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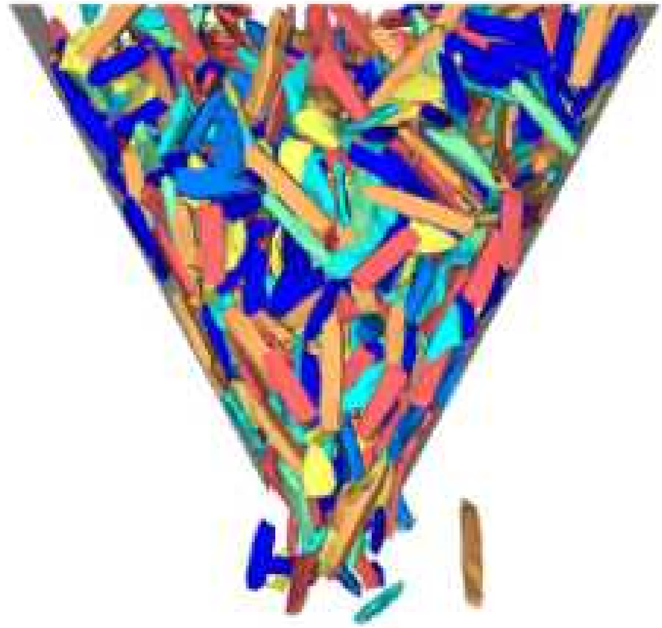
Idaho National Laboratory Relies on Complex-Shape Models to Analyze Milled Biomass Flow



The most abundantly available raw material on Earth — biomass, whose fodder ranges from woody residues to corn stover — has considerable potential as a renewable, sustainable, and environmentally friendly feedstock for conversion to fuels and consumer products. But despite considerable R&D efforts to date, commercial-scale conversion of biomass has remained limited.

One particular challenge that scientists and engineers face is robust design of material-handling equipment used during the milling/biorefinery process. Feeding operations tend to jam and clog components, largely influenced by biomass-particle flowability, resulting in increased downtime and higher costs.

Because biomass feedstocks are granular materials, their flowability is not easily represented by a single material property — their bulk physical behavior is inherently multi-scale. Particle and subparticle attributes, such as density, surface friction, elastic modulus and morphology (size and shape), collectively produce internal friction, wall friction, cohesion, and unconfined yield stress.

Current modeling approaches (including discrete element modeling, or DEM) offer some proven scientific insight, notably in pharmaceutical, mining and agricultural applications. These particles manifest relatively uniform material attributes (particle shapes, size distributions and material, mechanical properties). But the biomass industry has several major obstacles to creating an accurate modeling framework: how to capture complex behavior, how to account for variability of material attributes, and how to link those attributes to model parameters.

Idaho National Laboratory (INL), a U.S. Department of Energy national laboratory, is charged with improving and advancing bio-energy technologies. To that end, INL is investigating how to best leverage simulation tools to design optimal biorefinery equipment and processes. INL began its investigation with an exhaustive literature review on state-of-the-art modeling practices, the first-of-its-kind evaluation of DEM specifically for the biomass industry. It focuses on various particle-shape models' features and suitability for different types of milled biomass, because particle shape is the predominant attribute controlling flow behavior of complex-shaped granular material.

> "Our interest is understanding particle-flow behavior in biomass materials used to create bioenergy. We are one of the first laboratory teams to use the advanced shape models in Rocky DEM, exploring their suitability for modeling biomass particles and flow variability, within biomass handling equipment. We have already determined that Rocky DEM's flexible fiber model is suitable for corn stover tissue, and we will use it to perform complicated simulation scenarios for flow and shear tests to identify particulate behavior."
>
> — Yidong Xia, PhD
> Computational R&D Scientist
> U.S. DOE Idaho National Laboratory

As a particle-scale model, DEM can accurately track individual particles and resolves collisions. However, because discrete element modeling must perform calculations for every particle, it is limited by the total system size, especially when simulating nonspherical particles. And although there is a tremendous amount of literature on DEM model development and applications, there is only limited information on biomass DEM model development. Therefore, any biomass simulation instrumentation must be carefully examined, customized and validated by fully considering the flexible, deformable nature of milled biomass particles.

Biomass Particle and Shape Complexity

DEM biomass modeling requires a detailed understanding of interactions between particles under various load and shear conditions. Accurate physical parameters are critical, because many material properties are inherently coupled to each other.

Researchers consider particle shape and size, the root of complexity for milled biomass, as most key material properties (density, stiffness, moisture content) inherently depend on particle shape and size. Yet each particle is unique: A simple specification of length, width and thickness is not sufficient.

DEM Parameters Pertinent to Biomass Particles

Particle shape
Particle size distribution
Particle skeletal density
Particle envelope density
Skeletal elastic modulus
Effective elastic modulus
Poisson's ratio
Restitution coefficient
Static friction coefficient
Dynamic friction coefficient
Rolling friction coefficient
Damping coefficient
Contact cohesion
Bond stiffness

Investigators must represent materials as realistically as possible with the proper distribution of size, shape and material properties. Though **spherical** particle representation easily calculates contact detection/force and scales best in computing, biomass particles are naturally complex. Any simple model that decreases simulation time may lose accuracy in the process.

Composite-sphere particle models (multi-sphere, for non-deformable particles like peas and rice, and bonded-sphere, for flexible material including corn stover and switchgrass) consist of clusters of multiple spheres, sometimes a few hundred, to form a particle with relatively smooth- or flat-surface geometries. As a result, their use increases computational cost compared to spherical particle models.

Non-composite, non-spherical models — ellipsoids, super-quadrics, analytical shapes and level-set−based descriptive shapes — are more accurate and faster when modeling certain types of granular materials. These methods present a continuous, smooth particle surface, so they are not applicable to particles with sharp edges. Ellipsoids and super-quadric particle models contain symmetry that is rarely found in nature. **Polyhedral** particle models exhibit good potential for DEM investigation, particularly with woody materials like loblolly pine, as they offer better accuracy of complex particle-shape approximation, with element combinations such as vertex−vertex, vertex −edge, vertex−face, edge−edge, edge−face, and face−face. Some models include particle breakage, which allows modeling brittle material being crushed under strong impact. For example, Rocky DEM offers state-of-the-art polyhedral modeling (including fiber shapes), breakage-prediction capabilities, and GPU processing support that enables fast complex-scenario simulation.

For modeling fiber-like and thin shell-like particles with very large aspect ratios, such as corn stover and switchgrass, **sphero-cylindrical** and **shell** particle models take particle flexibility and efficiency into account.

Suitability of Different DEM Shape Models for Biomass Particles

Shape	Suitability
Spheres	Normally used for powdered biomass materials in fluidized bed reactors; potentially suitable as coarse-grained model with specially derived contact force models for biomass feedstock handling processes
Composite-spheres	Most-used model in nonspherical DEM; if computational cost is not considered, this model can be applied to any biomass particle shapes with sufficient accuracy. Contact detection and evaluation procedures developed for spherical DEM can be applied.
Custom-polyhedrons	Suitable for biomass particles with relatively sharp vertices, edges, faces (pine particles and chip-shape corn stover). Shapes of arbitrary complexity (concave convex) are possible provided with custom particle surface geometries; such shapes cannot be normally modeled with ellipsoidal or super-quadric equation.
Sphero-polyhedrons	Best for studying influence of aspect ratio of nonsymmetric rigid particles on characteristics of biomass feedstock feeding and handling systems. Both elongated and flat particles can be investigated; particle blockiness effects cannot be modeled.
Sphero-cylinders	Suitable for elongated flexible biomass particles (fiber-like corn stover and switchgrass fragments)
Composite-polygons (shells)	Suitable for flexible shell-shaped particles with virtual thickness. Shapes of arbitrary complexity are possible; can be used in mixture with sphero-cylinders for corn stover fragments.

Idaho National Laboratory's literature review identified the general strengths and weaknesses for models applicable to milled biomass modeling (shown here) as well as the computational efficiencies of same shape models.

Summary

Idaho National Laboratory's literature study demonstrates that DEM is a robust model to resolve the underlying particle−particle and particle−wall interactions in biomass granular flow, thanks to its natural ability to capture the complex geometries and deformation of individual particles. Rocky DEM's advanced polyhedral and breakage models offer real-world particle behavior, and GPU capabilities make simulation results achievable within a reasonable time frame.

Since biomass DEM modeling is an emerging area, it is not yet possible to identify the most suitable models for all known biomass particle systems. Defining the characteristics and potential strengths/weaknesses of the different models constitutes a step in the right direction.

For the future, multi-scale approaches are expected for the industry. Developing more-sophisticated DEM shapes/models in combination with CFD will contribute to accurate modeling of particle contact mechanics, as will general computational advances.

Problem

Researchers at Idaho National Laboratory have been tasked by the DOE's Bioenergy Technology Office to expand fundamental understanding of biomass materials and work on identifying/developing DEM simulation models and processes to advance best practices. Biomass materials have irregular particle shapes that can cause unpredictive flow patterns, which can jam and clog biorefinery equipment.

Solution

The research team at INL conducted a literature review to determine existing advanced material models and their suitability to particle flow behavior within biorefinery equipment and processes. Based on this first step, the project will next develop better modeling techniques using Rocky DEM realistic polyhedral/fiber models, then conduct pre-processing simulation studies that determine key parameters.

Benefits

Project results will be used to help industry players make decisions about optimizing biorefinery equipment/process design. The study has the potential to make equipment more efficient by eliminating downtime and, ultimately, reducing operational costs.

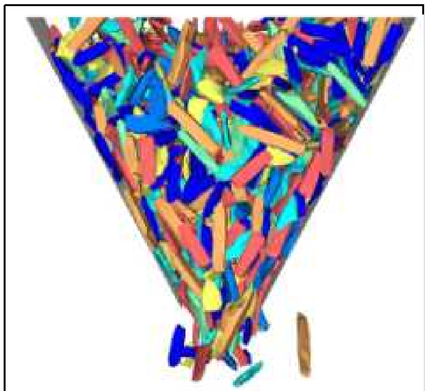
Yidong Xia, Ph.D.

Yidong Xia is a Computational R&D scientist for the U.S. Department of Energy Idaho National Laboratory's Energy and Environment Science & Technology Directorate. Xia obtained his PhD degree in aerospace engineering with a minor in general mathematics from North Carolina State University. At Idaho National Laboratory, his Xia's research and leadership experience lie in environmental subsurface science, nuclear energy, fossil energy, geothermal energy, bioenergy, and high-performance scientific computing. Xia's technical expertise spans several fields, including computational fluid dynamics and heat transfer, computational particle mechanics, computational chemistry, and nuclear material and thermal hydraulics.

Advancing Biorefinery Understanding Particle by Particle
By Silvia Carina Firmino

Idaho National Laboratory (INL), one of 17 U.S. Department of Energy national laboratories, performs research in support of DOE's mission to "discover the solutions to power and secure America's future.", Designated as the DOE's leading center for nuclear research, INL also receives program funding for other areas of interest, including funding from the DOE Bioenergy Technology Office (BETO). INL and BETO share a mission to advance fundamental understanding of biomass materials. The objective is to leverage research and development of feedstock and machinery to develop optimal biofuel technology — ultimately reducing the cost of biorefining and making it a viable renewable alternative to traditional fossil energy. INL's research is gathered in a database that can be utilized by industry to facilitate their own prospective designs.

As a computational R&D scientist at INL, Yidong Xia's role is to examine discrete element modeling (DEM) technology to learn how it can benefit the biomass industry. DEM has a natural ability to capture the complex geometries and deformation of individual particles, as it resolves the underlying particle−particle and particle−wall interactions in biomass granular flow.



Polyhedral shape approximation of chipped loblolly pine particles and application in hopper discharge DEM simulation

Potential feedstock material includes agricultural and forest residuals, such as pine and corn stover. Unfortunately, these ingredients can produce flowability issues — like arching, clogging, jamming — in feedstock-handling equipment. The materials exhibit a wide range of characteristics: highly flexible, fracture-prone, coarse-grained, elongated, and/or convex/concave/steep-verticed surface.

INL's project began with an exhaustive review of literature related to biorefinery applications. One of the engineering challenges is that biomass materials have complex, irregular particle shapes, and, therefore, flow pattern in refinery equipment is difficult to accurately predict. Identifying particle shape and size is important, yet each particle is unique: A simple specification of length, width and thickness is not sufficient. Proper modeling requires using complex shapes to better represent particle surface details — which adds to the computational cost. Though non-composite, non-spherical and spherical particle models easily calculate contact detection/force and scale best in computing, they are not complex enough to provide accurate results for biomass materials.

Literature defined and identified a number of models that, when used under the right conditions, can be applied to feedstock. Composite-sphere, custom-polyhedron, sphero-polyhedron, sphero-cylinder, shell and composite-polygon models are suitable to simulate biomass particle-flow behavior depending on their varying strengths/weaknesses (chart).

To learn details about the various models and their characteristics, click here.

Biomass DEM modeling is an emerging area, so it is not yet possible to identify the most suitable models for all known biomass particle systems. Defining the characteristics and potential strengths/weaknesses (including those related to computational cost) of the different models constitutes a step in the right direction.

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Idaho National Laboratory's literature review identified the general strengths and weaknesses for models applicable to milled biomass modeling.

Using this summary as a baseline, INL's work continues in evaluating which DEM models mimic biomass flow behavior better than others. The next step involves hands-on simulation experience, using Rocky DEM for a variety of assessment studies. For example, Yidong will need to determine that Rocky's flexible-fiber model is suitable for analyzing corn stover tissue and use it to perform flow and shear tests that can offer insight to engineering companies that design biomass handling equipment. Because it's critical that his study analyze complex particle shapes inherent to feedstock, Rocky DEM is the right tool, with its state-of-the-art polyhedral modeling (including fiber shapes), breakage-prediction capabilities, and GPU processing support that enables complex-scenario simulation.

Yidong's research will continue for another few years, yet already the software sector is already starting to recognize his success. One possibility is that we'll apply more-sophisticated DEM shapes and models. The scale-bridge between particle and scale might be the most challenging part in multiscale approaches, so it deserves significant research efforts. And advancing computational speed to crunch thousands of complex-shaped particles will always be part of the objectives.

Ideally, Yidong will develop a set of parameters that are critical to achieving accurate simulation results, which biorefinery pioneers can leverage to advance the industry.

About the Author

Yidong Xia is a Computational R&D scientist for the U.S. Department of Energy Idaho National Laboratory's Energy and Environment Science & Technology Directorate. Xia obtained his PhD degree in aerospace engineering with a minor in general mathematics from North Carolina State University. At Idaho National Laboratory, his Xia's research and leadership experience lie in environmental subsurface science, nuclear energy, fossil energy, geothermal energy, bioenergy, and high-performance scientific computing. Xia's technical expertise spans several fields, including computational fluid dynamics and heat transfer, computational particle mechanics, computational chemistry, and nuclear material and thermal hydraulics.