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A bonded sphero-cylinder model for the discrete element simulation of elasto-plastic fibers

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HIGHLIGHTS

- A bonded sphero-cylinder model is proposed to simulate elasto-plastic fibers.
- Elastic deformation and vibration of a fiber are validated against the beam theories.
- Plastic bending deformation of a fiber is validated against the FEM simulations.
- DEM implementation of loadinghistory-dependent fiber deformation model is proposed.

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ABSTRACT

Based on the Discrete Element Method (DEM), a bonded sphero-cylinder model is developed to simulate flexible fibers that can undergo plastic bending deformation. In the model, a fiber is formed by connecting a number of identical sphero-cylinders using virtual bonds, which can experience bending, axial extension/compression, and twisting deformations. The elastic deformation and vibration of a single fiber are simulated and validated against elastic beam theories. In addition, an elasto-plastic constitutive model is implemented to simulate the elasto-plastic bending deformation of a fiber. The DEM results compare well with Finite Element Method (FEM) simulations, verifying the proposed elasto-plastic fiber model. By using bonded sphero-cylinders as opposed to more traditional bonded spheres, large aspect ratio fibers with smooth surfaces can be simulated effectively with fewer elements. The new constitutive model allows for the simulation of elasto-plastic materials, such as metals, plastics, and biomass.

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1. Introduction

Flexible fibers are processed in numerous agricultural and industrial materials handling processes. For example, corn stover

* Corresponding author. *E-mail address:* guoyu03@gmail.com (Y. Guo). and switchgrass are treated in biomass reactors, crop stems are handled during harvesting, and carbon and glass fibers are processed in the manufacture of fiber-reinforced composites. Understanding the mechanical behavior of flexible fibers, such as flow, compression, packing, and breakage, is crucial for equipment optimization and product quality control. Most previous work focuses on rigid fibers without bending deformation (Favier et al., 1999;

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Grof et al., 2007; Hua et al., 2013, 2015). In recent years, computational simulations have been developed and applied to investigate flexible fiber flow (Guo et al., 2015), compression (Leblicg et al., 2016a), packing (Langston et al., 2015), breakage (Guo et al., 2017), and fiber-liquid suspensions (Wu and Aidun, 2010). For numerical modeling, a flexible fiber is typically represented by a chain of elements, which can be spheres, prolate spheroids, cylindrical rods, or sphero-cylinders. The adjacent elements are connected by bonds or ball-socket joints. The bending, axial extension/compression, and twisting of bonds results in the deformation of a fiber. Only elastic deformation is considered in most of the previous work on this topic. A comprehensive validation of the mechanical behavior, including both quasi-static loading and dynamic vibration, for an elastic fiber model was conducted by Guo et al. (2013). Recently, Leblicg et al. (2016b) simulated the plastic bending deformation and failure of flexible crop stems. They proposed a novel data-based approach to model the stem bending, in which the bending stiffness is obtained from look up tables of crop stem measurements based on the current bending angle and saved maximum historical bending angle. Since this bending model utilizes a large amount of experimental data for crop stems and has no explicit mathematical expression, it is not easily adaptable to other materials.

In this work, we propose a bonded sphero-cylinder model for Discrete Element Method (DEM) simulations of elasto-plastic fibers. The elastic deformation, including bending, axial extension/compression, and twisting of a single fiber under both static loads and dynamic vibrations are validated against theoretical predictions of an elastic beam. An elasto-plastic bond bending model is also derived analytically, assuming the fiber material behaves in an elastic-perfectly plastic manner. Three consecutive loading steps are used to allow the deformation in the following step to build upon the plastic deformation from the previous step. Finite Element Method (FEM) simulations of plastic deformation of a fiber with the same properties as those in the DEM simulations are also performed and compared with the DEM simulations in order to validate the DEM model. The proposed elasto-plastic fiber model may be easily adopted to model materials such as metal wires and plastic fibers.

Compared to the bonded sphere model (Fig. 1a), the bonded sphero-cylinder model (Fig. 1b) has some advantages: (i) The resulting fiber is smoother than the bumpy surfaces produced by



Fig. 1. Bonded sphere fiber model (a), bonded sphero-cylinder fiber model (b), and illustration of bonding forces and moments in the bonded sphero-cylinder model (c).

bonded spheres. The artificial roughness of a bonded sphere model can significantly affect the tangential contact force and sliding between two contacting fibers, as discussed in Guo et al. (2015). (ii) Fewer elements are required for a given aspect ratio fiber. For example, for a fiber aspect ratio $(AR_f = fiber length to cross$ sectional diameter) of 100, at least 100 spheres are needed to create a bonded-sphere fiber. However, fewer sphero-cylinders (two is the minimum) are required to generate a fiber of the same aspect ratio with the bonded sphero-cylinder model. Some drawbacks also exist for the bonded sphero-cylinder model: (i) A more complex contact detection algorithm is required for sphero-cylinders. Only the distance between two sphere centers needs to be determined for sphere-sphere contact detection, while the shortest distance between two major axes should be calculated for contact detection between two sphero-cylinders. A more complex algorithm generally implies higher computational cost. (ii) Smaller time steps are required for the bonded sphero-cylinder model. Large rotational velocities of the elongated sphero-cylinder elements may lead to a large relative translational velocity between the two connected end hemisphere centers of adjacent elements. A large relative velocity can lead to a large displacement and, consequently, an unrealistically large bonding force. As a result, a smaller time step is necessary to ensure numerical stability. This instability has been observed in prior work (Langston et al., 2015). Based on the pros and cons of the different models, one should choose a model that best fits the given application. In the present work, an elasto-plastic bending constitutive model is implemented in a bonded sphero-cylinder fiber model. Note that the same elasto-plastic model could also be implemented in a bonded sphere model.

2. Elastic fiber model

A fiber is modeled by connecting a number of identical spherocylinders in a straight line using virtual bonds, as shown in Fig. 1b. A sphero-cylinder element consists of a cylindrical band and two hemispherical ends. The bond connects to the centers of two elements. The centers of two hemispherical ends from two bonded sphero-cylinders initially coincide. The relative movement of the sphero-cylinder elements in a composite fiber leads to the deformation of the bonds and also the fiber. In response, bond forces/moments are induced and exerted on the sphero-cylinders to resist the deformation (Fig. 1c). For elastic deformation, the bond forces/moments and the bond deformation follow a linear relationship, and can be calculated using an incremental method as follows:

$$F_{\rm n} = \frac{E_{\rm b}A}{l_{\rm b}} \delta_{\rm n},\tag{1}$$

$$F_{\rm t} = \frac{G_{\rm b}A}{l_{\rm b}}\delta_{\rm t},\tag{2}$$

$$dM_{\text{twist}} = \frac{G_b I_p}{I_b} d\theta_{\text{twist}} = \frac{G_b I_p}{I_b} \dot{\theta}_{\text{twist}} dt, \qquad (3)$$

and,

$$dM_{\text{bend}} = \frac{E_{\text{b}}I}{l_{\text{b}}}d\theta_{\text{bend}} = \frac{E_{\text{b}}I}{l_{\text{b}}}\dot{\theta}_{\text{bend}}dt,\tag{4}$$

in which the bond normal force F_n and tangential force F_t are computed from the relative normal displacement δ_n and tangential displacement δ_t between the centers of hemispherical ends from two bonded sphero-cylinders, and the twisting moment M_{twist} and bending moment M_{bend} are determined incrementally from the twisting angular displacement θ_{twist} and bending angular displacement θ_{bend}

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