A methodology of calibrating flexible fibers in the discrete element method for simulating wheat straw shear

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A methodology of calibrating flexible fibers in the discrete element method for simulating wheat straw shear

by

Matthew Schramm

A dissertation submitted to the graduate faculty
in partial fulfillment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

Major: Agricultural and Biosystems Engineering

Program of Study Committee:
Mehari Z. Tekeste, Major Professor
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The student author, whose presentation of the scholarship herein was approved by the program of study committee, is solely responsible for the content of this dissertation. The Graduate College will ensure this dissertation is globally accessible and will not permit alterations after a degree is conferred.

Iowa State University
Ames, Iowa
2019

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DEDICATION

To my family and friends who cheered me on and told me that I would be able to complete this dissertation. To my family and friends who are no longer with us. To Brittany who showed love and great patience with me.
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ABSTRACT

A methodology for calibrating flexible fibers for use in discrete element method (DEM) simulations was developed, specifically for crop-machine simulations of wheat straw. The calibration procedure utilized three different tests, the cantilever beam test, the 3-point-bending test, and the uniaxial compression test. The calibration was validated with the direct shear test. The cantilever beam test and 3-point-bending test were utilized together to determine the Poisson’s ratio and the bond damping coefficient, while the uniaxial compression test determined the contact Young’s modulus, bond Young’s modulus, and particle-particle friction parameters.

To determine the calibration value of each particle parameter, surrogate models were developed by performing a simulated design of experiment (DOE) for each of the calibration simulations. The surrogate models were developed by fitting linear models to a specific output of a simulation that can be measured in a laboratory, given specific input DEM parameter values. The surrogate model for the cantilever beam test found a direct relationship between the global damping coefficient (how quickly a fiber loses its energy) and the local bond damping coefficient (the coefficient used in the DEM simulations that removes energy from a bond between two spheres). A direct relationship between the square root of the bond Young’s modulus and the frequency of oscillation of the fiber was also found. The surrogate models found from the cantilever beam tests were then used to find the DEM bond Young’s modulus and DEM bond local damping coefficient parameters that would reproduce a specific oscillation frequency and global damping value as a validation step. The validation simulation produced local bond damping coefficient and oscillation frequency values with percent errors of 0.9% and 1.8% respectively.
The 3-point-bending calibration test yielded a single surrogate model that related the calculated Young’s modulus strongly with the bond Young’s modulus and weakly with the Poisson’s ratio. With only a single equation, there exists infinitely many solutions due to the two free parameters of bond Young’s modulus and Poisson’s ratio. As this model incorporates the bond Young’s modulus, the surrogate model obtained from the cantilever beam test can be used in conjunction with the model obtained from the 3-point-bending test to obtain unique solutions. Using the surrogate model, obtained from the 3-point-bending test, to find the DEM parameters, a simulation of the 3-point-bending was performed to try to recreate the mean Young’s modulus result from the laboratory tests. The simulation was able to reproduce the mean calculated Young’s modulus, which was estimated from 3-point bending test, with a percent error of 3.11%.

To obtain bulk properties, the uniaxial compression test was used to create the surrogate models. Surrogate models were produced for each of three plunger sizes with diameters of 50 mm, 150 mm and 255 mm in which a specifically sized plunger was lowered onto a bed of fibers. The validation step for the uniaxial compression simulation and the overall validation utilizing the direct shear test, only the surrogate model for the 225 mm plunger was used. The surrogate models related the force on a plunger with the depth of the plunger insertion, bond Young’s modulus, contact Young’s modulus, and the particle-particle friction. Using the surrogate model to reproduce the mean forces obtained from the laboratory uniaxial compressions tests, a max percent error of 25% was found. The surrogate model over predicted the force versus displacement curve but was able to reproduce the overlying shape of the curve.

Having all the surrogate models, the direct shear test was used to validate the DEM methodology. The laboratory direct shear tests were done at three different normal stresses with three replicates at each normal stress while the simulation was done at eight different normal
stress. The values that the simulation was attempting to reproduce were the internal friction angle and the apparent cohesion. There was no evidence of a statistical difference between simulation and laboratory of either the internal friction angle or the apparent cohesion at a 95% confidence interval. This shows that the DEM methodology for calibrating DEM flexible-fiber of wheat straw was successful and can be applied to simulate crop (wheat straw)-machine simulations.
CHAPTER 1. GENERAL INTRODUCTION

The agricultural manufacturing industry is constantly looking for ways to better improve their crop processing machines, by either being able to improve the performance of current products, or by innovating new equipment. With the availability of lower cost and more powerful computers, simulation-based analysis utilizing computer aided engineering tools, offers enormous opportunities to accelerate the design of products and reduce physical prototyping. To ensure effective use of DEM tools, it is essential to properly characterize and understand the dynamic processes of crop-to-machine systems.

Equipment such as combines and hay and forage harvesters interact with different types of biological materials from flexible fibers (e.g., silage, and wheat straw) to rigid granular particles (e.g., corn, soybeans, and wheat grain) during crop gathering, threshing, separation, and handling processes. Broadly, the simulation of crop materials can be classified as particulate granular flow and dynamic crop-machine processing during which the crop is engaged in bending, cutting, frictional resistance, compression, and aero-dynamics separation (Srivastava et al., 1993; Miao et al., 2014).

Over the last decade, numerous studies have been conducted to model rigid-granular particles such as corn and soybeans, and successfully simulate crop processing systems, such as screw augers and hopper flow (Srivastava et al., 1993; Mousaviraad et al., 2016). However limited studies are available to develop models of flexible fibers, which are needed to model a wide range of materials ranging from silages, crop chops, crop stalks, and wheat straw. Such models are needed to simulate the flexible fiber crop-to-machine interaction (Miao et al., 2014) including processes such as the cutting of stems, transportation of stems via a conveyor or auger,
compression of stems, and grain separation from stems (Lenaerts et al., 2014; Nilsson 1999a; Nilsson 1999b; Miao et al., 2014; Peisong et al., 2008; Kovacs et al., 2018).

Model types include empirical models in which a surrogate model of the underlining physics is created through repeated tests, and numerical simulation based models that include models based on the finite element method (FEM), discrete element method (DEM), and computational fluid dynamics coupled with DEM (CFD – DEM). A surrogate model attempts to describe the output of a “black box function” given the inputs to the “black box function”. A “black box function” can be any processes (in this dissertation it will refer to a DEM simulation) that has a measurable response given specific inputs. It is not surprising that numerical based methods are more commonly used with improvements in computational capabilities.

Computational physics allows users to gain a better understanding of the underlying physics of a system. While FEM-based simulations can be used to model a single piece of straw, it cannot handle multiple fibers traveling through a system as FEM assumes the media being simulated is part of a continuum. While a DEM simulation software allows a user to simulate thousands of pieces of straw in a system. To better understand the interactions between a system and the material a user can run CFD – DEM simulations to compute the effect that a fluid has (CFD) on a wheat straw (DEM). With these simulations, accurate micro-mechanical properties of the material of interest must be determined.

The overall goals of this dissertation are to: 1) perform a thorough literature review of physics-based modeling techniques to simulate flexible particles, 2) develop a testing methodology required to characterize the physico-mechanical properties of flexible fiber, and 3) develop robust physics-based calibration of the constitutive relationships between forces and dynamics of particle behaviors. With the development of validated flexible particle models, the
methodology can be integrated into simulation-driven product engineering design and verification of new and better crop processing equipment systems.

**Introduction to the Discrete Element Method**

The discrete element method (DEM) is known as a meshless solver in which the user does not need to define a mesh over the domain to solve their problem. This fact differs DEM from both the finite element method (FEM) and finite volume method (FVM) in which the solvers require a mesh and the meshing of a system has a direct result on the outcome of the simulation. DEM was developed by Cundall and Strack (1979) to model the stresses inside a sample of sand. Analytical models predicted non-linear and hysteretic stress-strain behavior (Deresiewicz, 1958) but the approach was restricted to a cubic array of spheres with uniform size. While DEM would allow for the simulation of non-uniform spheres in more natural assemblies (randomly arranged structure).

DEM is implemented in both open source and commercial software products. One of the open source DEM software is called LIGGGHTS (LAMMPS Improved for General Granular and Granular Heat Transfer Simulations; which was implemented by DCS Computing Industriezeile 35, 4020 Linz, Austria). LIGGGHTS is built on top of another open-source DEM code, LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) which has been used to simulate molecular dynamics.

DEM is used to simulate the granular flow of simple numerical geometries, like spheres. Newton’s Second Law is applied to each particle in a collection of particles (Equations 1.1 and 1.2, for sake of clarity, particles will be assumed to be a sphere). For a collection of \( n \) particles, for each particle \( i \), the following relationships are used to update the particle’s position and velocity.
Where \( i \) is an index ranging from 0 to \( n \), \( M_i \) is the \( i \)th mass of a particle, \( \ddot{x}_i \) is the \( i \)th particle’s acceleration vector, \( F_i \) is the summation of all force vectors acting on the \( i \)th particle, \( I_i \) is the \( i \)th moment of inertia of a particle, \( \ddot{\theta}_i \) is the \( i \)th particles angular acceleration vector, and \( T_i \) is the summation of all torque vectors acting on the \( i \)th particle. Forces include sphere-sphere contacts (spheres colliding with another sphere), sphere-geometry contacts (sphere colliding with geometry walls), external forces (gravity, magnetic fields, air drag, etc.), cohesion/adhesion (a force that tends to keep in contact with other spheres and/or the geometry), and bond forces (forces that allow spheres to act as a mega-particle). Torques are applied to spheres either by the model itself like the bond model in which torques describe how the bond twists and bends, or by the contact model projecting the tangential force to the contact and calculating the cross product between the forces and the unit vectors and scaling by the distance to the contact. The system can now step through time utilizing an ordinary differential equation solver (ODE).

LIGGGHTS runs a simulation by first reading in an input file by the user that initializes the system geometry, particle shape(s), physics models, and the material properties. Physics updates are done by utilizing the symplectic ODE solver, the verlet update. This is a special solver that tries to maintain the energy in a system. A half step in time on the particle’s velocity is performed followed by a full step in time to estimate the particle’s new positions. Given these new positions, a neighbor search is performed to determine which particles will interact with other particles. Given these new neighbors, new forces and torques are found per sphere. Given these new forces, a final half step in time is performed on the particle’s velocity. This process continues until the simulation reaches the end time defined in the input file (Figure 1-1).
Figure 1-1: Flow chart of a DEM simulation in the software LIGGGHTS.
DEM Particle-Particle Contact Constitutive Laws

When Cundall and Strack (1979) introduced DEM, the first approximations of granular materials were introduced. The original contact normal force models the force between two spheres (i and j) was approximated as a linear spring (Equation 1.3).

\[ \mathbf{F}_{c,n(i,j)} = K_n \delta_{n(i,j)} \]  

(1.3)

Where

- \( \mathbf{F}_{c,n(i,j)} \) is the (c)ontact (n)ormal force vector between sphere i and sphere j
- \( K_n \) is the normal stiffness
- \( \delta_{n(i,j)} \) is the normal overlap vector between sphere i and sphere j

The normal overlap is the distance between the sphere centers of i and j minus the radii of i and j. This normal force model was later improved upon by the non-linear Hertzian theory model (Di Renzo, 2004) (Equation 1.4) that better approximated the force relationship between two spheres. The model contains a normal and tangential spring dampener system in which the coefficients are calculated from a non-linear equation (Equation 1.4, Equation 1.7, Equation 1.11, and Equation 1.14). Friction is also modeled in the tangential direction (Figure 1-2). It is important to remember that while some of the parameter names correspond with physical names (Young’s modulus, Shear Modulus, Poisson’s ratio), these values may not be the DEM parameter values used in a simulation.
Figure 1-2: The normal and tangential force model representation between two spheres.

\[
F_{c,n(i,j)} = \frac{4}{3} E^* \sqrt{R^*} \delta_{n(i,j)}^2
\]

\[
\frac{1}{E^*} = \frac{1 - \nu_i^2}{E_{c,i}} + \frac{1 - \nu_j^2}{E_{c,j}}
\]

\[
\frac{1}{R^*} = \frac{1}{R_i} + \frac{1}{R_j}
\]

Where

- \( E^* \) is the effective Young’s modulus between the two spheres
- \( E_{c,i} \) and \( E_{c,j} \) is the contact Young’s modulus from sphere i and sphere j respectively
- \( \nu_i \) and \( \nu_j \) is the Poisson’s ratio of sphere i and sphere j respectively
- \( R^* \) is the effective radius of the spheres in contact
- \( R_i \) and \( R_j \) is the radius from sphere i and sphere j respectively

Equation 1.4 defines a modified non-linear spring while Equation 1.7 defines the (d)amping (c)ontact (n)ormal force vector between sphere i and sphere j \( (F_{c,n(i,j)}^d) \).
\[ \mathbf{F}^d_{c,n(i,j)} = -2 \sqrt{\frac{5}{6}} \beta_c S_n M^* \dot{x}_n \]  
\[ S_n = 2 E^* \sqrt{R^* \delta_{n(i,j)}} \]  
\[ \beta_c = \frac{\ln(e)}{\sqrt{\ln(e)^2 + \pi^2}} \]  
\[ \frac{1}{M^*} = \frac{1}{M_i} + \frac{1}{M_j} \]

Where

- \( \beta_c \) is the contact damping coefficient
- \( S_n \) is the normal stiffness
- \( M^* \) is the effective mass between the two spheres
- \( \dot{x}_n \) is the relative normal velocity vector between sphere i and sphere j
- \( e \) is the coefficient of restitution between sphere i and sphere j

With Equations 1.4 and 1.7, the normal contact force between spheres is defined. However, additional information is needed for the tangential forces that also produce torques on the spheres.

The tangential forces are approximated by utilizing a simplification of the Mindlin-Deresiewicz theory (Mindlin, 1949; Mindlin and Deresiewicz, 1953) (Equation 1.11). This simplification is often used in DEM simulation software, like EDEM (DEM Solutions Ltd., 2004) and LIGGGHTS (Kloss et al., 2012).

\[ \mathbf{F}_{c,t(i,j)} = S_t \delta_t \]  
\[ S_t = 8G^* \sqrt{R^* \delta_n} \]
\[
\frac{1}{G^*} = \frac{2(2 - \nu_i)(1 + \nu_i)}{E_{c,i}} + \frac{2(2 - \nu_j)(1 + \nu_j)}{E_{c,j}}
\]  
(1.13)

Where

- \( F_{c,t(i,j)} \) is the contact tangential force vector
- \( S_t \) is the tangential stiffness
- \( G^* \) is the effective shear modulus between the two spheres
- \( \delta_t \) is the tangential overlap vector between sphere \( i \) and sphere \( j \)

Tangential contact damping is defined by Equation 1.14.

\[
F_{c,t(i,j)}^d = -2 \sqrt{\frac{5}{6}} \beta_c \sqrt{S_t M^*} \dot{x}_t
\]  
(1.14)

Where \( \dot{x}_t \) is the relative tangential velocity between sphere \( i \) and sphere \( j \). Given the tangential forces, the torques that are placed on a sphere can be calculated. It should be noted that additional normal and tangential models exist like the Edinburgh, Hooke, Hooke hysteresis, Luding, Thornton models (Kloss et al., 2012). Given the contact equations, the variables that are needed to define the simulation are a sphere’s Poisson’s ratio, Young’s modulus, and the coefficient of restitution between two spheres.

**DEM Particle-Particle Bond Constitutive Laws**

To create a flexible fiber in DEM a “bond” must be created between spheres to form a mega-particle (multiple spheres bonded together in a line). While it is possible to model a cylinder in LIGGGHTS (superquadratic particles), these particles do not allow bending. The bond force and torque equations are based on Potyondy and Cundall’s (2004) work in which they defined a bond to model cemented rock (Equations 1.15 – 1.20).
\[ F_{b,n} = K_{b,n} A_b \delta_{n,b} \]  
(1.15)

\[ F_{b,t} = K_{b,t} A_b \delta_{t,b} \]  
(1.16)

\[ M_{b,n} = K_{b,t} I_p \theta_{n,b} \]  
(1.17)

\[ M_{b,t} = K_{b,n} I \theta_{t,b} \]  
(1.18)

Where

- \( F_{b,n} \) is the bond normal force vector
- \( F_{b,t} \) is the bond tangential force vector
- \( M_{b,n} \) is the bond moment normal vector
- \( M_{b,t} \) is the bond moment tangential vector
- \( A_b \) is the bond cross sectional area with radius = \( \lambda \) \( \min(R_i, R_j) \)
- \( \delta_{n,b} \) is the change in the normal distance between spheres since bond creation
- \( \delta_{t,b} \) is the change in the tangential distance between spheres since bond creation
- \( \theta_{n,b} \) is the change in the normal angle between spheres since bond creation
- \( \theta_{t,b} \) is the change in the tangential angle between spheres since bond creation
- \( I_p \) is the moment of inertia
- \( I \) is the polar moment of inertia
- \( l_b \) is the length of the bond at bond creation

\( \lambda \) is used as a multiplier to adjust the effective radius of the bond to change the stiffness coefficients. For this research, \( \lambda \) was set to one so it did not change how the bond stiffness
coefficients are calculated. Due to the difficulty in tracking the overall changes in relative position and relative angles between bonded spheres, it is common to rewrite Equations 1.15 – 1.18 with Equations 1.21 – 1.28. This representation comes at the cost of increased numerical errors as rounding errors can cause the appearance of plastic deformation in the bond when none exists.

\[
\begin{align*}
\delta F_{b,n,i} &= K_n A_b \dot{x}_n \Delta t \\
\delta F_{b,t,i} &= K_t A_b \dot{x}_t \Delta t \\
\delta M_{b,n,i} &= K_t I_p \dot{\theta}_n \Delta t \\
\delta M_{b,t,i} &= K_n I \dot{\theta}_t \Delta t \\
F_{b,n} &= \sum_{\forall i} \delta F_{b,n,i} \\
F_{b,t} &= \sum_{\forall i} \delta F_{b,t,i} \\
M_{b,n} &= \sum_{\forall i} \delta M_{b,n,i} \\
M_{b,t} &= \sum_{\forall i} \delta M_{b,t,i}
\end{align*}
\]

The bond damping equations used in this manuscript are defined by Equations 1.29 – 1.33 and described as linear dampeners between forces and displacements (Guo et al. 2013a).

\[
\begin{align*}
F^d_{b,n} &= 2\beta_b \sqrt{K_n A_b M^*} \dot{x}_n \\
F^d_{b,t} &= 2\beta_b \sqrt{K_t A_b M^*} \dot{x}_t \\
M^d_{b,n} &= 2\beta_b \sqrt{K_t I_p J^*} \dot{\theta}_n \\
M^d_{b,t} &= 2\beta_b \sqrt{K_n I J^*} \dot{\theta}_t
\end{align*}
\]
\[
\frac{1}{J^*} = \frac{5}{2M_i R_i^2} + \frac{5}{2M_j R_j^2}
\]  

(1.33)

Where

- \( \beta_b \) is the local bond damping coefficient
- \( J^* \) is the effective inertia of the spheres

The parameters that need to be defined for the bond equations are the bond Young’s modulus, local bond damping coefficient, bond Poisson’s ratio, and the area cross sectional area of the bond. This specific bond model was chosen due to its high accuracy in reproducing results obtained from Euler-Bernoulli beam theory (Guo et al. 2013b).

**DEM Rolling Friction Model**

Since DEM methods often utilize spheres as the material being simulated, additional forces are needed to better approximate a physical material. An example is when modeling a soybean. Soybeans are not perfectly spherical, and each have a unique “shape”. This shape resists rolling differently from one soybean to another. Rolling friction is often added to the contact forces and torques to help better describe the “shape” of the original material. In the software LIGGGHTS, there exists four rolling friction models that could be applied to a wheat straw simulation. These models include the constant directional torque (CDT) model, the elastic-plastic spring-dashpot (EPSD) model, the EPSD2 model, and the EPSD3 model (Kloss et al., 2012). The CDT model is described by Equation 1.34 while the EPSD family is described by Equations 1.35 – 1.40.

\[
M_{rf} = \frac{\mu_{rf} S_n \delta_n R^* \dot{\theta}_{shear}}{\left| \dot{\theta}_{shear} \right|}
\]

(1.34)

Where

- \( M_{rf} \) is the rolling friction moment vector
• \( \mu_{rf} \) is the coefficient of rolling friction between sphere i and sphere j

• \( \dot{\theta}_{\text{shear}} \) is the projection, from sphere i, of the relative angular velocity, between sphere i and sphere j, into the shear plane

\[
M_{rf} = M_r^k + M_r^d
\]  
(1.35)

\[
\Delta M_r^k = -K_r \Delta \theta_r
\]  
(1.36)

\[
M_r^k = M_r^k + \Delta M_r^k
\]  
(1.37)

\[
|M_r^k| \leq \mu_{rf} R^* F_n
\]  
(1.38)

\[
M_r^d = \begin{cases} 
-2 \eta_{rf} \sqrt{I_r K_r} \dot{\theta}_r & \text{if } |M_r^k| < \mu_{rf} R^* F_n \\
-2 f \eta_{rf} \sqrt{I_r K_r} \dot{\theta}_r & \text{if } |M_r^k| = \mu_{rf} R^* F_n
\end{cases}
\]  
(1.39)

\[
1 \over I_r = \left( 1 \over I_i + M_i R_i^2 + I_j + M_j R_j^2 \right)
\]  
(1.40)

Where

• \( M_r^k \) is the rolling friction moment

• \( M_r^d \) is the damping rolling friction moment

• \( K_r \) is the rolling stiffness coefficient

• \( \eta_{rf} \) is the coefficient of damping rolling friction between sphere i and sphere j

• \( I_i \) is the moment of inertia of the \( i^{th} \) particle

• \( f \) is equal to zero when the spheres are in full mobilization

The differences between the EPSD family comes down to how \( K_r \) is described. For EPSD and EPSD3, the value is described by Equation 1.41 while EPSD2 uses the value as described in Equation 1.42.

\[
K_r = \gamma_{\text{EPSD}} S_n \mu_{rf}^2 R^* R^2
\]  
(1.41)

\[
K_r = S_t R^* R^2
\]  
(1.42)
Where $\gamma_{EPSD}$ is set to 2.25 for EPSD while the user chooses this value in EPSD3.

For the purposes of simulating flexible fibers, it was assumed that the bonding of spheres together would reproduce the “shape” of the real fiber and thus chosen not implement a rolling friction model.

**DEM Cohesion**

Another way to add physics to a material to better approximate the true behavior of a material in DEM is to add an attractive force when particles are close to each other that makes it difficult for the spheres to separate. LIGGGHTS makes available two liquid bridge models (easo/capillary/viscous and washino/capillary/viscous) and two simplified Johnson-Kendall-Roberts (sJKR) models (sJKR and sJKR2) (Kloss et al., 2012). While the Easo and Washino models (Kloss et al., 2012) both model a liquid bridge, the processes are very different, and their descriptions will be skipped.

The simplified JKR methods both try to approximate the forces seen in the JKR normal contact model when the spheres are in contact ($\delta_n < 0.0$), while the full JKR method also has an attractive force when the spheres are close. The full JKR method is given by Equation 1.43 – 1.44 and replaces Equation 1.7 as the normal contact model and cohesion model.

$$F_{c,n} = -4\sqrt{\pi \gamma_{jkr} E^*} a^3 + \frac{4E^*}{3R^*} a^3$$

$$\delta_n = \frac{a^2}{R^*} - \sqrt{\frac{4\pi \gamma_{jkr} a}{E^*}}$$

Where $\gamma_{jkr}$ is the surface energy between sphere i and sphere j. The main issue when utilizing the full JKR equation, is that $a$ in Equation 1.44 must be determined. Some methods in doing this is to use a root solver and create a look-up table at the start of a simulation or to use the
complete solutions directly. To mitigate this, LIGGGHTS simply adds a value to the Hertzian normal force (Equations 1.45 – 1.46) to create the sJKR models (Kloss et al., 2012).

\[ F_{c,n} = \frac{4}{3} E^{*} \sqrt{R^{*}} \delta_{n(i,j)}^{Z} + K_{sJKR} A \]  

(1.45)

\[ A = \begin{cases} \frac{\pi (r - R_i - R_j) (r + R_i - R_j) (r - R_i + R_j) (r + R_i + R_j)}{r^2} & \text{for SJKR} \\ \frac{4 \pi (R_i + R_j - r) R^{*}}{r^2} & \text{for SJKR2} \end{cases} \]  

(1.46)

Where

- \( K_{sJKR} \) is the cohesion energy density
- \( A \) is the area of overlap between the two spheres
- \( r \) is the distance between the two spheres \( (R_1 + R_2 - \delta_n) = r \)

From Equations 1.45 – 1.46, when the distance between the two spheres is equal to the sum of their radii, the resulting force is equal to 0.0. This is not the case for the full JKR method. The simplified JKR method first requires contact between two spheres before a change in force is observed. Cohesion was not used for the study to simplify the interactions and initial characterization of the wheat straw did not demonstrate cohesive behavior.

**Calibration of DEM Parameters**

DEM calibration methodology can be defined as a systematic process whereby the material parameters of the DEM contact laws are calibrated by comparing the results from DEM simulations and physical bulk laboratory tests. The DEM simulation runs are obtained from design of experiments of DEM material parameters at multiple design points. The calibration of DEM parameters can take most of the time dedicated to a simulation, and much care must be taken to assure an accurate simulation. For granular simulations, there exists simple tests to calibrate the particles, such as the angle of repose, hopper discharge, and direct shear. The
difficulty lies in the fact that not all laboratory measured values can be directly used for the simulation. As an example, the laboratory may measure a particle density for a fiber, but this value cannot be used in simulation. The reason is that the fiber can be approximated as a hollow cylinder while a flexible fiber is made of solid spheres. Using the bulk density of the simple tests is often used as the density value in simulations.

Calibration simulations are often performed in which a variable is measured in the laboratory and the same process is duplicated inside a DEM virtual experiment. Values are compared and a calibration model for a specific test is created. These laboratory experiments and simulations are often follow the ASTM standard tests (Coetzee, 2017). However, most ASTM standards cannot be directly used for wheat straw and must be modified or new standards are required. As an example, Coetzee and Els (2009) suggests the use of a shear cell to calibrate the coefficients of friction and the particle stiffness. The hurdle here is that their measurements were for corn, a particle in which the aspect ratio is less than three. This forces the wheat straw to be cut short but long enough to get bond parameter values in addition to the particle contact parameters. Wheat straw samples preparation including cleaning and cutting of wheat straw for small size tests (such as uni-axial compression and direct shear) are very time consuming which could take many weeks to prepare for the simple tests.

References


CHAPTER 2. APPROACH TO WHEAT STRAW CHARACTERIZATION

A general characterization was done on a sample of winter wheat straw harvested from the Iowa State University research farm located in Boone IA to get a distribution of material properties. Thirty stems were selected randomly from the harvested straw. The stem’s outer layer was removed, and stem heads were removed (Figure 2-1) as these were not modeled in the simulations.

![Figure 2-1: A wheat stem before and after being processed.](image)

**Wheat Straw Physical Properties**

The mean mass of the grain heads was found to be 1.05 grams with a 95% confidence interval of 0.9 to 1.2 grams (Figure 2-3). The cleaned stems’ mean mass was found to be 0.66 with a 0.59 to 0.72 grams C.I. (Figure 2-4) and a mean length of the cleaned stem of 797.2 mm with a 765.3 to 829.0 mm C.I. (Figure 2-5). Approximating the stem as a hollow cylinder, the mean density of the stems was calculated to be between 380 and 456 Kg m$^{-3}$ (Figure 2-6). The stems were then separated into segments (Figure 2-2) at the stem nodes. Of the 30 samples, six were found to only have four segments while all other samples had five. For the stems that had only four nodes, all characteristics assigned to the first segment were not included in the analysis.
Figure 2-2: Representation of section breakdown of a piece of wheat straw.

Figure 2-3: Distribution of stem grain head mass of 30 randomly selected stems of wheat straw from Iowa State University Research Farm in Boone, IA.
Figure 2-4: Distribution of stem mass without head of grain of 30 randomly selected stems of wheat straw from Iowa State University Research Farm in Boone, IA.

Figure 2-5: Distribution of the stem length of the 30 randomly selected stems of wheat straw from Iowa State University Research Farm in Boone, IA.
Along with the full stem characteristics, segment characteristics were also found for segment length (Figure 2-7), segment density (Figure 2-8), segment diameter (Figure 2-9), and segment thickness (Figure 2-10). Utilizing these values can lead to a creation of randomized flexible fibers that can be imputed into a DEM simulation. Depending on the simulation type, different levels of detail can be utilized. When dealing with single flexible fibers a high detail fiber model can be utilized (Figure 2-11a) while a low detail fiber model (Figure 2-11b) can be used when a simulation requires many fibers. High detail fibers can be utilized to simulate cutting behaviors of a flexible fiber. However, high detail fiber models would be impracticable to simulate when many fibers are needed. This is due to the number of spheres needed and the simulation time associated with many spheres in a system. In Figure 2-11, both fibers are simulating the same characteristics, but the low detail fiber requires 111 spheres while the high detail fiber required 6366 spheres.
Figure 2-7: Histogram of length of stem by segment of wheat straw for 30 randomly selected wheat plants from Iowa State University Research Farm in Boone, IA.

Figure 2-8: Histogram of density of stem by segment of wheat straw for 30 randomly selected wheat plants from Iowa State University Research Farm in Boone, IA.
Figure 2-9: Histogram of diameter of stem by segment of wheat straw for 30 randomly selected wheat plants from Iowa State University Research Farm in Boone, IA.

Figure 2-10: Histogram of stem thickness by segment of wheat straw for 30 randomly selected wheat plants from Iowa State University Research Farm in Boone, IA.
Figure 2-11: Single fiber in low detail using 111 spheres (a) and a single fiber in high detail using 6366 spheres (b) for a wheat straw stem where the colors represent a change in fiber diameter.

**Wheat Straw Coefficient of Friction and Coefficient of Restitution Estimation**

Along with physical measurements the coefficient of friction and the coefficient of restitution were estimated for both particle-particle interactions and particle-geometry interactions. The coefficient of friction values were estimated by calculating the static friction (Equation 2.1) from an incline plane test, where the angle between the plane and horizontal would continuously increase until the straw began to slide (Figure 2-12). The inclined plane was tested for both particle-particle interactions and particle-stainless steel interactions. Both experiments used 18 different segments of straw with a mean length of 30.54 mm and mean diameter of 2.19 mm.

\[
\mu_f = \tan(\phi) = \frac{h}{L} \tag{2.1}
\]
Figure 2-12: Incline plane test to estimate particle-particle friction and particle-geometry friction.

When testing for particle-geometry interactions, some of the pieces of straw did not slide down the plane, even once the plane became vertical. This suggests that additional forces may need to be developed for simulating wheat straw in DEM. Figure 2-13 shows the results of the friction calculations with errors caused by performing the measurements. Errors were calculated by Equation 2.2.

\[ E\mu_f = \sqrt{\left(\frac{\sigma_h}{L}\right)^2 + \left(\frac{\sigma_L h}{L^2}\right)^2} \]  

(2.2)

Where

- \( \sigma_h \) is the error in measuring \( h \) (0.5 mm)
- \( \sigma_L \) is the error in measuring \( L \) (0.5 mm)
Figure 2-13: Coefficient of static friction results for particle-particle interactions (a), and particle-geometry interactions (b) of wheat straw.

The coefficient of restitution was estimated by analyzing high speed video (120 fps) and calculating the velocity of the piece of wheat straw before and after a collision of either a packed bed of straw or a piece of stainless steel. This is done by tracking the center of mass of a stem two frames before impact and the two frames after impact. Given the two frames before impact, velocity of the segment can be approximated \( v_{in} \). This can be repeated for the last two frames to get \( v_{out} \). Taking the ratio of these velocities gives the coefficient of restitution (Equation 2.3).

\[
C_r = \frac{v_{out}}{v_{in}}
\] (2.3)
The difficulty in measuring the coefficient of restitution was the high variability observed during impact of the wheat straw. This variability can be seen from Figure 2-14. Error in the measurement was calculated from Equation 2.4.

\[
E_{Cr} = \sqrt{2 \left( \frac{\sigma_{dt} v_{out} dt}{v_{in}} \right)^2 + 2 \left( \frac{\sigma_{CM} v_{out}}{v_{in}} \right)^2 + 2 \left( \frac{\sigma_{CM} v_{out}}{v_{in}} \right)^2}
\] (2.4)

Where

- \( \sigma_{dt} \) is the error in calculating the time between frames
- \( \sigma_{CM} \) is the error in determining the center of mass of a segment

Figure 2-14: Coefficient of restitution results for particle-particle interactions (a) and particle-geometry interactions (b) for wheat straw stems.
Conclusions

Experimental procedures to characterize the physical properties of wheat straw were developed. Wheat straw parameters are measured, and their statistical distributions are presented. With these distributions, randomized flexible fibers representing wheat straw DEM particle model was generated for use in DEM simulations. The coefficients of friction and coefficient of restitution from wheat straw-wheat straw interactions and wheat straw-steel interactions were successfully measured with low repeatability error.
CHAPTER 3. BOND DAMPING AND BOND YOUNG’S MODULUS ESTIMATION FOR FLEXIBLE WHEAT STRAW DEM MODEL

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Abstract

A method to calculate the local damping coefficient and the bond Young’s modulus of a flexible fiber for use in the Discrete Element Method (DEM) is proposed and validated. Segments of harvested wheat straw were clamped on one end while the other end was deflected a set distance, released, and allowed to vibrate freely. This cantilever beam motion was captured by a high-speed camera (960 fps). The red-band of the images were isolated and used to calculate the x-section height (mm) along the stem in time. This data was then fit to a non-linear function, which conforms to beam theory. The global bond damping coefficient, as a function of x-section height, was then calculated and found to be in the range of 0.5 to 0.2. The cantilever beam experiment was then repeated in the DEM software LIGGGHTS, where the wheat straw was modeled as a single line of spheres connected by stiff-flexible bonds. A Design of Experiment (DOE) was ran varying bond Young’s modulus and local bond damping (damping coefficient between spheres), to determine the linear relationships with the global bond damping coefficient (damping coefficient found from the mega-particle) and the frequency of oscillation of the DEM particle respectively. With the proposed method the DEM local bond damping coefficient and the DEM bond Young’s modulus were calibrated with relative errors of 0.9% and 1.8% respectively to laboratory estimated values. Utilizing the linear relationships found from
the DEM simulations, the bond Young’s modulus was found to be in the range of 0.42 to 4.84 GPa.

Keywords: DEM Calibration, Flexible fiber, LIGGGHTS, Discrete Element Method

Introduction

With the continued improvements in computational speed, researchers have begun to utilize simulation-based design for complex engineering problems. The Discrete Element Method (DEM) has recently been shown to be a powerful tool in simulating discrete flows of granular and fibrous systems. One of the many challenges to overcome in DEM, is the determination of the micro-interaction parameters that determine particle-particle and particle-geometry interactions. This is due to how both particles and interactions of particles are numerically approximated in the simulation. DEM codes approximate a material by a simple numerical geometric shape, commonly a sphere (e.g. soybean) or clumped/glued spheres to approximate irregular shaped particles (e.g. corn). Using these to approximate a given material, it is common to use laboratory acquired material properties as a starting point in calibrating a DEM particle model. Potyondy and Cundall (2004) provided a way to approximate rock as a dense packing of non-uniformly sized spheres bonded together. This bond model has since been extended to approximate fibrous materials (e.g. wheat straw) but provided no means of capturing the damping behavior observed in fibrous material. Using Potyondy’s and Cundall’s model as a steppingstone, multiple bond models began to be implemented by the DEM community. These models ranged from cohesion models (Wittel et al., 2006), spring and damper models (Park & Kang, 2009; Lenaerts et al., 2014), to bond elastic wave models (Guo et al., 2013a). With the additions of these bond models, a method to determine the damping coefficient has yet to be brought forward. In most of the above methods, the authors either choose an arbitrary value for
the local bond damping coefficient or tuned the coefficient until the simulation of the material matched the behavior observed in physical experiments (Lenaerts et al., 2014).

Park and Kang (2009) used a relationship including the spring coefficient and the coefficient of restitution to calculate the normal damping coefficient while the coefficient of friction is used for tangential energy dissipation. While the coefficient of restitution and friction can be measured, it is often difficult to have a flexible fiber behave in such a matter to collect reliable data. There do exist multiple sources where material properties for fibers can be experimentally estimated (Galedar et al., 2008; Adapa et al., 2010; Afzalinia & Roberge, 2007).

The objective of this study was to (1) determine global damping of wheat straw based on cantilever beam theory, (2) develop a relationship between the global damping coefficient (as measured by the entire fiber) and the local damping coefficient (as measured between two spheres) for DEM simulations, and (3) develop a relationship between the period of oscillation and the bond stiffness coefficient. By providing calibration techniques, manufacturers can run more accurate simulations to reduce the time and money associated with bringing a product to market.

**Methods and Materials**

**Data Acquisition**

Winter wheat straw were harvested from the Iowa State University Research Farm located in Boone Iowa, 50036. Individual wheat straw stems were separated from the shell and cut such that there were no samples of the wheat straw containing a node (each wheat straw was a hollow cylinder). Thirty samples of the hollow cylindrical processed wheat straw were randomly selected and cut such that a mean length of 156 mm was observed above the clamp (wire clamp) holding the stem. An aluminum pin (2.25 mm diameter) was placed inside the hollow wheat straw at one fixed end such that a wire clamp did not crimp the straw (Figure 3-1).
The wheat straw with fixed end was put on a flat plane and the other end was deflected horizontally to a mean deflection of 25 mm by hand by using the tip of a finger on the top of the straw. The straw was then released by hand immediately allowing the straw to oscillate. This oscillation was recorded by a high-speed camera (Sony NEX-FS700) at 960 frames per second (fps).

**Figure 3-1**: Schematic of laboratory test. A hollow wheat straw has an aluminum pin placed inside of it to stop crimping caused by the wire holder clamp.

**Data Analysis**

MATLAB (version R2017b, www.mathworks.com) was used to analyze the high-speed video data. The video frames were split into the red, blue, and green spectrums of light. The red band was then used to create logical video frames of the wheat straw stems during the oscillation (Figure 3-2a) as the red band provided a clearer image for analysis. The raw median of the
logical image was then used as the stem’s central location and was used to fit a second order linear model of the wheat stem position in the x-direction (Figure 3-2b). The median was used to minimize artifacts of the logical image. The linear model was used as a preliminary step to calculate the trajectory of the wheat stem as a function of stem height (x) during damping.

Figure 3-2: Logical image of wheat straw in red band (a). Second order fit of the median pixel location as a function of height of the logical image of the wheat straw (b).

The displacement of the stem was then tracked with time per stem height (Figure 3-3a) and the dataset was then trimmed to just before stem release to when the oscillation of the stem ceased (Figure 3-3b). The time axis was normalized by setting the time to zero at the moment that the stem was released and divided dividing the time by the period of the observed oscillation, and the deflection was normalized by the maximum deflection (Figure 3-3c). This was done as a preliminary step to fit the non-linear function (Equation 3.1).

\[ y(t) = b_0 e^{b_1 t} \cos(2\pi b_2 t) \]  

(3.1)

Where

- \( y(t) \) is the deflection of the stem at time equal to \( t \) at a specific height along the wheat stem
- \( b_0 \) is the initial deflection of the wheat stem
- \( b_1 \) is the global damping coefficient
• $b_2$ is the oscillation frequency

Equation 2.1 was used as it is a proposed solution to the differential equation that describes damped harmonic motion (Equation 3.2).

$$\frac{d^2y}{dt^2} + 2\zeta \omega \frac{dy}{dt} + \omega^2 y = 0 \quad (3.2)$$

Where

• $y$ is the deflection distance
• $\omega$ is the oscillation frequency
• $\zeta$ is the damping ratio

Although $\omega$ and $b_2$ both describe the frequency in which the fiber oscillates, $b_2$ can be calculated directly while $\omega$ can only be calculated knowing the bond stiffness value. Ideally, the relationship $\omega = \frac{b_2}{2 \pi}$ should hold but cannot be guaranteed.

Figure 3-3: Displacement (measured) of wheat straw at a specific height of stem (a). Dataset reduced to just before release and stem has reached equilibrium (b). Dataset normalized in both time and deflection. Time is normalized by observed period of oscillation and displacement is divided by max deflection (c).
DEM Simulation of Wheat Straw Cantilever Test

A Discrete Element Method (DEM) simulation design of experiments (DOE) was ran to investigate the DEM parameters sensitive to the cantilever test and to compare simulation to the observed wheat straw laboratory experiments. The open-source DEM software LIGGGHTS (version 3.7) (Kloss et al., 2012) was chosen to perform the DEM simulations. A modified version of LIGGGHTS developed by Richter (2015) that included the bond equations was further developed to include the bond damping equations (Equations 3.3 – 3.10) (Guo et al., 2013a). For the DEM simulation, a mega-particle comprised of 56 spheres (2.83 mm diameter) was used to represent a piece of wheat straw (Figure 3-4). This fully modified copy of LIGGGHTS gave comparable results to Guo et al. (2013b). The diameter of 2.83 mm was chosen due to the results of an earlier straw characterization sampling.

One end of the mega-particle was held fixed by a single sphere while the other end was deflected to 15mm, once the mega-particle came to rest, the deflected end was then allowed to vibrate freely for 0.01 seconds. The discrepancy between the simulation and laboratory deflection distances was to allow the simulations to finish in a reasonable amount of time. This process was repeated for eight different values of the bond damping coefficients and ten different values of bond Young’s modulus. The values, 25, 50, 75, 100, 125, 150, 175, and 200 were used in equations 3.3 – 3.10 as the DEM local bond damping coefficient ($\beta_b$), and the values 1 GPa, 2 GPa, 3 GPa, 4 GPa, 5 GPa, 6 GPa, 7 GPa, 8 GPa, 9 GPa, and 10 GPa were used for the bond
Young’s modulus, to calculate the DEM bond forces \((F_{b,n} \text{ and } F_{b,t})\) and bond moments \((M_{b,n} \text{ and } M_{b,t})\) for both normal and tangential components (Equations 3.3-3.10). Utilizing these ranges of values, a full factorial DOE was done for a total of 80 runs. Equation 3.11 is used to calculate \(K_n\) and \(K_t\).\n
\[
\delta F_{b,n,i} = K_n A_b \dot{x}_n \Delta t \\
\delta F_{b,t,i} = K_t A_b \dot{x}_t \Delta t \\
\delta M_{b,n,i} = K_t l_p \dot{\theta}_n \Delta t \\
\delta M_{b,t,i} = K_n l \dot{\theta}_t \Delta t
\]

\[
F_{b,n} = \sum_{\forall i} \delta F_{b,n,i} + 2 \beta_b \sqrt{M^* A_b K_n} \dot{x}_n \\
F_{b,t} = \sum_{\forall i} \delta F_{b,t,i} + 2 \beta_b \sqrt{M^* A_b K_t} \dot{x}_t \\
M_{b,n} = \sum_{\forall i} \delta M_{b,n,i} + 2 \beta_b \sqrt{J^* l_p K_n} \dot{\theta}_n \\
M_{b,t} = \sum_{\forall i} \delta M_{b,t,i} + 2 \beta_b \sqrt{J^* l K_n} \dot{\theta}_t
\]

\[
K_n = \frac{E}{i_b}, K_t = \frac{K_n}{2(1 + v)}
\]

Where (Guo et al. 2013a)

- \(F_{b,n}, F_{b,t}\) are the normal and tangential bond forces, respectively
- \(M_{b,n}, M_{b,t}\) are the normal and tangential bond moments, respectively
- \(\delta F_{b,n,i}, \delta F_{b,t,i}\) are the normal and tangential \(i\)th incremental bond forces caused by the linear spring, respectively
- \(\delta M_{b,n,i}, \delta M_{b,t,i}\) are the normal and tangential \(i\)th incremental bond moments caused by the linear spring, respectively
- $K_n$ and $K_t$ are the normal and tangential bond stiffness constants, respectively
- $A_b$ is the bond cross sectional area
- $\Delta t$ is the time step
- $\beta_b$ is the local bond damping coefficient
- $M^*$ and $J^*$ are the equivalent mass and equivalent moment of inertial of the particles, respectively
- $\dot{x}_n$ and $\dot{x}_t$ are the normal and tangential relative velocities between the two particles, respectively
- $\dot{\theta}_n$ and $\dot{\theta}_t$ are the normal and tangential relative angular velocities between the two particles, respectively
- $l$ and $l_p$ are the second area moment and polar area moments of inertia, respectively
- $E$ is the bond Young’s modulus
- $\nu$ is the Poisson’s ratio
- $l_b$ is the equilibrium bond length

It should be noted that there is a discrepancy between the above equations and what is found in Guo, et al (2013a). The authors chose to use a factor of 2 rather than a factor of $\sqrt{2}$ as the constant 2 more closely resembles the form of Equation 3.2.

This bond model assumes that two particles are bonded together via a spring and damper system. Guo, et al (2013b) has shown that the non-damped bonds reproduce beam behaviors as described by the Euler-Bernoulli beam equations (Guo, et al, 2013b). A shortcoming to the bond equations in the handling of damping. If the local bond damping coefficient $\beta_b$ is large, the bond equations become stiff and require very small time steps to be stable. While Guo et al. (2013b)
gave an equation to determine the time step required for a simulation, it did not include the damping coefficient.

After the DEM simulations, the global damping coefficient ($b_1$) and oscillation frequency ($b_2$) was estimated using the same process as used for the laboratory experiment of wheat straw mentioned above (Equation 3.1). Table 3-1 shows the DEM material parameters that were used for the simulations. Bond diameter and bond length were selected to be the stem’s diameter. The particle density was found from a random sample of stems utilizing the average mass and average volume (assuming the stem was a solid cylinder) of this sample. Density was then calculated taking the average mass and dividing it by the average volume. Poisson’s ratio and contact Young’s modulus were selected from literature (Hamman et al., 2005; O’Dogherty et al., 1995; Stasiak, 2003).

Table 3-1: DEM parameters for wheat stem DEM simulation

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<tr>
<th>Parameters</th>
<th>Values</th>
<th>Units</th>
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<td>mm</td>
</tr>
<tr>
<td>Bond diameter</td>
<td>2.83</td>
<td>mm</td>
</tr>
<tr>
<td>Bond length</td>
<td>2.83</td>
<td>mm</td>
</tr>
<tr>
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<td>Kg m$^{-3}$</td>
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<tr>
<td>Particle Contact Young’s Modulus</td>
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<td>GPa</td>
</tr>
<tr>
<td>Particle Poison's Ratio</td>
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<td></td>
</tr>
<tr>
<td>Time Step ($\Delta t$)</td>
<td>1.0e-10</td>
<td>Seconds</td>
</tr>
</tbody>
</table>
Results and Discussion

Laboratory Results

The mean wheat straw length was measured to be 156 mm (standard deviation of 4.5 mm), a mean diameter of 2.57 mm (standard deviation of 0.45 mm) and a mean thickness of 0.34 mm (standard deviation of 0.08 mm). The moisture content of the wheat was measured to be 5.8% dry basis. The maximum deflection of each stem utilizing the captured video was found to have a mean of 23.6 mm (standard deviation of 5.3 mm). The global damping coefficient ($b_1$) and frequency of oscillation ($b_2$) as a function of x-section stem height was then calculated for 29 samples. One test was removed due to the stem breaking during the deflection process. Figure 3-5 shows the results of the global bond damping coefficient and the observed frequency of oscillation. For the wheat stems that were tested, the global damping coefficient normalized by the max deflection of a given stem was found to have a mean value of -0.46 (standard deviation of 0.17) and the mean frequency was found to be 64.6 Hz (standard deviation of 21.2 Hz).

![Figure 3-5](image.png)

**Figure 3-5:** Histogram of observed frequencies of oscillations of wheat stems (a). Histogram of observed global bond damping coefficient of wheat straw stems normalized by max deflection (b).

Figure 3-6 displays the normalized global bond damping coefficient as a function x-section stem height and as a function of the stem’s aspect ratio. The aspect ratio was calculated by dividing
the stem length by the stem diameter. As can be seen in Figure 3-6a, there appears to be no clearly defined relationship between the global damping coefficients ($b_1$) and the stem dimensional properties. However, in Figure 3-6a, banding was observed in the form of a linear dependency if looking at an individual stem, as a function of x-section stem height. Viewing the data circled (from stem #22), the base of the stem has a damping ratio of -0.2 and linearly decreases to the tip of the stem. Aspect ratio of a stem’s length to its diameter showed no correlation to the normalized global damping coefficient (Figure 3-6b).

![Graph showing interaction of stem height on the global damping coefficient ($b_1$). Bounding is seen from stem #22 (circled) (a). Graph showing the effect of aspect ratio on the global damping coefficient (b).](image)

**DEM Simulation**

Figure 3-7a illustrates the effect of the bond Young’s modulus ($E$) on the period of oscillation of the wheat stem while Figure 3-7b illustrates the effect of the local bond damping coefficient ($\beta_b$) on the global damping coefficient ($b_1$) of the wheat stem. Both figures are using selective values as to not over saturate the figures. For Figure 3-7a a value of 150 was held constant for the local bond damping coefficient and the bond Young’s modulus was set to 1, 5, and 10 GPa. In Figure 3-7a it was observed that as the bond Young’s modulus increased, so did
the frequency of oscillation while appearing to have no effect on the global damping of the wheat stem per oscillation as the heights appeared to be similar for each plot per full cycle. This was later confirmed during model selection. For Figure 3-7b a value of 10 GPa was held constant for the bond Young’s modulus while the local bond damping coefficient was set to 25, 100, and 200. From Figure 3-7b, it was observed that as the local bond damping coefficient was increased, so did the global bond damping coefficient of the simulated wheat stem.

Figure 3-7: Plot showing the effect of selective bond Young’s modulus on the frequency of the oscillation of the fiber while holding the local bond damping coefficient at a constant value of 150 (a). Plot showing the effect of selective local bond damping coefficient on the rate of observed global damping of the flexible fiber while holding the bond Young’s modulus at a constant value of 10 GPa (b).

Figure 3-8 shows the histograms of the percent error of two linear models that predict the DEM parameters of bond Young’s modulus (Figure 3-8a) and the local bond damping coefficient (Figure 3-8b). Where the percent error was calculated by taking the difference of the laboratory measured value and the model predicted value and dividing the difference by the maximum observed laboratory value. The linear model for the bond Young’s modulus, in Pascals, can be seen in Equation 3.12 using normalized displacement and not normalized time, and the local bond damping coefficient linear model can be seen in Equation 3.13 using both normalized displacement and normalized time. Models were developed by first fitting the full
interaction linear model and then linear terms were removed utilizing a nested model selection F-test where the reduced model was rejected if the p-value was less than 0.05.

\[
\sqrt{E_b} = 574.3 \, b_2 + 91.4 \tag{3.12}
\]

\[
\beta_b = -261.4 \, b_1 + 2.5 \tag{3.13}
\]

Where \( b_1 \) and \( b_2 \) are the coefficients found using Equation 3.1 in the laboratory. Both models (Equations 3.12 and 3.13) yielded an adjusted \( R^2 \) greater than 0.99. Utilizing equation 3.12, it was found that 90% of stems maintained a Young’s modulus between 0.42 and 4.84 GPa. Using Equations 3.12 and 3.13, one can now estimate what the DEM simulation parameters. As an example, given a stem yielded a normalized global damping coefficient \( (b_1) \) of 0.64, and a frequency of oscillation \( (b_2) \) of 113.1 Hz, the estimated DEM simulation parameters will be 4.23 GPa and 164.80 for the bond Young’s modulus and local bond damping coefficient, respectively.

Running a DEM simulation of the cantilever beam using the bond Young’s modulus value of 4.23 GPa, local bond damping coefficient of 164.80 and the remaining DEM parameters in Table 3-1, the simulated wheat stem yielded an error of the frequency of oscillation \( (b_2) \) measurements of 1.8% between the simulation and laboratory, and an error 0.9% between the simulated and laboratory measured normalized global bond damping coefficients \( (b_1) \).
Figure 3-8: Absolute Error histogram of the residuals in the linear models for the prediction of the bond Young’s modulus (a) and the local bond damping coefficient (b).

Conclusions

The bond damping model as described by Guo et al. (2013a) was implemented in the DEM software LIGGGHTS. The bond DEM model was used to simulate a cantilever beam test of a wheat straw. The simulation was able to reproduce the exponential decay of the global damping $\left(b_1\right)$ that was observed in laboratory experiment. Furthermore, the simulation was able to reproduce the global bond damping coefficient that matches the observed mean local bond damping coefficients within 0.9% relative error. This was mirrored for the bond Young’s modulus with a relative error of 1.8%. With the measurement and calibration of bond damping proposed in this study, future works will be conducted to investigate how such measurements and calibration techniques can be integrated into bulk DEM simulations of flexible fibers and investigate the time step sensitivity and how it is affected by the local bond damping coefficient.

References


CHAPTER 4. CALCULATING THE BOND YOUNG’S MODULUS AND THE POISSON’S RATIO UTILIZING 3-POINT BENDING

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Modified from a manuscript to be submitted to Biosystems Engineering

Abstract

A method to determine the bond Young’s modulus and the Poisson’s ratio for use in DEM simulations is presented and validated, utilizing the 3-point-bending test. Segments of harvested wheat straw were cut and placed onto two supports and a plunger descended onto the straw segment at a velocity of 20 mm/s. The force of the plunger interacting with the straw segment was recorded. The linear portion of the data was extracted and used to calculate the Young’s modulus of the straw segment and the mean Young’s modulus was found to be in a 95% confidence interval of 2.66 and 4.87 GPa. The 3-point-bending tests were then repeated in the DEM software LIGGGHTS where the wheat straw were modeled as a stiff-flexible fiber. A design of experiment (DOE) was used to determine linear relationships between the measured Young’s modulus and the bond Young’s modulus and Poisson’s ratio from the DEM particle. From the DOE, a linear equation was found and used to validate the method utilizing the mean Young’s modulus (3.77 GPa) found from the laboratory experiments. The resulting validation simulation provided a measured Young’s modulus of 3.64 GPa resulting to a percent error of 3%.

Keywords: DEM Calibration, Flexible fiber, LIGGGHTS, Discrete Element Method, 3-Point-Bending
Introduction

As more powerful computer hardware is made available, so does the desire for manufacturers to perform simulation-based design to solve complex engineering problems. A tool that has recently been shown to be a powerful option is the Discrete Element Method (DEM) to simulate discrete flows of granular and fibrous systems. A drawback to utilizing DEM is determining the micro-interactions between particles and the geometry of the system. This limitation is caused by how the physics are approximated in DEM software. DEM approximates a material by utilizing simple numerical shapes. A popular numerical shape is a sphere. Material is then approximated by a single sphere (e.g. soybeans) or by gluing multiple spheres together to approximate irregularly shaped particles (e.g. corn). Once the shape of a particle is described, laboratory obtained material properties, (Young’s modulus, Poisson’s ratio, density, etc.), are used as a starting point to calibrate the model for use in the simulation.

A starting point to model flexible fibers came from Potyondy and Cundall (2004) in which they provided a means to simulate concrete by bonding close spheres together. From this model, multiple bond models began to be implemented by the DEM community. These models range from cohesion models (Wittel et al., 2006), spring and damper models (Park & Kang, 2009; Lenaerts et al., 2014), to bond elastic wave models (Guo et al., 2013a). With these bond models, a method to determine the bond Young’s modulus and Poisson’s ratio of the bond still needs to be investigated.

The objectives of this study were:

1) Relate the measured Young’s modulus from the 3-point-bending method to the DEM parameters bond Young’s modulus and Poisson’s ratio.

2) Validate the calibration method results with results found in lab.
Methods and Materials

Experimental Design

Winter wheat straw material were harvested from Iowa State Research Farm Boone, Iowa. Straw were hand cut at ground height from the field to minimize damage to the straw. The straw was then processed to remove the head of the straw at the top most node and the leaves (Figure 4-1).

Figure 4-1: Wheat stem before and after being processed from the Iowa State University Research Farm in Boone, IA.

Sixty samples were randomly selected from sections 2, 3, 4, and 5 of the stems (Figure 4-2) and cut to a length of 55 mm. Thirty samples were randomly selected from the sections such that they contained no nodes and 30 samples were randomly selected from the sections such that a node was included. The node was located randomly on the segment (uniformly distributed).

Figure 4-2: Representation of section breakdown of a stem of wheat straw.
Stems were cut by hand using shear cutting mechanism. Diameters of the samples were measured three times throughout the length of the stem. The diameter and thickness of the stem were measured utilizing a digital caliper. Density of each sample was then calculated by approximating the segment as a hollow cylinder. Using ASTM D 790 (2003) as a guide, samples were placed on two supports separated by 40 mm (Figure 4-3). A plunger was lowered 20 mm from an initial height just above the sample at a rate of 2 mm s\(^{-1}\). Force on the plunger and displacement of the plunger data were recorded at a 100 Hz sampling rate. The plunger speed and data collection was done by a Sintech 60|D (MTS, 14000 Technology Drive, Eden Prairie, MN USA). The supports of the 3-point structure have a diameter of 3 mm. These supports allowed the fiber to rotate but the deflection was fixed. After tests were completed, the moisture (dry basis) of the samples were recorded after leaving a sample of the tested wheat straw in an oven at 221 degrees Fahrenheit for 24 hours (ASTM, 2010).

Figure 4-3: 3-Point bending apparatus where supports are separated by 40 mm and the plunger is set to be 20 mm from a support.
DEM Simulation

A discrete element method (DEM) simulation was used to simulate a design of experiments (DOE). The DEM software used was the open-source software LIGGGHTS (version 3.7) (Kloss et al., 2012). Equations 4.1-4.9 show the equations that describe the bond interaction of a fiber.

\[
\delta F_{b,n,i} = K_n A_b \dot{x}_n \Delta t \quad (4.1)
\]

\[
\delta F_{b,t,i} = K_t A_b \dot{x}_t \Delta t \quad (4.2)
\]

\[
\delta M_{b,n,i} = K_t I_p \dot{\theta}_n \Delta t \quad (4.3)
\]

\[
\delta M_{b,t,i} = K_n I \dot{\theta}_t \Delta t \quad (4.4)
\]

\[
F_{b,n} = \sum_{\forall i} \delta F_{b,n,i} + 2 \beta_b \sqrt{M^* A_b} K_n \dot{x}_n \quad (4.5)
\]

\[
F_{b,t} = \sum_{\forall i} \delta F_{b,t,i} + 2 \beta_b \sqrt{M^* A_b} K_t \dot{x}_t \quad (4.6)
\]

\[
M_{b,n} = \sum_{\forall i} \delta M_{b,n,i} + 2 \beta_b \sqrt{J^* I_p} K_t \dot{\theta}_n \quad (4.7)
\]

\[
M_{b,t} = \sum_{\forall i} \delta M_{b,t,i} + 2 \beta_b \sqrt{J^* K_n} \dot{\theta}_n \quad (4.8)
\]

\[
K_n = \frac{E}{l_b}, K_t = \frac{K_n}{2(1 + \nu)} \quad (4.9)
\]

Where (Schramm et al. 2019)

- \(F_{b,n}, F_{b,t}\) are the normal and tangential bond forces, respectively
- \(M_{b,n}, M_{b,t}\) are the normal and tangential bond moments, respectively
- \(\delta F_{b,n,i}, \delta F_{b,t,i}\) are the normal and tangential \(i^{th}\) incremental bond forces caused by the linear spring, respectively
• \( \delta M_{b,n,i} \) and \( \delta M_{b,t,i} \) are the normal and tangential \( i^{th} \) incremental bond moments caused by the linear spring, respectively

• \( K_n \) and \( K_t \) are the normal and tangential bond stiffness constants, respectively

• \( A_b \) is the bond cross sectional area

• \( \Delta t \) is the time step

• \( \beta_b \) is the local bond damping coefficient

• \( M^* \) and \( J^* \) are the equivalent mass and equivalent moment of inertia of the particles, respectively

• \( \dot{x}_n \) and \( \dot{x}_t \) are the normal and tangential relative velocities between the two particles, respectively

• \( \dot{\theta}_n \) and \( \dot{\theta}_t \) are the normal and tangential relative angular velocities between the two particles, respectively

• \( I \) and \( I_p \) are the second area moment and polar area moments of inertia, respectively

• \( E \) is the bond Young’s modulus

• \( \nu \) is the Poisson’s ratio

• \( l_b \) is the equilibrium bond length

The DOE for the simulation looked at the bond Young’s modulus and Poisson’s ratio to capture their effect on the measured Young’s modulus of the fiber. The bond Young’s modulus varied from 1 – 10 GPa at five levels (1, 2, 3, 4, 5, 6, 7, 8, 9, and 10 GPa) and the Poisson’s ratio varied from 0.1 to 0.4 at five different levels (0.100, 0.175, 0.250, 0.325, 0.400). The overall DOE was a full factorial design leading to 25 simulations. Similar to the laboratory tests, a mega-particle DEM fiber representing a mean wheat straw fiber (obtained from the laboratory measured data), was placed onto two support structures (represented as 3 mm wide half cylinders) separated by
40 mm and a plunger (represented as a 3 mm wide half cylinder) descended onto the fiber at 2 mm s\(^{-1}\) (Figure 4-4). Table 4-1 shows the remaining constant DEM parameters that were used for the study. Particle diameter, bond diameter, and bond length were chosen to be the same as the laboratory sample’s mean diameter. Due to the plunger being in the center of two spheres, a half sphere was used to put forces onto the sphere and not cause extra separation of the spheres that would have been caused by the angled plunger. Contact Young’s modulus was chosen to be the same as the bond Young’s modulus. The contact Young’s modulus is in reference to the stiffness factor that is used when calculating the forces associated with the external geometry and/or other fibers. Since there is only one fiber being tested and that this is a semi-static test, it was assumed that the contact properties of the simulation would not be sensitive to the study. Damping was not used due to the low dynamics found in the 3-point-bending test. Particle density was also chosen to be the mean of the laboratory calculated density (density was calculated by measuring the mass of an individual wheat straw and dividing by the volume of the wheat straw which was assumed to be a hollow cylinder).

Figure 4-4: DEM simulation consisted of a simulated fiber consisting of a row of 20 spheres 2.81 mm in size that were numerically bonded together based on equations 4.1 – 4.9. The horizontal supports was provided between the 2\(^{\text{nd}}\) and 3\(^{\text{rd}}\) spheres and the 18\(^{\text{th}}\) and 19\(^{\text{th}}\) spheres. The plunger interacted between the middle spheres.
Table 4-1: DEM parameters for wheat stem DEM simulation

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<td>Laboratory Measured</td>
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<tr>
<td>Particle Density</td>
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<td>Taken to be the same as the bond Young’s Modulus</td>
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<tr>
<td>Bond Diameter</td>
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<td>Laboratory Measured</td>
</tr>
<tr>
<td>Bond Length</td>
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<td>Laboratory Measured</td>
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<td>Seconds</td>
<td></td>
</tr>
</tbody>
</table>

Data Analysis

Equation 4.10 was utilized to calculate the Young’s modulus of the laboratory tests and the simulation results.

\[
E = \frac{m L^3}{48 I} \tag{4.10}
\]

\[
I = \begin{cases} 
\frac{\pi}{4} (R^4 - (R - t)^4), & \text{Laboratory} \\
\frac{\pi}{4} R^4, & \text{Simulation}
\end{cases} \tag{4.11}
\]
Where $E$ is the Young’s modulus, $L$ is the separation of the two supports (40 mm), $I$ is the area moment of inertia and is calculated according to Equation 4.11, $R$ is the radius of the sample, $t$ is the sample’s thickness, and $m$ is the linear slope of the displacement vs force curve. The thickness of the stem is not part of the bond equations thus it is assumed that the bond forms a filled cylinder between the spheres. To estimate the Young’s modulus, the linear portion of the displacement and force data prior to the maximum axial force (yield strength) was used. The data (all simulated and laboratory obtained) used for the linear fit includes the data range such that the force values are non-zero, and less than the maximum measured force. Data was then removed near the maximum force until the linear fit $R^2$ value is greater than 0.999 (Figure 4-5).

![Figure 4-5: Axial displacement and forces data for wheat straw showing the linear portion of 3-point bending with the data used for the linear fit (blue spheres) and data removed for linear fit (black stars) for the Young’s modulus estimation. The linear fit with $R^2$ value greater than 0.99 is shown as a solid red line.](image)

With the approximated values of the Young’s modulus calculated, a two-sample t-test was used to determine if there exists a significant difference between the mean Young’s modulus values of
the laboratory samples with and without a node at a 95% confidence value, and the node location was tested by fitting a linear model approximating the Young’s modulus as a function of the node location.

Once simulations were completed, a linear model was developed, utilizing MATLAB’s stepwiselm (MATLAB, 2019b) function, relating the bond Young’s modulus and Poisson’s ratio to the measured Young’s modulus using Equation 4.10. The stepwiselm function removes additional terms of a quadratic linear model function with interactions depending if there is no statistical differences between the “full” model or the “reduced” model. Using this linear model, optimized values for bond Young’s modulus and Poisson’s ratio were approximated utilizing MATLAB’s fmincon nonlinear constrained optimization function (MATLAB, 2019a). The initial guess used for the optimizer will be 0.3 and 1.4 GPa for the Poisson’s ratio and bond Young’s modulus respectively. Constraints used for the Young’s modulus is that the value must be greater than 0.0 GPa and the constraints for Poisson’s ratio forces it to be in the range 0.01 – 0.49. Comparisons will then be made between the observed mean value of the Young’s modulus from laboratory data and the value obtained from the simulations.

**Results and Discussion**

Laboratory samples were cut to a mean length of 55.18 mm with the mean being in the 95% confidence interval of 55.03 and 55.34 mm. The diameter of the fibers was found to have a mean 2.81 mm [2.72, 2.91]. The mean thickness of the stems tested was found to be 0.35 mm [0.33, 0.37]. The measured mean density of the particles was found 314.5 Kg m$^{-3}$ [277.6, 351.3]. The moisture content of the straw was measured to be 5% in the dry basis.

Figure 4-6 shows the calculated Young’s modulus values from the laboratory data. Applying the two-sample t-test, it was found that there existed no statistical difference in the mean of the two sample classes of section with and without nodes (p > 0.05). Testing if the node
location affected the Young’s modulus was also found to be insignificant at p > 0.05. The mean calculated Young’s modulus was found to be 3.76 GPa, with the 95% confidence interval placing the mean between 2.66 and 4.87 GPa. The measured Young’s modulus using the 3-point bending was similar to the value predicted by Schramm et al. (2019) using the cantilever beam test and to the range given by Lenaerts (2014).

![Graph showing distribution of Young's modulus values](image)

Figure 4-6: Plot showing the distribution of Young’s modulus values from all wheat straw sections separated by having and not having a node (a), and all obtained Young’s modulus values (b).

Table 4-2 shows the calculated Young’s modulus values per stem section. From the table there appears to be no difference in the Young’s modulus from one section segment to another segment with 95% certainty (confidence intervals were calculated utilizing the student-t distribution and the number of samples indicated in Table 4-2). Due to the lack of differences between stem segments, it can be assumed that the stem has a uniform Young’s modulus. This allows researchers to use the assumption of uniform Young’s modulus during DEM simulations.
Table 4-2: Tabulated Young’s modulus values per wheat stem segment.

<table>
<thead>
<tr>
<th>Section Number</th>
<th>Number of Samples</th>
<th>Young’s Modulus (GPa)</th>
<th>95% Confidence Interval</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Mean</td>
<td>Stdev.</td>
</tr>
<tr>
<td>2</td>
<td>17</td>
<td>2.84</td>
<td>1.69</td>
</tr>
<tr>
<td>3</td>
<td>12</td>
<td>2.42</td>
<td>2.67</td>
</tr>
<tr>
<td>4</td>
<td>16</td>
<td>3.11</td>
<td>2.16</td>
</tr>
<tr>
<td>5</td>
<td>15</td>
<td>6.56</td>
<td>7.18</td>
</tr>
</tbody>
</table>

Equation 4.12 shows the linear equation found by performing the DOE, by finding a linear relationship between the measured Young’s modulus, and the DEM parameters: bond Young’s modulus and Poisson’s ratio. The presented coefficients were all found to be significant with a p-value < 0.05.

\[ E = E_b \left( 0.63 - \frac{0.043}{1 + v} \right) \]  

(4.12)

From Equation 4.12, it is seen that the Poisson’s ratio plays a small role in the calculation of the measured Young’s modulus even though its value is significant in the linear model.

While Equation 4.12 does not provide a method to calculate a unique value for the bond Young’s modulus and Poisson’s ratio directly, it can be used part as an optimization scheme to find an adequate bond Young’s modulus and Poisson’s ratio. Utilizing Equation 4.12 and minimizing the error between the measured mean and the linear equation, it was found that a bond Young’s modulus of 6.25 GPa and a Poisson’s ratio of 0.23 minimized this error. Running the simulation, the simulation measured Young’s modulus was found to be 3.64 GPa, which is an error of 3.11%. Figure 4-7 shows the solution spaces for the measured mean Young’s modulus and the optimized DEM bond Young’s modulus as there exists and infinite number of solutions.
Figure 4-7: Solution space for the mean laboratory Young's modulus and the DEM predicted bond Young's modulus. Blue line shows the solution space for a measured value of 3.76 GPa obtained from laboratory data, while the red dashed line shows the solution space for a measured value of 3.64 GPa obtained from the optimized DEM simulation. Curves are created using Equation 4.12 and shows the infinite solutions that can be obtained.

Conclusions

The 3-point bending test was implemented in the DEM software LIGGGHTS utilizing a bond model to simulate wheat straw. The Young’s modulus was calculated utilizing the linear section of the stress strain curve and a model was developed to reproduce laboratory results. The presented calibration method was able to replicate the mean Young’s modulus obtained from laboratory data with an error of 3.11%. With this proposed calibration scheme for bond Young’s modulus and Poisson’s ratio, future works will investigate how to incorporate the calibration
scheme to better simulate wheat straw in bulk simulations, and investigate alternative measurement methods to find a scheme that better estimates the Poisson’s ratio.

References


https://github.com/richti83/LIGGGHTS-WITH-BONDS


CHAPTER 5. SIMULATION OF UNIAXIAL COMPRESSION FOR FLEXIBLE FIBERS OF WHEAT STRAW USING THE DISCRETE ELEMENT METHOD

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Modified from a manuscript to be submitted to Biosystems Engineering

Abstract

The uniaxial compression test was investigated as a potential test to be used for Discrete Element Method (DEM) calibration for bulk behavior of fibrous material. Wheat straw was cut to 100 mm and was loosely filled into a cylindrical container (225 mm diameter) with a mean mass of 65 grams. A plunger was inserted into the wheat straw filled container at 15 mm/s to collect uniaxial compression forces and plunger displacement. A total of nine tests, on newly prepared wheat straw material bed, were conducted using three different sized cylindrical plungers, 50, 150, and 225 mm in diameter. All tests were initially preloaded using the 225 mm plunger to a normal stress of 1 kPa. A DEM Design of Experiments (DOE) of uniaxial compression, with similar setup as the laboratory tests, were conducted in LIGGGHTS (an open source DEM software) to determine the DEM parameters which are sensitive to the uniaxial compression test. These DEM parameters included the local bond damping coefficient, bond Young’s modulus coefficient, particle-particle friction coefficient, and particle-geometry friction coefficient. It was found that bond Young’s modulus, particle-particle friction, and particle-geometry friction were sensitive to the uniaxial compression. However, the local bond damping coefficient was not sensitive to the uniaxial compression test. This is assumed to be due to the semi-dynamic nature of the compression test and a higher plunger speed may be required. This may prove to be problematic as most uniaxial compression tests are run at lower speeds. The
uniaxial compression test could be used to calibrate the bond Young’s modulus and the contact Young’s modulus coefficient, and particle-particle and particle-geometry friction coefficient values.

Keywords. Calibration, DEM, DOE, Flexible DEM Particle, Uniaxial Compression, Wheat Straw

Introduction

The Discrete Element Method (DEM) has been a major computational technique in granular machine design and has recently began to be used in agricultural machine design, with an example being the modeling of flexible fibers (Lenaerts et al., 2014). Utilizing contact and bond equations to describe the micro-interactions and DEM numerical shape approximations of the granular material, such as soybean, corn, or wheat straw. DEM can also predict particle flow, compression, and damping of bulk behaviors. Utilizing DEM allows manufacturers to create multiple designs and simulate crop-to-machine interactions to evaluate their performance before building physical prototypes, saving time and money. A main hurdle with DEM models is that the DEM model material parameters must be calibrated before being deployed for simulation of large applications. The calibration may begin with laboratory measured bulk material behavior values, even though the values are not uniquely related to the DEM micro-interaction equation parameters, they do provide useful starting points. Application based simple tests are needed to perform sensitivity of the DEM micro-interaction parameters and to calibrate the DEM model.

Potyondy and Cundall (2004) applied a bond DEM model to simulate cemented rocks response under loading. This model was later expanded to create fibrous biomass materials (Guo et al., 2013a; Lenaerts et al., 2014). Guo et al. (2013a) added bond damping equations for the DEM bond model. Guo et al.’s (2013a) DEM model has been shown to approximate flexible rod like particles and follow beam theory (Guo et al., 2013b). While there does exists material
properties for wheat straw, (Afzalinia & Roberge, 2007; Galedar et al., 2008; Adapa et al., 2010), there is little work on how to find bond properties. A systematic approach to find bond damping and bond Young’s modulus properties exists for single fibers utilizing a cantilever beam test (Schramm et al., 2019). As bulk material properties cannot be determined from a single fiber test, a uniaxial compression test is proposed to help calibrate DEM parameters that influence bulk behavior of wheat straw. The uniaxial compression test was chosen to further validate the DEM model of wheat straw in a compression setting and due to its simplicity in both a laboratory and a DEM setting. By determining which DEM parameters are sensitive to a specific test, a calibration procedure may be developed which incorporates differing laboratory tests that will fully characterize a DEM model. DOE based virtual experiments have been a useful technique to perform sensitivity studies, and to create meta-models of the dependent and independent variables measured from the DOE to optimize DEM parameters to reproduce laboratory test data (Mousaviraad et al., 2016).

The objectives of this study are to:

1. Investigate the effect of plunger diameter on uniaxial compression tests of wheat straw
2. Investigate which DEM parameters are sensitive to a uniaxial compression test

**Methods and Materials**

**Experimental Design and Apparatus**

Winter Wheat straw material were hand harvested from the Iowa State University Research Farm located in Boone, Iowa. Straw was hand cut, just above the ground (25 mm to 50 mm), to ensure the straw remained undamaged. Straw was then processed by removing the stem head of the straw and the straw husk shielding the stem (Figure 5-1). The cleaned straw was then separated into stem sections that did not include the inter-nodes (Figure 5-2). The sections were
then randomly selected from the middle sections, excluding the bottom section (section 1) and the top section (section 5) (Figure 5-2). Representative samples from sections 2, 3, and 4 were then cut to a mean length of 100.2 mm (standard deviation of 0.30 mm) prior to conducting the experiment.

Figure 5-1: Cut wheat straw collected from Iowa State University Research Farm and a cleaned stem that has had its head and leaves removed.

Figure 5-2: Representation of section breakdown of a piece of wheat straw with head and leaves removed.

A 225 mm diameter cylindrical clear acrylic container was loosely filled to a mean mass of 65 grams with the cut wheat straw sections (Figure 5-3a). An Instron 4502 (Instron, 825 University Ave Norwood, MA, 02062-2643, USA) was then used to insert a 225 mm steel disk at low speed to a pre-loading stress of 1 kPa. Once this normal stress was reached, the plunger was raised quickly. For the primary loading step, each of the cylindrical plunger sizes (50, 150, or 225 mm) (Figure 5-3b) each disk was inserted into pre-compressed straw at 15 mm/s. Nine separate tests were ran in total, three for each plunger. The plunger size was randomly selected by taking a normal permutation of sizes, [50, 50, 50, 150, 150, 150, 225, 225, 225], and applying
a random permutation to the array to obtain the sampling order [150, 225, 50, 225, 150, 50, 150, 225, 50]. Uniaxial compression forces and vertical plunger displacement were captured at a sampling rate of 10 Hz for all tests. The three different sized plungers were investigated to find if a specific plunger size was statistically better for the calibration the DEM bond parameters.

Figure 5-3: Laboratory test particle bed inside a clear acrylic container filled with wheat straw (a). 50, 150, and 225 mm diameter plungers used in tests (b).

DEM Simulation of Uniaxial Compression

The open-source Discrete Element Method (DEM) software LIGGGHTS (version 3.7) (Kloss et al., 2012) was used to simulate the design of experiments (DOE) of uniaxial compression to determine which DEM parameters are sensitive in the tests, and to compare simulations results, by extracting the forces acting on the plunger and the plunger’s vertical displacement, to those found in the laboratory experiments. LIGGGHTS DEM bond model, initially developed by Richter (2015) was modified according to Guo et al. (2013a) to include the damping equations (Equations 5.1-5.9). This fully modified version of LIGGGHTS gave comparable results to Guo et al’s (2013b) bond model as was found in Schramm et al. (2019).
For fiber-fiber and fiber-geometry contacts, the LIGGHTS built-in Hertz-Mindlin contact model was chosen.

\[
\delta \hat{F}_{b,n,i} = K_n A_b \hat{x}_n \Delta t \tag{5.1}
\]

\[
\delta \hat{F}_{b,t,i} = K_t A_b \hat{x}_t \Delta t \tag{5.2}
\]

\[
\delta \hat{M}_{b,n,i} = K_t I_p \hat{\theta}_n \Delta t \tag{5.3}
\]

\[
\delta \hat{M}_{b,t,i} = K_n I \dot{\theta}_t \Delta t \tag{5.4}
\]

\[
F_{b,n} = \sum_{\forall i} \delta \hat{F}_{b,n,i} + 2 \beta_b \sqrt{M^* A_b K_n} \hat{x}_n \tag{5.5}
\]

\[
F_{b,t} = \sum_{\forall i} \delta \hat{F}_{b,t,i} + 2 \beta_b \sqrt{M^* A_b K_t} \hat{x}_t \tag{5.6}
\]

\[
M_{b,n} = \sum_{\forall i} \delta \hat{M}_{b,n,i} + 2 \beta_b \sqrt{J^* I_p K_n} \hat{\theta}_n \tag{5.7}
\]

\[
M_{b,t} = \sum_{\forall i} \delta \hat{M}_{b,t,i} + 2 \beta_b \sqrt{J^* I K_n} \hat{\theta}_t \tag{5.8}
\]

\[
K_n = \frac{E}{l_b} , K_t = \frac{K_n}{2(1 + \nu)} \tag{5.9}
\]

Where (Schramm et al. 2019)

- \( F_{b,n}, F_{b,t} \) are the normal and tangential bond forces, respectively
- \( M_{b,n}, M_{b,t} \) are the normal and tangential bond moments, respectively
- \( \delta \hat{F}_{b,n,i}, \delta \hat{F}_{b,t,i} \) are the normal and tangential \( i^{th} \) incremental bond forces caused by the linear spring, respectively
- \( \delta \hat{M}_{b,n,i}, \delta \hat{M}_{b,t,i} \) are the normal and tangential \( i^{th} \) incremental bond moments caused by the linear spring, respectively
- \( K_n \) and \( K_t \) are the normal and tangential bond stiffness constants, respectively
- \( A_b \) is the bond cross sectional area
• $\Delta t$ is the time step
• $\beta_b$ is the local bond damping coefficient
• $M^*$ and $J^*$ are the equivalent mass and equivalent moment of inertia of the particles, respectively
• $\dot{x}_n$ and $\dot{x}_t$ are the normal and tangential relative velocities between the two particles, respectively
• $\dot{\theta}_n$ and $\dot{\theta}_t$ are the normal and tangential relative angular velocities between the two particles, respectively
• $l$ and $l_p$ are the second area moment and polar area moments of inertia, respectively
• $E$ is the bond Young’s modulus
• $\nu$ is the Poison’s ratio
• $l_b$ is the equilibrium bond length

Figure 5-4: DEM representation of a wheat straw stem with bonds (dark yellow) with 35 spheres with a diameter of 2.91 mm.

To create a wheat stem in DEM, 35 spheres, each with a diameter of 2.91 mm were bonded together (Figure 5-4). These numbers were obtained by determining the mean diameter of the laboratory wheat straw used in the uniaxial compression tests. The 35 spheres comes from trying to get as close to the 100 mm length that was used in the laboratory tests. The DOE used for this study was a Box-Behnken design (Box & Behnken, 1960) to test for main effects, interaction effects and quadratic effect terms on the following DEM parameters: bond Young’s modulus
(low = 0.1 GPa and high = 10 GPa), local bond damping coefficient (low = 0.1 and high = 10),
and particle-particle friction coefficient (low = 0.1 and high = 0.6). This design gives 13
simulation design points per plunger. For the three plungers, a total of 39 simulations were run in
LIGGGHTS. Runs were competed on a MPI cluster where each machine contained a quad core
Intel Xeon processor (E3-1240 v3 @ 3.40 GHz) with 16 GB of memory. The simulations took
two weeks to complete.

The Young’s modulus ranges were decided to have the same range and that range should
include ranges found in the literature (Hamman et al., 2005; O’Dogherty et al., 1995; Stasiak,
2003). The particle-particle friction range was found by testing the sliding friction in laboratory
utilizing an inclined plane. Table 5-1 shows the remaining DEM material parameters that were
used for the simulations and were held constant such that only sensitivities brought out by the
bond equations were investigated. Particle diameter was chosen to be the average stem diameter,
measured at the center of each sample, of the random wheat stem samples. Particle bond
diameter and bond length were selected to be the same as measured stem diameter. The particle
density was calculated using an average mass and assuming the stem was a solid cylinder. The
Poisson’s ratio was selected from literature (Hamman et al., 2005; O’Dogherty et al., 1995;
Stasiak, 2003). The material properties were measured from a sample size of 30 of unused wheat
straw. Each of the DOE runs started with the same particle insertion. Each run was then pre-
compressed to 1 kPa using the 225 mm diameter plunger (Figure 5-5). The plunger was lowered
onto the sample initially at 1 m s\(^{-1}\) until a pressure of 50 Pa was reached. The plunger speed was
reduced by 25% (to 0.75 m s\(^{-1}\)). This processes repeated every additional 50 Pa until the plunger
velocity reached 0.025 m s\(^{-1}\), where the speed of the plunger was kept the same. Once the pre-
compression was complete, the plunger was raised until no force was measured on the plunger
and the kinetic energy of the system was less than 1.0E-6 Joules. After this period, the plunger was replaced with either the 50, 150, or 225 mm plunger and the plunger would begin its descent into the simulated container at 40 mm/s to 40% of the height when the pre-compression simulation finished. The vertical force applied to the plunger and the distance traveled by the plunger were recorded at 1000 Hz. This process was repeated for each of the 39 DOE experimental tests.

Table 5-1: Fixed DEM material parameters for the uniaxial compression simulation.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
<th>Source/Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle Diameter</td>
<td>2.91</td>
<td>mm</td>
<td>Laboratory Measured</td>
</tr>
<tr>
<td>Particle Density</td>
<td>125</td>
<td>kg m(^{-3})</td>
<td>Laboratory Measured</td>
</tr>
<tr>
<td>Poison's Ratio</td>
<td>0.2</td>
<td>NA</td>
<td>Hamman et al., 2005; O'Dogherty et al., 1995; Stasiak, 2003</td>
</tr>
<tr>
<td>Bond Diameter</td>
<td>2.91</td>
<td>mm</td>
<td>Laboratory Measured</td>
</tr>
<tr>
<td>Bond Length</td>
<td>2.91</td>
<td>mm</td>
<td>Laboratory Measured</td>
</tr>
<tr>
<td>Particle-Particle Coefficient of Restitution</td>
<td>0.160</td>
<td></td>
<td>Laboratory Measured via Drop Test</td>
</tr>
<tr>
<td>Particle-Geometry Coefficient of Restitution</td>
<td>0.320</td>
<td></td>
<td>Laboratory Measured via Drop Test</td>
</tr>
<tr>
<td>Particle-Geometry Coefficient of Friction</td>
<td>0.530</td>
<td></td>
<td>Laboratory Measured via Inclined Plane Test</td>
</tr>
<tr>
<td>Time Step</td>
<td>1.00E-07</td>
<td>Seconds</td>
<td></td>
</tr>
</tbody>
</table>
Figure 5-5: DEM representation of plunger test with 225 mm plunger into a bin of wheat straw. Insertion was done in two stages hence the banding seen. Color of fibers indicate their id number in the simulation.

**Data Analysis**

Given the vertical displacement \((z)\) in mm and the vertical force \((F)\) in Newtons, Equation 5.10 was used to fit the vertical force as a function of displacement. Equation 5.10 was fit utilizing multiple calls to MATLAB’s lsqnonlin non-linear optimization function (MATLAB, 2019a) altering the initial guess of the function. These guesses were randomly chosen using a uniform distribution between the lower and upper bounds. The lsqnonlin function minimizes the non-linear least squares problem by minimizing the sum of square errors (SSE) of a function.

\[
F = (A + Bz)(1 + e^{cz})
\]  

(5.10)

Once equation 5.10 is used to fit the vertical force \((F)\) versus the vertical displacement \((z)\) of each DOE data sets, equations 5.11 to 5.13 will be used to attempt to find a linear relationship between the model coefficients \((A, B,\) and \(C)\) in Equation 5.10 to the DEM input parameters. All
linear models start as a full quadratic with interaction model. These models are then reduced based on the hypothesis test that there is no significant difference in prediction between the full and reduced model. If this hypothesis fails at \( p < 0.05 \) then the full model is used. If it does not fail, then the reduced model becomes the full model, and this is repeated until terms are not able to be removed (MATLAB, 2019b).

\[
A = \Lambda_A(D_{plung}, E_c, E_b, ppf) \quad (5.11)
\]

\[
B = \Lambda_B(D_{plung}, E_c, E_b, ppf) \quad (5.12)
\]

\[
C = \Lambda_C(D_{plung}, E_c, E_b, ppf) \quad (5.13)
\]

Where

- \( D_{plung} \) is a categorical variable of the size of the plunger being used
- \( E_c \) is the contact Young’s modulus used in the simulation
- \( E_b \) is the bond Young’s modulus used in the simulation
- \( ppf \) is the particle-particle friction used in the simulation
- \( \Lambda[i] \) is the minimum linear regression model for a model parameter

Data trimming was utilized to provide better fits. Data began once the vertical force held a value greater than 1.0 N. Data was stopped once the plunger reached max depth (40% of the height of the plunger from the initial compression) for simulations while data was manually trimmed for the laboratory results or if the plunger traveled further than in a simulation. This was done to isolate just the compressing of material and not the buckling of material (Figure 5-6).
Figure 5-6: Technique showing selection of laboratory data. Compression data was kept (open circles) while data that is contributed to crushing the stems were removed (filled circles).

**DEM Simulation Verification**

Once equations 5.11 – 5.13 are found, a verification run was attempted to verify the processes utilizing the 225 mm plunger data. Equation 5.14 is used to attempt to minimize the error between the model and the laboratory obtained model by adjusting the DEM parameters. Once the verification run completes, the verified run will be compared to the laboratory runs and the error between the predicted run and the verification run will be calculated.

\[
\min \left( \left| F(z) - (A_A(\lambda) + A_B(\lambda) z)(1 + e^{A_C(\lambda) z}) \right| \right)_z
\]

\[
\lambda = [225, E_c, E_b, ppf]
\]
Results and Discussion

Figure 5-7 shows the results of the laboratory test separated by plunger size for 50 mm (a), for 150 mm (b) and for 225 mm (c). Table 5-2 shows the mean and standard deviation of the coefficients in Equation 5.10. From Figure 5-7, the laboratory samples do follow a similar trend, but variability exists. This variability is evidenced by the large standard deviation values seen in Table 5-2.

Table 5-2: Mean and standard deviation values for the fitted coefficients obtained from the laboratory data for the uniaxial compression tests.

<table>
<thead>
<tr>
<th>Plunger</th>
<th>Coefficient (Units)</th>
<th>Mean</th>
<th>Stdev.</th>
</tr>
</thead>
<tbody>
<tr>
<td>50 mm Plunger</td>
<td>A (N)</td>
<td>3.08</td>
<td>0.94</td>
</tr>
<tr>
<td></td>
<td>B (N/m)</td>
<td>0.73</td>
<td>0.29</td>
</tr>
<tr>
<td></td>
<td>C (m$^{-1}$)</td>
<td>0.02</td>
<td>0.01</td>
</tr>
<tr>
<td>150 mm Plunger</td>
<td>A (N)</td>
<td>2.18</td>
<td>2.45</td>
</tr>
<tr>
<td></td>
<td>B (N/m)</td>
<td>0.76</td>
<td>0.44</td>
</tr>
<tr>
<td></td>
<td>C (m$^{-1}$)</td>
<td>0.07</td>
<td>0.05</td>
</tr>
<tr>
<td>225 mm Plunger</td>
<td>A (N)</td>
<td>3.33</td>
<td>2.89</td>
</tr>
<tr>
<td></td>
<td>B (N/m)</td>
<td>1.23</td>
<td>1.53</td>
</tr>
<tr>
<td></td>
<td>C (m$^{-1}$)</td>
<td>0.07</td>
<td>0.03</td>
</tr>
</tbody>
</table>
Figure 5-7: Plots of laboratory obtained data of the uniaxial compression test with the 50 mm plunger (a), 150 mm plunger (b), and the 225 mm plunger (c) for wheat straw.

Figure 5-8 shows the results of all the DOE simulations and demonstrates the exponential behavior that Equation 5.10 predicts between the plunger vertical displacement and the uniaxial compression force. Applying Equation 5.10 to the data from the differing sized plungers showed very good fits with an average $R^2$ value of 1.00, 1.00, and 1.00 for the 50, 150, and 225 mm plungers, respectively. Linear models were then obtained from the fitted data in accordance to Equations 5.11 – 5.13. Table 5-3 shows which DEM parameters were sensitive in the linear models and their adjusted $R^2$ values.
Table 5-3: Coefficients deemed sensitive in the linear model.

<table>
<thead>
<tr>
<th>Plunger</th>
<th>Coefficient</th>
<th>$E_c$</th>
<th>$E_b$</th>
<th>$ppf$</th>
<th>Adj-R$^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>50 mm Plunger</td>
<td>A</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>0.94</td>
</tr>
<tr>
<td></td>
<td>B</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>1.00</td>
</tr>
<tr>
<td></td>
<td>C</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>0.92</td>
</tr>
<tr>
<td>150 mm Plunger</td>
<td>A</td>
<td>NS</td>
<td>NS</td>
<td>NS</td>
<td>NA</td>
</tr>
<tr>
<td></td>
<td>B</td>
<td>X</td>
<td>X</td>
<td>NS</td>
<td>0.96</td>
</tr>
<tr>
<td></td>
<td>C</td>
<td>X</td>
<td>X</td>
<td>NS</td>
<td>0.70</td>
</tr>
<tr>
<td>225 mm Plunger</td>
<td>A</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>0.99</td>
</tr>
<tr>
<td></td>
<td>B</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>1.00</td>
</tr>
<tr>
<td></td>
<td>C</td>
<td>X</td>
<td>X</td>
<td>NS</td>
<td>0.85</td>
</tr>
</tbody>
</table>

(X == Sensitive at $p < 0.05$, and NS means that the coefficient was found to not be sensitive in the linear model)

Ppf – particle-particle friction coefficient

Applying Equation 5.14 it was found that the optimal values to reproduce the 225 mm plunger data, was to use 112 MPa for the contact Young’s modulus, 301 MPa for the bond Young’s modulus, and 0.7968 for the particle-particle friction coefficient. This value for the particle-particle friction seems high and lies outside the range that was initially tested in the DOE. This may be caused by the lack of a rolling friction model and/or a cohesion model. Figure 5-9 shows the result of the optimized value run and the mean of the 225 mm plunger data (a), and the optimized value run results along with what was the predicted value via the optimization process from Equation 5.14 (b).
Figure 5-8: Plots showing all DEM runs with the 50 mm plunger (a), the 150 mm plunger (b), and the 225 mm plunger (c) for wheat straw.

Figure 5-9: Plot showing the fitted values of the optimized run and mean of 225 mm plunger data as a function of their raw data (a). Plot showing the difference between what the optimization scheme predicted to be and what the optimization scheme produced (b) for wheat straw segments.
From Figure 5-9b, the optimization under predicted the simulation with a max percent error of 25%. This shows promise in the optimization scheme being a potential tool to be used to calibrate future models for bulk simulations.

**Conclusions**

A method for calibrating flexible wheat straw in DEM is presented and validated against laboratory measurements. Utilizing the calibration for a 225 mm plunger, the simulations was able to obtain the laboratory measured mean with a max error of 25%. While the optimization scheme described can be useful, the time required for sample preparation may be too great. The preparation of the wheat straw to be used in the nine tests took multiple weeks. Further work will need to be done to determine if the husks of the wheat straw have a large influence on the results obtained.

**References**


CHAPTER 6. VERIFYING THE CALIBRATION OF WHEAT STRAW MODELED AS A FLEXIBLE FIBER IN DEM BY SIMULATING THE DIRECT SHEAR TEST OF WHEAT STRAW

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Modified from a manuscript to be submitted to Biosystems Engineering

Abstract

The calibration of a wheat straw flexible fiber for use in a DEM simulation of a direct shear test was validated against laboratory direct shear tests. The direct shear test was conducted on a 101.6 mm by 101.6 mm square cell and loosely filled with precut wheat straw (10 mm long with an average width of 2.91 mm). The wheat straw was measured to have a moisture content of 8.6 % in the dry basis. The wheat straw filled shear cells were sheared at 6 mm min⁻¹ to a horizontal displacement of 18 mm while maintaining a normal load applied to the top of the shear cell. This test was replicated three times at normal load levels of 2.76, 5.49, and 8.28 kPa. Data on normal stress, shear stress, and horizontal and vertical displacement were acquired once per second. The maximum shear stress was estimated from each of the direct shear tests. Then a linear fit was applied to the maximum shear stress as a function of the normal load to find the internal friction angle and the apparent cohesion of the wheat straw. The experimental procedure was reproduced in DEM simulation where the wheat straw was modeled as a flexible particle model. In the DEM simulation, eight normal loads (2.76, 3.55, 4.34, 5.13, 5.91, 6.71, 7.49, and 8.28 kPa) were used to obtain a better regression model and a shear speed of 40 mm sec⁻¹ was used to reduce the computational effort. The internal friction angle and cohesion value for the wheat straw measured in laboratory was found to be in the 95% confidence interval 24.72 – 44.72 degrees and -1.14 – 2.01 kPa respectively. The DEM predicted an internal friction angle and cohesion value in the ranges of 19.18 – 29.10 degrees and -1.66 – 1.05 kPa respectively.
Introduction

With the release of more powerful computer hardware, there still exists a need to be able to quickly calibrate flexible fiber models for use in discrete element method (DEM) simulations (Lenaerts et al., 2014). This is needed to allow manufactures the ability to quickly optimize and implement new products. Modeling flexible fibers to simulate wheat straw was demonstrated by Potyondy and Cundall (2004) by developing a method to simulate concrete. From Potyondy and Cundall’s (2004) original method, methods to simulate flexible fibers have been introduced including cohesion models (Wittel et al., 2006), spring and damper models (Park & Kang, 2009; Lenaerts et al., 2014), and bond elastic wave models (Guo et al., 2013a). With these models the underlining problem of defining DEM properties have not been addressed. Calibration of the DEM model is still needed to address the micro-interactions that are approximated by replacing a hollow cylinder (wheat straw) with bonded spheres.

Presented is a systematic approach utilizing previous chapter tests and results to tune the wheat straw model in DEM and validate the calibrated model utilizing a shear simulation. Validation is an important step in calibration as it is able to show the short comings of calibration methods. Assumptions were made that the DEM parameter values could be estimated from the initialization measurements taken from the drop test and sliding test, single particle estimation using the cantilever beam test and 3-point-bending test, and that bulk properties could be estimated from the uniaxial compression test. The objectives of the study are to: (1) simulate the shear behavior of flexible wheat straw in DEM to predict the internal friction angle and the apparent cohesion, and (2) compare the DEM simulated material properties (internal friction angle and apparent cohesion) to laboratory data.
Methods and Materials

Experimental Design and Apparatus

Winter wheat straw material were harvested from the Iowa State University Research Farm in Boone Iowa. Straw by hand to minimize damage during harvest. Straw was then cleaned (Figure 6-1) to remove the head and outer leaves. The straw was then cut to a mean length of 10 mm utilizing a Dremel cutting disk to minimize the chance of crushing the straw (Figure 6-2) as using shears caused the fiber to buckle.

![Figure 6-1](image1.png)

Figure 6-1: Cut wheat straw collected from the Iowa State University Research Farm and a cleaned stem that has had its head and leaves removed.

![Figure 6-2](image2.png)

Figure 6-2: Template of cutting apparatus with disk cutting attachment to trim wheat stems.
Lengths were chosen from the straw stem such that contained no nodes (connecting points between segments of straw). Once pieces of straw were cut, they were used to randomly fill a 101.6 mm by 101.6 mm (4-inch by 4-inch) shear cell to a mean mass of 26.5 grams of straw (Figure 6-3). A 401 g top plate was placed on top of the straw and either 2.75, 5.5, or 8.25 kPa was applied as a normal load to the top plate. Loads were chosen such that the high normal load did not cause all of the fibers to buckle due to the pressure, and the low end was chosen by dividing the high value by three. The shear cell was then sheared at 6 mm min⁻¹, until a shear distance of 18 mm (18% shear) was reached. Three replicates were run for each of the normal loads and data was recorded once per second.

Figure 6-3: A 101.6 mm by 101.6 mm shear cell filled just below half-way with 10mm long cut wheat straw.
DEM Simulation of the Shear Cell

A discrete element method (DEM) simulation was used to simulate the shearing process described above. The DEM software used was the open-source software LIGGGHTS (version 3.7) (Kloss et al., 2012). Equations 6.1-6.9 define how the particles are bonded together.

\[
\delta \dot{F}_{b,n,i} = K_n A_b \dot{x}_n \Delta t \tag{6.1}
\]

\[
\delta \dot{F}_{b,t,i} = K_t A_b \dot{x}_t \Delta t \tag{6.2}
\]

\[
\delta \dot{M}_{b,n,i} = K_t l_p \dot{\theta}_n \Delta t \tag{6.3}
\]

\[
\delta \dot{M}_{b,t,i} = K_n l \dot{\theta}_t \Delta t \tag{6.4}
\]

\[
F_{b,n} = \sum_{\forall i} \delta \dot{F}_{b,n,i} + 2 \beta_b \sqrt{M^* A_b K_n} \dot{x}_n \tag{6.5}
\]

\[
F_{b,t} = \sum_{\forall i} \delta \dot{F}_{b,t,i} + 2 \beta_b \sqrt{M^* A_b K_t} \dot{x}_t \tag{6.6}
\]

\[
M_{b,n} = \sum_{\forall i} \delta \dot{M}_{b,n,i} + 2 \beta_b \sqrt{J^* I_p K_n} \dot{\theta}_n \tag{6.7}
\]

\[
M_{b,t} = \sum_{\forall i} \delta \dot{M}_{b,t,i} + 2 \beta_b \sqrt{J^* K_n} \dot{\theta}_t \tag{6.8}
\]

\[
K_n = \frac{E}{l_b}, K_t = \frac{K_n}{2(1 + \nu)} \tag{6.9}
\]

Where (Schramm et al. 2019)

- \(F_{b,n}, F_{b,t}\) are the normal and tangential bond forces, respectively
- \(M_{b,n}, M_{b,t}\) are the normal and tangential bond moments, respectively
- \(\delta \dot{F}_{b,n,i}, \delta \dot{F}_{b,t,i}\) are the normal and tangential \(i^{th}\) incremental bond forces caused by the linear spring, respectively
- \(\delta \dot{M}_{b,n,i}, \delta \dot{M}_{b,t,i}\) are the normal and tangential \(i^{th}\) incremental bond moments caused by the linear spring, respectively
• $K_n$ and $K_t$ are the normal and tangential bond stiffness constants, respectively
• $A_b$ is the bond cross sectional area
• $\Delta t$ is the time step
• $\beta_b$ is the local bond damping coefficient
• $M^*$ and $J^*$ are the equivalent mass and equivalent moment of inertia of the particles, respectively
• $\dot{x}_n$ and $\dot{x}_t$ are the normal and tangential relative velocities between the two particles, respectively
• $\dot{\theta}_n$ and $\dot{\theta}_t$ are the normal and tangential relative angular velocities between the two particles, respectively
• $I$ and $I_p$ are the second area moment and polar area moments of inertia, respectively
• $E$ is the bond Young’s modulus
• $\nu$ is the Poisson’s ratio
• $l_b$ is the equilibrium bond length

Figure 6-4: Mega-particle model of a flexible fiber for the direct shear cell DEM simulations. There were four spheres per mega-particle. Each sphere had a diameter of 2.5 mm and the bond length was 2.5 mm.

Collisions between the flexible fiber mega-particles and collisions between the fibers and geometry were handled by the Hertz-Mindlin method with no rolling model or cohesion model. Particles were created by bonding four 2.5 mm diameter spheres together (Figure 6-4) utilizing
the bond equations show above (Equations 6.1 – 6.9). Twenty-six grams of particles were inserted into the shear cell randomly, allowed to settle, and a top plate was given a predefined normal load. Once the simulation has settled (kinetic energy of the system falls below 1.0e-4 Joules), the bottom half of the shear cell will travel at 40 mm s⁻¹ while forces are read from the top half of the shear box, similar to the laboratory tests (Figure 6-5). The particles were sheared until a shear distance of 18 mm were reached. While the laboratory tests looked at three different normal loads, the simulation was ran at eight differing stresses (2.76, 3.55, 4.34, 5.13, 5.91, 6.71, 7.49, and 8.28 kPa). These values were chosen after the laboratory tests and reflect the end values of the loads obtained. Multiple loads were ran to better approximate the internal angle of friction and apparent cohesion values.

![101.6 mm by 101.6 mm shear cell](image)

Figure 6-5: 101.6 mm by 101.6 mm shear cell used in simulations of the direct shear tests.

The DEM parameters, Poisson’s ratio, bond Young’s modulus, contact Young’s modulus, and the particle-particle friction were obtained by optimizing values obtained from previous tests (cantilever beam test, 3-point bending test, and the uniaxial compression test) while the remaining DEM parameters were based on literature and laboratory measurements. For bond and
contact Young’s modulus and particle-particle friction, the uniaxial compression results were used (Equation 6-10), while Poisson’s ratio was decided by the cantilever beam and the 3-point bending tests (Equation 6-11).

\[
\min \left( \left| F(z) - (A_1(\lambda) + A_2(\lambda) \cdot z)(1 + e^{A_3(\lambda) \cdot z}) \right|_2 \right) \\
\lambda = [225, E_c, E_b, ppf] \\
\min \left( \left| \sqrt{E_b} - 574.3 \cdot b_2 + 91.4 \right|_2 + \left| E - E_b \left( 0.63 - \frac{0.043}{1 + \nu} \right) \right|_2 \right)
\]

Where

- \( F(z) \) is the mean force from the 225 mm plunger tests with respect to the displacement of the plunger from a uniaxial compression test
- \( z \) is the displacement of the plunger
- \( \Lambda_i \) is the linear model that describes the \( i \)th coefficient from Equations 5.11 – 5.13
- \( E_c \) is the contact Young’s modulus
- \( E_b \) is the bond Young’s modulus
- \( E \) is the mean value for the Young’s modulus found from the 3-point bending test
- \( b_2 \) is the mean frequency of oscillation of a fiber found from the cantilever beam test
- \( ppf \) is the particle-particle friction
- \( \nu \) is the Poisson’s ratio

Equation 6.11 is only used to determine the Poisson’s ratio as the assumption is made that this value does not change between bulk and single fiber simulations. Utilizing these equations, the optimized values found were 0.112 GPa for the contact Young’s modulus, 0.301 GPa for the bond Young’s modulus, 0.797 for the particle-particle friction, and 0.253 for the Poisson’s ratio. Table 6-1 holds the DEM parameter values for the simulation. Data was recorded at 1000 Hz.
Table 6-1: DEM parameter values for the direct shear simulation of wheat straw.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
<th>Source/Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle Diameter</td>
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<td>mm</td>
<td>To Fit Laboratory Measured Length</td>
</tr>
<tr>
<td>Particle Density</td>
<td>125</td>
<td>kg m⁻³</td>
<td>Laboratory Measured</td>
</tr>
<tr>
<td>Bond Diameter</td>
<td>2.5</td>
<td>mm</td>
<td>To Fit Laboratory Measured Length</td>
</tr>
<tr>
<td>Bond Length</td>
<td>2.5</td>
<td>mm</td>
<td>To Fit Laboratory Measured Length</td>
</tr>
<tr>
<td>Particle Contact Young’s Modulus</td>
<td>111.5</td>
<td>MPa</td>
<td>Optimized Value</td>
</tr>
<tr>
<td>Particle Bond Young’s Modulus</td>
<td>300.9</td>
<td>MPa</td>
<td>Optimized Value</td>
</tr>
<tr>
<td>Particle Poisson’s Ratio</td>
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<td></td>
<td>Optimized Value</td>
</tr>
<tr>
<td>Steel Contact Young’s Modulus</td>
<td>197.5</td>
<td>GPa</td>
<td>Thinky Corporation (2018)</td>
</tr>
<tr>
<td>Steel Poisson’s Ratio</td>
<td>0.27</td>
<td></td>
<td>Thinky Corporation (2018)</td>
</tr>
<tr>
<td>Particle-Particle Coefficient of Restitution</td>
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<td></td>
<td>Laboratory Measured Using Drop Test</td>
</tr>
<tr>
<td>Particle-Particle Coefficient of Friction</td>
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<td></td>
<td>Optimized Value</td>
</tr>
<tr>
<td>Particle-Geometry Coefficient of Restitution</td>
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<td></td>
<td>Laboratory Measured Using Drop Test</td>
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<tr>
<td>Particle-Geometry Coefficient of Friction</td>
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</tr>
<tr>
<td>Time Step</td>
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<td>Seconds</td>
<td></td>
</tr>
</tbody>
</table>
Data Analysis

The following values were measured during both from the laboratory tests and the DEM simulations, the top plate height, the horizontal shear displacement, and the shear force of the top half of the shear box. The shear forces are generated from the wheat straw/mega-particles in the top plate shearing the stationery wheat straw/mega-particle bed in the bottom plate according to ASTM D 3080M (ASTM, 2011). The horizontal forces are converted into shear stress by dividing the forces by the area of the top plate (101.6 mm by 101.6 mm). The maximum shear was then found from the data by visual inspection. Data was considered to be at the maximum once the value reached a steady state. These max shear values are then plotted with respect to their corresponding normal pressure to calculate the internal friction angle and the cohesion of the system by the Mohr-Coulomb equation. (Equation 6.12). The internal friction angle and the apparent cohesion predicted from the DEM simulation were then be compared to the values obtained from the laboratory tests.

\[ \tau = \sigma \tan(\phi) + c \]  

(6.12)

Where

- \( \tau \) is the measured max shear strength.
- \( \sigma \) is the total stress applied normal to the shear plane.
- \( \phi \) is the internal friction angle.
- \( c \) is the apparent cohesion of the sample material.

Due to Equation 6.12 representing a linear line, the 95% confidence intervals of the linear coefficients (\( \tan(\phi) \) for slope and \( c \) for the intercepts) were used for all comparisons.
Results and Discussion

The mean particle mass of the samples was found to be 26.33 grams with a standard deviation of 0.9 grams. The fibers were found to have a moisture content of 8.6% (dry basis). Figure 6-6 shows the shear stress versus horizontal strain curves of the laboratory data which were generated from the direct shear tests at the three normal loads of 2.76, 5.49, 8.28 kPa. Results show that the 101.6 mm by 101.6 mm shear cell may be too small for the size of particles being used for the 8.28 kPa load. Figure 6-7 shows the vertical deformation as a function of the horizontal deformation of the sample. From Figure 6-7, it can be seen that as the normal load increases the vertical deformation increases.

Figure 6-6: Stress strain curves for shear cell laboratory tests of wheat straw segments being sheared to 18% of the length of the shear cell (4 inch) at 2.76 kPa (a), 5.49 kPa (b), and 8.28 kPa (c).
Figure 6-7: Vertical deformation of wheat straw as a function of horizontal deformation of the top plate of the 101.6 mm square shear cell at three normal loads of 2.76 kPa (a), 5.49 kPa (b), and 8.28 kPa (c).

Figure 6-8: Maximum shear stress versus normal pressure (stress) showing the internal friction angle and the apparent cohesion of wheat straw from laboratory data, linear fit with $R^2$ of 0.86 and the 95% confidence interval.
Given the maximum shear stress values shown in Figure 6-6, the internal friction angle was estimated utilizing a linear regression to fit Equation 6.12 (Figure 6-8). Fitting the data to the equation, an internal friction angle of 35.95 degrees was found with a 95% confidence interval of 24.72 to 44.72 degrees. The apparent cohesion value was found to be 0.44 kPa but was found to be not significant due to the interval containing the value 0.0 kPa (-1.14 to 2.01 kPa).

After completing the DEM simulation runs, the results of the shear stress versus the shear displacement are shown in Figure 6-9. For the simulations, it appears that the shear stress reaches an equilibrium at approximately equal to 10% of the strain value, whereas the laboratory results showed that the shear stress from the wheat straw tests were not reaching the equilibrium. The horizontal strain corresponding to the initial steady state shear stress (equipment) from the simulation occurred at higher horizontal strain values that the laboratory data (Figure 6-7).

Figure 6-10 shows the simulation results for the displacement of the top plate. There can be seen vast movement of the top plate when compared to the laboratory shear cell results. An explanation of this could be that the DEM simulation particles cannot buckle and be compressed whereas a real wheat straw can be crushed.
Figure 6-9: Shear stress versus horizontal displacement from the 101.6 mm by 101.6 mm square direct shear DEM simulation at normal stresses of 2.76 kPa (a), 3.55 kPa (b), 4.34 kPa (c), 5.13 kPa (d), 5.91 kPa (e), 6.71 kPa (f), 7.49 kPa (g), and 8.28 kPa (h) for wheat straw.
Figure 6-10: Vertical deformation as a function of horizontal deformation of the top plate of the 101.6 mm square shear cell at eight normal loads of 2.76 kPa (a), 3.55 kPa (b), 4.34 kPa (c), 5.13 kPa (d), 5.91 kPa (e), 6.71 kPa (f), 7.49 kPa (g), and 8.28 kPa (h) for wheat straw.
Figure 6-11 shows the internal friction angle and the cohesion value estimates. The internal friction angle was found to be 24.34 degrees with a 95% confidence interval of 19.18 to 29.10 degrees. While this value is lower than what was found earlier with the laboratory data, with an error of 32.3%, the simulation obtained value’s confidence interval does fall within the confidence interval obtained from the laboratory experiment. The cohesion value was found to be insignificant due to the 95% confidence interval including 0.0 kPa for the apparent cohesion (-0.17 to 1.05 kPa).

![Maximum shear stress versus normal pressure](image)

Figure 6-11: Maximum shear stress versus normal pressure (stress) showing the internal friction angle and the apparent cohesion of the wheat straw from laboratory data, linear fit (R² of 0.95) and the 95% confidence intervals.

**Conclusions**

Direct shear simulation of flexible wheat straw particle was successfully simulated using DEM in LIGGGHTS. Values of the DEM parameters optimized from the uniaxial compression, 3-point-bending, and cantilever beam were able to predict the internal friction angle and apparent cohesion, which are bulk material properties, within the laboratory estimated values. The direct
shear testing of wheat straw provided good data for verification of DEM simulations. ASTM standard measurement of wheat straw shear tests gave promising results to be utilized as a simple tests for modeling flexible fibers. Additional work is needed to reduce additional potential errors in the simulation of the direct shear test. Further work for example, improving the rolling models for flexible fibers, buckling model and elasto-plastic models may be necessary to improve the prediction behaviors of wheat straw as they engage with crop processing equipment.

References


CHAPTER 7. GENERAL CONCLUSIONS

Following the methodology explained in the previous chapters to first characterize wheat straw, and systematic DEM parameter initialization and calibration procedures, the following conclusions can be made.

Cantilever Beam

Presented in this work was an overview of the bond model for simulating flexible fibers, like wheat straw, in the discrete element method (DEM) framework. It was found that the cantilever beam allowed for the calculation of bond Young’s modulus and the bond damping coefficient. The cantilever beam test, being a dynamic test, was successfully used to calculate the bond damping coefficient.

Due to the plunger needing to be slowly lowered into a sample, the 3-point-bending test was not found to be an appropriate calibration experiment to determine the bond damping coefficient. The uniaxial compression and shear cell simulations simply had too many particles in the simulation to be able to perform a simulation in a reasonable amount of time (less than a month). This is due to the time step needed for a highly dampening fiber to be very small (0.1 nanoseconds).

It was found that the bond damping coefficient and bond Young’s modulus are not coupled and can be solved for directly (Equations 7.1 – 7.2). Where Equation 7.1 relates the square-root of the bond Young’s modulus ($E_b$) with the frequency of oscillation ($b_2$) of the fiber, and Equation 7.2 relates the bond damping coefficient ($\beta_b$) with the global damping coefficient ($b_1$) of the fiber.

$$\sqrt{E_b} = 574.3 \ b_2 + 91.4 \quad (7.1)$$
\[ \beta_b = -261.4 \, b_1 + 2.5 \quad (7.2) \]

**3-Point-Bending**

Using the 3-point-bending test a relationship between the measured Young’s modulus and the bond Young’s modulus and the Poisson’s ratio. While the Poisson’s ratio cannot normally be determined using a standard 3-point-bending test, it was assumed that the Poisson’s ratio in the DEM simulation could be sensitive due to its addition into the shear strength calculation. It was found that the measured Young’s modulus \( (E) \) in the simulations were weakly dependent on the Poisson’s ratio \( (\nu) \) and strongly dependent on the bond Young’s modulus \( (E_b) \) (Equation 7.3).

\[
E = E_b \left( 0.63 - \frac{0.043}{1 + \nu} \right) \quad (7.3)
\]

Equation 7.3 allows for infinitely many solutions due to the two free parameters, bond Young’s modulus and Poisson’s ratio. Equation 7.3 needs to be coupled with Equation 7.1 to obtain a unique solution.

**Uniaxial Compression**

Uniaxial compression was the first bulk test used to find bond and contact DEM properties of the flexible fiber model. DOE analysis from the uniaxial compression runs allowed the estimation of the particle-particle friction, contact Young’s modulus, and bond Young’s modulus properties. Bond and contact Young’s modulus were included to determine if there was a statistical difference between them. In order to find the surrogate models for the DEM parameters, the Force \((F)\) – displacement \((z)\) curves were fitted using Equation 7.4.

\[
F = (A + B \, z)(1 + e^{C \, z}) \quad (7.4)
\]

Where \(A\), \(B\), and \(C\) were free parameters that would be related to the DEM parameters and the plunger size, using linear relationships (Equations 7.5 – 7.7).
\[ A = \Lambda_A(D_{plung}, E_c, E_b, ppf) \]  
\[ B = \Lambda_B(D_{plung}, E_c, E_b, ppf) \]  
\[ C = \Lambda_C(D_{plung}, E_c, E_b, ppf) \]

With linear equations found to relate the free parameters to DEM particle property parameters, an optimization problem can be defined that minimizes the error between laboratory obtained force – displacement curves with Equation 7.4 utilizing the linear equations found in Equations 7.5 – 7.7 (Equation 7.8).

\[
\min \left( |F(z) - (\Lambda_A(\lambda) + \Lambda_B(\lambda)z)(1 + e^{\Lambda_C(\lambda)z})|^2 \right) \]

\[ \lambda = [225, E_c, E_b, ppf] \]

This optimization was done for the 225 mm wide plunger. It was found that the contact Young’s modulus was statistically different to the bond Young’s modulus and that both were needed to minimize Equation 7.8. It was found that the optimized values gave a max error between the mean force – displacement curve found from the laboratory data and the optimized simulation was 25%. This could have been caused by the fiber’s insertion orientation. Assuming that Equation 7.4 can be approximated by a quadratic equation \( F(z) = \gamma_0 + \gamma_1 z + \gamma_2 z^2 \) a mixed random effects linear model can be ran on the laboratory obtained data to determine if random effects are statistically prevalent to the results. It was found that random effects are present with 95% certainty. This raises questions on how can orientation be accounted for in both laboratory tests and simulations.

**Direct Shear Test**

The direct shear (101.6 mm by 101.6 mm shear cell) DEM simulation was used as a way to validate the calibration process outlined throughout the dissertation utilizing Equations 7.1,
7.3, and 7.8. The contact Young’s modulus, bond Young’s modulus, and particle-particle friction were found using Equation 7.8, Equations 7.1 and 7.3 were used to estimate the Poisson’s ratio. The DEM simulation had good agreement with the laboratory estimated internal friction angle. The laboratory measured value was found to be 35.95 degrees while the DEM simulation predicted it to be 24.34 degrees, giving a relative percent error of 32.3%. While the 95% confidence interval of each friction angle led to them not be statistically different (simulation had a 95% confidence interval in the internal friction of 19.18 – 29.10 while the range for the laboratory measured friction angle was 24.72 – 44.72) another attempt was made to try to lower the prediction error. Instead of utilizing Equation 7.8 to find the contact Young’s modulus, bond Young’s modulus, and the particle-particle friction, it was assumed that the contact Young’s modulus equaled the bond Young’s modulus, and the particle-particle friction was equal the mean static friction value obtained using the inclined plane test. Running the new simulation yielded an internal friction angle of 36.04 degrees, a percent error of only 0.25%.

**Future Recommendations**

Flexible fibers are often part of highly dynamic systems while most of the calibrations are done using semi-static experiments and processed wheat straw (i.e. without the husk and nodes). This is due to the high dynamic systems such as crop processing in forage harvesting operations might need higher bond damping coefficients and which would imply using too small of time steps to simulate the flexible fibers. For applications that involve highly dynamic crop behaviors, further research will be required to develop calibration experiments fit for highly dynamic tests and develop new damping methods to increase stable time steps.