 J m^{-2} and 433 ± 292 J m^{-2} for unretted and retted samples, respectively. This range of values was comparable to that (100 and 400 J m^{-2}) obtained by Booth et al. (2004).

Simulation results

Model behavior Preliminary tests were performed on the model to determine whether the simulation was behaving as expected using different magnitudes for the coefficients of the internal energy constants of F, U and G. For scenario (a), the fibre and core were strong enough to allow for clean peeling (Fig. 9). For scenario (b), the



(a) **(b)**

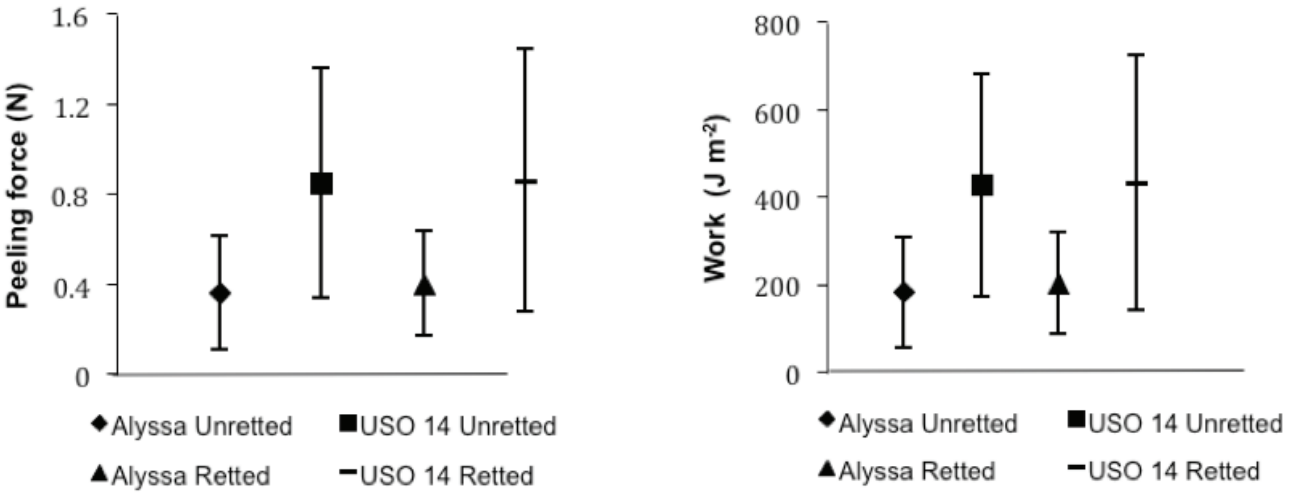
Fig. 7. Observed behaviour of mechanical test: a) small oscillation range; b) large oscillation range.

fibre-core interface is significantly stronger than the cohesive energy of the core-core interface, which resulted in some of the core material to be peeled off in conjunction with the fibre. For scenario (c), the fibre itself was too weak to withstand peeling, which resulted in the fibre breaking before the peeling could occur. The model behaved as expected for each scenario.

Simulated peeling forces The peeling force versus displacement curves for each scenario are shown in Figs. 10a, b and c. The output for scenario (a) produced load oscillations about an average value, which behaved similarly to a mechanical peel test. The output for scenario (b) resulted in load oscillations similar to (a), but with a larger average value of the peeling force. Scenario (c) shows how the peeling force increased until the fibre breakage occurred and no force was recorded afterwards.

Model parameter adjustment The results of the peeling test were used to determine the parameters, T, U and G for hemp. As only one parameter could be determined, one had to make assumptions for the other two parameters. The only form of peeling observed during the peeling test was the behaviour described as scenario (a), clean peeling, therefore, the coefficients of cohesive energy for the fibre, T, and core, U, were assigned a large value of 1000 J m^{-2}. This value serves the purpose of ensuring that neither fibre breaking nor core pull out will occur as the simulation took place. With this assumed value for T and U, the value of G was determined through matching the average forces measured in the peeling tests and those simulated using the model.

Since the available data for the peeling test did not yield differences between retting conditions, the value of G was only adjusted to account for differences between hemp varieties. Through trial and error, the G values of 352 and 200 J m^{-2} resulted in the best match between the measured and simulated forces for USO 14 and Alyssa

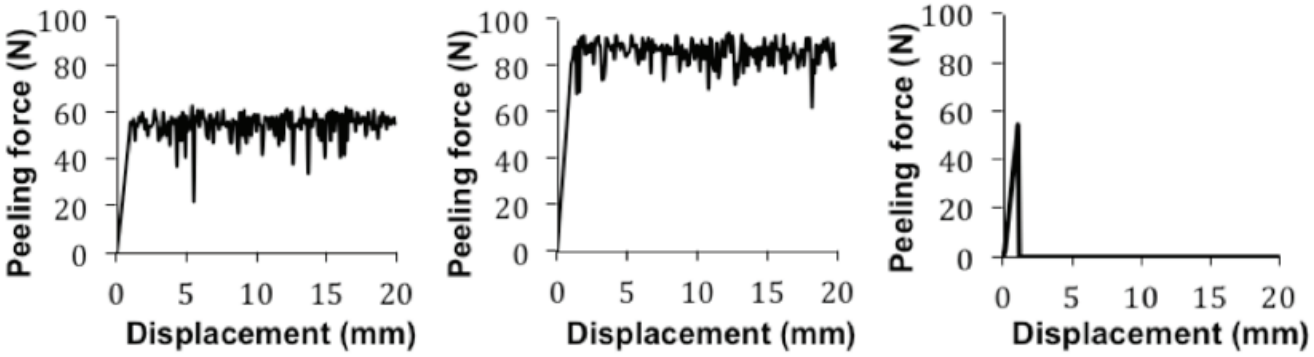


(a) **(b)**

Fig. 8. Summary of peeling test results with SD: a) Average peel force and b) Average work to peel.

(a) (b) (c)

Fig. 9. Computer model sample output: (a) F=50, U=15, G=20; (b) F=50, U=2, G=20; (c) F=10, U=15, G=20.



(a) (b) (c)

Fig. 10. Simulated peeling forces for different scenarios: (a) F=50, U=15, G=20; (b) F=50, U=2, G=20; (c) F=10, U=15, G=20.

respectively. With these coefficients of adhesive energy, the resulting output of the stochastic model is presented in Fig. 11. The stochastic model produced average peel forces of 0.86 N for USO 14 and 0.39 N for Alyssa.

Overall, the results of the stochastic model for fibre peeling were in accordance with the analysis of the peeling test, which further validated the application of the proposed method. Future research could potentially investigate magnitudes for the input parameters for a larger array of varieties and retting conditions. This would provide industry and researchers additional tools to compare the energy requirements of hemp-fibre separation as well as benefit the future design of decorticators for hemp. The versatility of this method could potentially be applied in researching energy requirements for peeling other types of natural fibres, such as flax, or to create mathematical models describing the energy required to break bonds uniting natural fibres to resins in a pull out test.

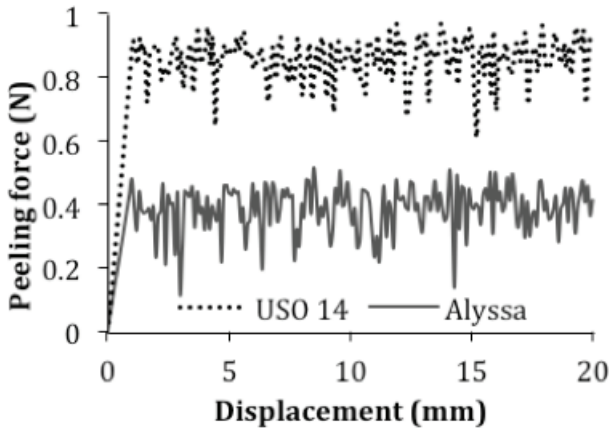


Fig. 11. Stochastic model peeling force output.

CONCLUSION

The peel test evaluating the strength required to separate the hemp fibre and core components was successfully conducted. The peeling forces and work required to peel hemp fibre were significantly different between the two hemp varieties tested, but not between the retting and unretting conditions. The average peeling force of fibre was 0.39 ± 0.24 N, for Alyssa, and 0.86 ± 0.55 N, for USO 14. The proposed stochastic model was accurate in describing the behaviour observed during the peel tests, where the peeling force reached a peak value followed by a load oscillation approximate to an average value until the test was completed. Model parameters can be easily adjusted to model peeling of different hemp varieties and retting conditions. Additionally, this approach could potentially be applied to describe other material behaviours under conditions similar to those observed in a pull out test.

ACKNOWLEDGEMENT

The Strategic Grants Program of the Natural Sciences and Engineering Research Council of Canada (NSERC) financially supported this work.

LIST OF SYMBOLS

W_{ept} = Experimental work to peel (J m^{-2})
R_e = Average force (N)
X_e = Peeling distance (m)
A = Area of Peel (m^2)
E = Internal energy of the system (J)
e_i = Internal energy of cell i (J)
m_i = Number of subsystems with internal energy e_i
H = Hamiltonian (J)
W = Extrinsic work (J)
F_i = Fibre cell i
f_i = Fibre cell i bond status
C_i = Core cell i
c_i = core cell i bond status
T = Cohesive energy between fibre cells (J m^{-2})
U = Cohesive energy between core cells (J m^{-2})
G = Adhesive energy between fibre and core (J m^{-2})
S_{ij} = Interaction area between cells i and j (m^2)
b = Number of fibre bundles per peel
d = diameter of fibre bundle (mm)
R = Tensile force (N)
X_s = Simulated peeling distance per step (mm)
P = Probability of state change in the system
r = Random number
β = Thermodynamic constant (kJ $mol^{-1}K^{-1}$)

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