Application of Numerical Simulation Technology in the Biomass Densification and Molding Field: A Review

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Biomass densification and molding technology can compress and densify crushed materials into portable solid fuels with a certain shape and density. Such densification has the advantages of high combustion efficiency, high calorific value, environmental protection, and cleanliness. In recent years, scholars have used the finite element method and discrete element method to simulate biomass densification and molding technology, revealing the flow and deformation laws of materials in the biomass densification and molding process from different perspectives. This work has provided reference and guidance for the optimization of biomass densification and molding mechanism and molding dies. This article first reviews the basic ideas of finite element method, as well as the application of ANSYS and ABAQUS in biomass densification and molding technology. Secondly, it reviews the basic ideas of discrete element method and the application of EDEM and PFC in biomass densification and molding technology. Finally, it reviews the application of combined finite element method with discrete element method in biomass densification and molding technology. The content of the article has certain reference and guidance significance for the numerical simulation of future biomass densification and molding technology.

DOI: 10.15376/biores.21.1.Ning

Keywords: Biomass densification; Numerical simulation; Finite element method; Discrete element method

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INTRODUCTION

Biomass refers to various biological material that is formed through photosynthesis, including all animals, plants, and microorganisms. It has the characteristics of renewability, low pollution, and wide distribution (Chen *et al.* 2024; Ye *et al.* 2025). Biomass densification and molding technology can compress crushed biomass materials into block or granular fuels with a certain density. Biomass densified fuels have the advantages of high combustion efficiency, high calorific value, environmental friendliness and cleanliness (Arulprakasajothi *et al.* 2020; Anukam *et al.* 2021; Silva *et al.* 2022), and they are widely used in heating furnaces, hot water boilers, biomass power plants, and so on.

The earliest developed biomass forming machine was the screw extrusion forming machine. It primarily relies on external heating of the molding die to maintain a forming temperature between 150 and 300 degrees °C. Through the reciprocating advancement and compression of biomass material by the screw, it compresses and densifies the material into block-shaped biomass fuels (Ning and Qian 2023). Piston stamping forming machines usually do not require external heating. They mainly rely on the back-and-forth movement of the piston to compress and form biomass materials. This type of forming machine is mainly used for producing solid block or rod-shaped fuels (Ning *et al.* 2025). The ring die (or flat die) and pressure roller are the two key components of a die roller forming machine. When biomass material enters the space between the pressure rollers and the ring die (or flat die), the relative motion between these components continuously forces the material into the forming holes of the ring die (or flat die) before being extruded out. Due to the cutting device installed at the discharge port, it is cut into biomass granular fuel with a certain length under its action (Wang *et al.* 2023; Li *et al.* 2023). Figure 1 shows typical biomass densified fuels formed by such processing.

Fig. 1. Biomass densified fuels

The biomass material after crushing exhibits discreteness. In the process of biomass densification and molding, the material comes into contact and friction with the molding die, and the boundary conditions exhibit nonlinearity. The material undergoes significant deformation and flow, exhibiting geometric nonlinearity. At the same time, the stress-strain curve of the material is also nonlinear, resulting in material nonlinearity (Wang *et al.* 2024). When scholars have studied the flow deformation laws during the compression molding process of biomass materials, some of them have considered discrete biomass materials as continuous media for simulation, whereas others have used discrete element method for simulation, and others have used a combination of finite element method and discrete element method for simulation.

This article reviews the current status of numerical simulation research on biomass densification and molding technology, analyzes the application of finite element method and discrete element method in biomass densification and molding technology, and provides reference and guidance for the biomass densification and molding mechanism and optimization of biomass densification and molding dies.

NUMERICAL SIMULATION OF BIOMASS DENSIFICATION AND MOLDING TECHNOLOGY BASED ON FINITE ELEMENT METHOD

The finite element method (FEM) is a numerical calculation method for solving mathematical equations and is a powerful numerical calculation tool for solving practical engineering problems. It is a numerical analysis technique that organically combines mechanics theory, matrix theory, and computer software. Recently, it has been widely applied in many disciplines and practical engineering problems (Du *et al.* 2024; Yang *et al.* 2024; Zheng *et al.* 2024).

The basic idea of the finite element method is to discretize a continuous solution area into a combination of finite elements that are interconnected in a certain way. Because the elements can be combined into Boolean combinations in different ways, and the elements themselves can have different shapes, it is possible to model complex geometric solving domains. Another important feature of the finite element method as a numerical analysis method is the use of approximate functions assumed within each element to represent the unknown field function to be solved on the entire solution domain in a fragmented manner. The approximate function within a unit is usually expressed by the values of the unknown field function or its derivatives at each node of the unit and its interpolation function. In this way, in the finite element analysis of a problem, the values of the unknown field function or its derivatives at each node become new unknowns, thereby transforming a continuous infinite degree of freedom problem into a discrete finite degree of freedom problem. Once these unknowns are solved, the approximate values of the field functions within each element can be calculated through interpolation functions, thereby obtaining an approximate solution for the entire solution domain. Obviously, as the number of units increases, the approximation of the solution will continue to improve. If the unit meets the convergence requirements, the approximate solution will eventually converge to the exact solution.

Application of ANSYS in Biomass Densification and Molding Technology

ANSYS software

ANSYS software is a large-scale general finite element analysis (FEA) software developed by the American company ANSYS. It is the fastest growing computer-aided engineering (CAE) software in the world and can interface with most computer-aided design (CAD) software to achieve data sharing and exchange, such as Creo, NASTRAN, Algor, I-DEAS, AutoCAD, and so on (Zhang *et al.* 2024). It is a large-scale universal finite element analysis software that integrates structure, fluid, electric field, magnetic field, and sound field analysis. It has a wide range of applications in mechanical manufacturing, automotive transportation, aerospace, energy, civil engineering, shipbuilding, and other fields. ANSYS is powerful and easy to operate and has become the most popular finite element analysis software internationally, ranking first in FEA evaluations over the years.

Material constitutive model- (1) Yield criterion

The crushed biomass materials fall into the category of elastic-plastic materials. Their most important characteristic is that when the material yields, its stress-strain relationship exhibits nonlinearity. When conducting elastic-plastic analysis on complex stress state materials, it is necessary to meet the following requirements: the established yield rule must not only comply with the material properties, but also the determination of the flow rule must comply with the relative relationship between the stress and plastic strain increment of the elastic-plastic body, as well as the law of stress state hardening after determining the material yield. The establishment of yield criteria is crucial in the compression molding process of biomass materials.

During the process of bearing loads, the stress state of materials gradually transitions from elastic state to plastic state, and such phenomena are called yielding. The yield criterion of a material is the necessary condition for plastic deformation to occur at a certain point within the material. Currently, there are two commonly used yield criteria: the Mohr Coulomb criterion and the Drucker Prager criterion. Due to the difficult convergence of the Mohr Coulomb criterion in calculations, the Drucker Prager criterion is widely used in elastic-plastic finite element analysis (Xu 2012).

The expressions for the Drucker Prager yield criterion are as follows,

$$f = aI_1 + \sqrt{J_2} - K = 0 \tag{1}$$

$$I_1 = \sigma_{ii} = \sigma_1 + \sigma_2 + \sigma_3 = \sigma_x + \sigma_y + \sigma_z \tag{2}$$

$$J_2 = \frac{1}{2} S_i S_i = \frac{1}{6}\left[(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2\right] \tag{3}$$

$$a = \frac{\sin\varphi}{\sqrt{3}(3 - \sin\varphi)} \tag{4}$$

$$K = \frac{6c\cos\varphi}{\sqrt{3}(3 - \sin\varphi)} \tag{5}$$

where I_1 represents the first invariant of stress tensor; J_2 represents the second invariant of stress deviation; c represents the cohesion of materials, kPa; φ represents the internal friction angle of materials, °.

The Drucker Prager yield criterion and the Mohr Coulomb criterion are relatively similar, and they are used to modify the Mises criterion. This criterion is mainly used for granular materials, such as rock and soil, and the corresponding equivalent stress expression is as follows,

$$\sigma_e = 3\beta\sigma_m + \left[\frac{1}{2}\{S\}^T\{M\}\{S\}\right]^{\frac{1}{2}} \tag{6}$$

where σ_m represents the static water pressure or average stress, $\sigma_m=1/3(\sigma_x+\sigma_y+\sigma_z)$; $\{S\}$ represents the deviation stress; $\{M\}$ represents $\{M\}$ in the Mises yield criterion,

$$M = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 \end{bmatrix}.$$

The expression for material constant β is as follows,

$$\beta = \frac{2\sin\varphi}{\sqrt{3}(3 - \sin\varphi)} \tag{7}$$

The expression for the material yield parameter σ_y is as follows,

$$\sigma_y = \frac{6c\cos\varphi}{\sqrt{3}(3 - \sin\varphi)} \tag{8}$$

Therefore, the expression for the yield criterion can also be expressed as follows:

$$F = 3\beta\sigma_m + \left[\frac{1}{2}\{S\}^T\{M\}\{S\}\right]^{\frac{1}{2}} - \sigma_y = 0 \tag{9}$$

In the principal stress space, if $\varphi > 0$, then the yield surface of the Drucker Prager criterion is an external cone with a Mohr Coulomb hexagonal cone shape, as shown in Fig. 2. If $\varphi = 0$, the Drucker Prager criterion transforms into the Mises criterion.

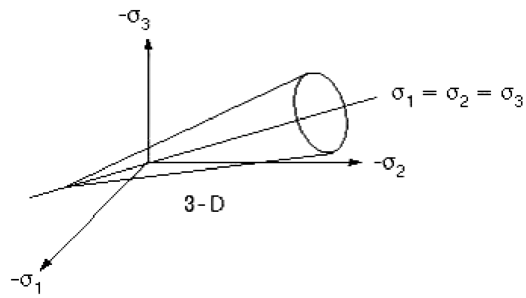

Fig. 2. Drucker Prager yield criterion

(2) The law of flow

With continuous loading, the plastic zone of the material will gradually expand and continue to undergo plastic deformation, ultimately leading to its failure. During the continuous loading process of materials entering the plastic zone, the direction of plastic strain increment is defined by the flow law. Under stress, any hardened/softened material has different states with varying degrees of plastic strain potential energy. In the space of principal stress, the plastic potential surface is defined as the potential point of the bending surface connected by the same plastic strain. The law of flow stipulates that in the principal stress space, the increment of plastic strain at any point must always be orthogonal to the plastic potential surface passing through that point. Furthermore, the expression for plastic strain increment can be obtained,

$$\{d\varepsilon^{p}\} = d\lambda \frac{\partial Q(\sigma)}{\partial\{\sigma\}} \tag{10}$$

where $Q(\sigma)$ represents the plastic potential function; $d(\lambda)$ represents the single sign multiplier, mainly used to determine the magnitude of strain increment.

The yield surface $F(\sigma)$ of a material usually does not coincide with the plastic potential surface $Q(\sigma)$. If the yield surface of the material coincides with the plastic potential surface, then the resulting flow law is called the adaptive flow law, while the opposite is called the non-adaptive flow law. The following expression can be used to describe the adaptive flow rule:

$$\{d\varepsilon^{p}\} = d\lambda \frac{\partial F(\sigma)}{\partial\{\sigma\}} \tag{11}$$

(3) Hardening law

The hardening law is mainly used to describe the development of the subsequent yield surface and plastic strain of a material entering the plastic zone in the principal stress space. It is used to analyze the stress-strain state of materials in the plastic zone. If a material has hardening properties, its stress-strain state undergoes plastic deformation as it increases from a yield surface. Because the plastic potential energy changes, the yield surface will gradually expand outward and obtain a new yield surface, which is called the successor yield surface. The stress path cannot fully reflect the hardening degree; the stress level corresponds one-to-one with the total plastic potential energy.

In the law of flow, this factor $d\lambda$ can be assumed to be as follows,

$$d\lambda = \frac{1}{A}\frac{\partial f}{\partial \sigma_{ij}}d\sigma_{ij} = (-)\frac{1}{A}\frac{\partial f}{\partial H}dH \tag{12}$$

where f represents the yield condition function; A represents the function of hardening parameter H.

Related works

Gao (2004) focused on the research of loose biomass hot pressing molding technology, addressing the issues of low density and difficult molding in biomass densification and molding. Through finite element simulation, the temperature field and mechanical behavior during the extrusion process were analyzed. The study employed the Drucker-Prager criterion to establish an elastoplastic constitutive equation and used ANSYS software to simulate the temperature field distribution and extrusion molding process at 300 and 250 °C. The results indicated that heating at 300 °C resulted in a more reasonable temperature field distribution, facilitating lignin plasticization and molding. During the extrusion process, hydrostatic pressure was identified as the key factor for densification, with negative hydrostatic pressure promoting material densification, while excessive shear stress could easily lead to product cracking. The study provided a theoretical basis for optimizing biomass densification and molding process parameters and revealed the interaction mechanisms among temperature, pressure, and material flow.

Li *et al.* (2009) used the widely used finite element analysis software ANSYS, which had a high market share, to simulate the process of biomass densification and molding. The main factors affecting the molding process, such as different length-to-diameter ratios of molding dies and different opening taper angles of molding holes, were obtained to study the influence of internal stress-strain of raw materials. Compared with the experimental results of the main factors affecting biomass densification and molding, it was found that finite element software could simulate the internal changes of biomass during compression molding process well, which was effective for studying compression molding laws. Using the thermal analysis module of ANSYS to simulate the distribution of temperature field inside the heated biomass, the influence of temperature factors on biomass densification and molding was investigated, and the softening and melting of lignin in each section of biomass were inferred, providing reference for extrusion technology. The force analysis of the molding hole wall is important for determining the distribution of molding holes in the molding die. Through simulating the deformation and stress of the forming hole, the displacement deformation and maximum stress of the inner wall of the forming hole showed a small-scale continuous variation law, providing a reference for the design of the forming hole structure.

Gu *et al.* (2012) used finite element theory analysis to establish a molding hole strength model and conducted numerical simulation analysis and failure analysis on the mechanical properties of the model using basic data. From the Von Mises equivalent stress cloud map, it could be seen that the stress at the node 305 corresponding to the equivalent stress in the connection area between the feeding cavity and the forming cavity of the molding hole was relatively concentrated, indicating that the Von Mises equivalent stress at this location was the highest, which was the dangerous point of the molding hole, with the largest deformation and easy occurrence of fatigue failure. The stress of this node was stored for fatigue analysis. Based on the established finite element model of the molding hole, fatigue life analysis was conducted on molding holes with different structural parameters, and fatigue life data of the molding hole under different structural parameters were obtained, providing theoretical support for the design of high life ring die and verifying the key technical parameters of the optimal design of the molding die determined in the experiment.

Celik *et al* (2018) established a three-dimensional model of the flat die using SolidWorks and conducted finite element analysis through ANSYS Workbench to explore the structural response of the flat die of the biomass pelleting machine under high compressive loads. Twelve sets of empirical models constructed based on the response surface method showed that the exit radius of the die hole and the compressive pressure had a significant impact on the maximum stress, while the effective length mainly affected the deformation amount. The goodness of fit of all models reached more than 98%. The results showed that optimizing the compression ratio could balance the particle density and the die life, providing a quantitative basis for the flat die design. The design exploration method adopted in the study verified the feasibility of numerical simulation in the optimization of agricultural machinery components, and at the same time pointed out that it was necessary to further combine experimental verification and consider the influence of porous layout.

Application of ABAQUS in Biomass Densification and Molding Technology

ABAQUS software

ABAQUS is a powerful engineering simulation finite element software that not only can solve relatively simple linear problems, but also many more complex nonlinear problems (Wang *et al*. 2023). The unit library of the software is more abundant, which can simulate arbitrary geometric shapes, and has different types of material libraries inside, which can be used to simulate the performance of typical engineering materials (such as metal, rubber, reinforced concrete, geotechnical materials, composite materials, polymer materials, and compressible super-elastic foam materials). ABAQUS, as a universal numerical simulation software, can solve many structural problems, such as stress or displacement. It also can be used for simulating many problems in other engineering fields such as piezoelectric analysis, acoustic analysis, heat conduction, thermoelectric coupling analysis, mass diffusion, and geotechnical analysis.

Material constitutive model

The Drucker Prager model cannot reflect the material yield problems caused by hydrostatic pressure. ABAQUS provides the Drucker Prager Cap model, which adds a cap-shaped yield surface based on the Drucker Prager model, thereby introducing yield caused by compression and controlling the wireless shear dilation phenomenon of the material under shear action. Therefore, the Drucker Prager Cap model has been widely applied in the extrusion molding process of bulk materials (Si *et al.* 2013).

(1) Yield surface

The yield surface of the Drucker Prager Cap model is shown in Fig. 3. The model is mainly composed of the shear failure surface and cap surface provided by Drucker Prager. ABAQUS uses a gradient surface to smoothly connect the shear failure surface and the cap surface, serving as a transition surface.

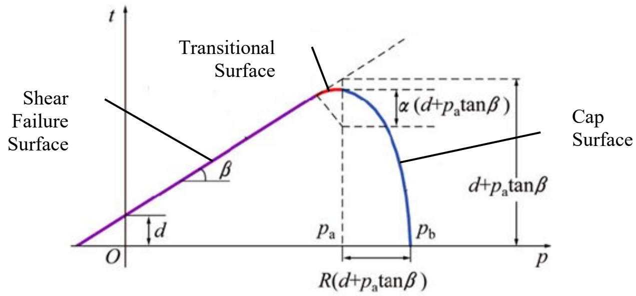

Fig. 3. Drucker Prager Cap model yield surface

The yield function of the shear failure surface is as follows:

$$F_s = t - p\tan\beta - d = 0 \tag{13}$$

where d represents the friction angle of the material; β represents the cohesion of the material.

The yield function of the cap surface is as follows:

$$F_c = \sqrt{(p - p_a)^2 + \left[\frac{Rt}{1+\alpha-\alpha/\cos\beta}\right]^2} - R(d + P_a\tan\beta) = 0 \tag{14}$$

where R represents the parameter that controls the geometric shape of the cap; α represents the parameter that determines the shape of the transition zone; p_a is the intersection point between the cap surface and the p axis, controls the size of the cap, which is called the yield compression average stress, determined by the following equation:

$$p_a = \frac{p_b - Rd}{1 + R\tan\beta} \tag{15}$$

The yield function of the transition surface is as follows:

$$F_t = \sqrt{(p - p_a)^2 + \left[t - \left(1 - \frac{\alpha}{\cos\beta}\right)(d + p_a\tan\beta)\right]} - \alpha(d + \tan\beta) = 0 \tag{16}$$

(2) Plastic potential surface

The plastic potential surface of the Drucker Prager Cap model is also composed of several segments (as shown in Fig. 4), which are correlated on the cap surface, but not correlated in the transition zone and shear failure surface.

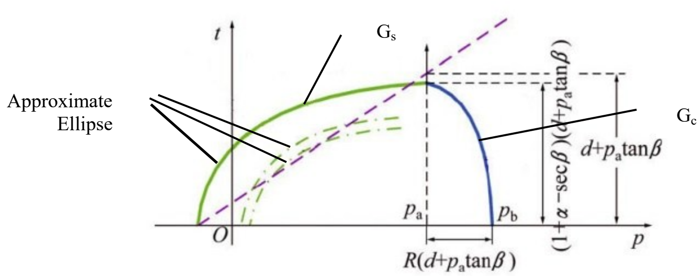

Fig. 4. Plastic potential surface of Drucker Prager Cap model

The plastic potential surface function on the cap surface is as follows:

$$G_c = \sqrt{(p - p_a)^2 + \left[\frac{Rt}{(1+\alpha-\alpha/\cos\beta}\right]^2} \tag{17}$$

The plastic potential surface function of the transition zone and shear failure surface is as follows:

$$G_s = \sqrt{\left[(p_a - p)\tan\beta\right]^2 + \left[\frac{t}{(1+\alpha-\alpha/\cos\beta}\right]^2} \tag{18}$$

Related works

Wang (2013) used the Drucker Prager Cap constitutive model to describe the mechanical properties of the powder. Based on ABAQUS, a rolling and die-hole extrusion model of the material was established. Through changing simulation parameters, such as friction coefficient, die-roller gap, and die-roller diameter ratio, the influence of various die-hole extrusion model factors on the rolling process was explored. The results showed that as the friction coefficient and die-roller diameter ratio increased and the die-roller gap decreased, the equivalent stress of the material after compression increased, indicating better compression quality. Among these three influencing factors, the friction coefficient had a relatively large impact and was easy to change, so it should be the main optimization object to consider.

Zhu (2014) analyzed the stress and material flow conditions at the conical hole of the ring die, and optimized its structure based on TRIZ innovative theory. Using ABAQUS software to simulate the material extrusion before and after structural optimization, the results showed that the optimized structure reduced the extrusion pressure of the roller, reduced the energy consumption of granulation, and ensured the quality of particles.

In view of the material nonlinearity, geometric nonlinearity, and boundary condition nonlinearity present in the material molding process of the roller plunger forming machine, Ning *et al.* (2016) conducted numerical simulation research on the particle process of the roller plunger forming machine based on the nonlinear finite element analysis software ABAQUS. The results showed that the stress and displacement at the bottom of the roller plunger at the 30° installation line were the highest, and the material at this location was more prone to plastic deformation. At the same time, based on ABAQUS nonlinear finite element analysis software, numerical simulations were conducted for two types of roll forming techniques. The results showed that the maximum stress value of the traditional roll forming method was 18.74 MPa, which occurred at the contact between the roller and the ring die without opening holes, while the maximum stress value of the roll plunger forming method was only 5.966 MPa, which occurred at the bottom of the roller plunger, was extremely advantageous for materials entering the ring die hole with a tapered opening to participate in compression forming.

Wilczynski *et al* (2021) investigated the influence of process parameters (compressive stress, temperature, moisture content) on the properties of biomass pellets during single-piston compaction of pine sawdust. Based on experimental data, the Drucker-Prager-Cap (DPC) model was used to parametrically describe the mechanical behavior of sawdust, and the reliability of the experimental results was verified through ABAQUS simulation. ABAQUS was employed to analyze pellet density distribution, energy consumption, and compressive force variations under different process conditions. Simulation results showed good agreement with experimental data, indicating the model's effectiveness in predicting key compaction parameters. The research showed that ABAQUS combined with the DPC model could serve as an effective tool for optimizing the biomass compaction process, providing theoretical support for equipment design and process parameter selection, while reducing experimental costs. The optimal process parameters were determined to be 150 MPa, 150 °C, and 10% moisture content, yielding the highest particle density and strength.

NUMERICAL SIMULATION OF BIOMASS DENSIFICATION MOLDING TECHNOLOGY BASED ON DISCRETE ELEMENT METHOD

The discrete element method (DEM) is another powerful numerical calculation method used to analyze the dynamics of material systems, following the finite element method and computational fluid dynamics. The discrete element method provides a platform for solving various comprehensive problems involving particles, structures, fluids, electromagnetics, and their coupling by establishing a parameterized model of solid particle systems for particle behavior simulation and analysis. It has become a powerful tool for process analysis, design optimization, and product development. The application of discrete element method in the industrial field has gradually matured, and it has expanded from the research of bulk mechanics, geotechnical engineering, geological engineering and other engineering applications to the design and development of industrial processes and industrial products (Xu *et al.* 2013).

The basic idea of the discrete element method is to separate the discontinuity into a set of rigid elements, so that each rigid element satisfies the motion equation. The next step is to solve the motion equation of each rigid element using a time step iterative method and then obtain the overall motion form of the discontinuity. This method allows for relative motion between units without necessarily satisfying the conditions of displacement continuity and deformation coordination. It has fast calculation speed and requires small storage space, making it particularly suitable for solving large displacement and nonlinear problems.

Application of EDEM in Biomass Densification and Molding Technology

EDEM software

With the development of computer visualization technology and computational methods, the application software of discrete element method has reached a new stage, and its representative product is the discrete element analysis software EDEM (Shi *et al.* 2023). EDEM is a commercial new 3D discrete element software developed by DEM Solutions in the UK, which has the following features: (1) External geometric models can be imported for quick modelling, and the boundaries can be solid; (2) Strong visualization ability; (3) Easy to operate; and (4) The post-processing capability of parameters is powerful. These characteristics are not present in previous discrete element software, making discrete element simulation analysis more convenient and feasible. Moreover, the analysis function of EDEM software also includes a coupling analysis module for solid particles and liquids, which expands the field of discrete element analysis.

Related works

Based on the soft ball model contact theory, Li *et al.* (2015) established a discrete element simulation model for the material molding process. They simulated the densification and molding process of powder under different compression speeds, compression displacements, forming cavity apertures, and cone angles of the compression rod. The compression and stress relaxation curves of each group were obtained, and the influence of compression speed on compression force could be ignored. For preventing the loosening of straw compacts, it was recommended to choose a molding die with an aperture of Φ_d = 8 mm and a cone angle of θ = 45°, and to maximize the downward displacement of the compression rod. At the same time, the 25th and 54th seconds of the molding process were selected for analysis of the displacement, velocity, force, and torque between the particles and the contact wall. The results showed that after the loading of the particle system stopped, stress relaxation occurred in the straw-formed blocks, and the internal straw particles continued to undergo small movements instead of immediately coming to a standstill. The lower end surface of the compression rod and the cone angle of the molding die were subjected to the maximum force, and damage to these areas should be avoided as much as possible. Therefore, during the design and manufacture of the mold, to minimize damage to both the compression rod and the molding die, special attention should be given to enhancing the mechanical properties of the lower end surface of the pressure rod and the conical surface of the molding die.

Gao (2019) used the discrete element method to simulate the densification and molding process of single mode pores in *Salix* particles. The simulation data was compared with experimental data and one-way ANOVA was conducted to verify the effectiveness of the established discrete element model. The contact force distribution at different stages of the compression process could be obtained through EDEM software, and the compression transmission mechanism and force chain evolution mechanism were studied in detail. Frictional force between particles and between particles and molding dies were explained through the force chain distribution state. The motion trajectories of particles of different sizes during the compression process were investigated, the influences of different factors on the forming quality and energy consumption were analyzed, the micro-mechanical behaviors and molding mechanism of *Salix* shavings during the densification and molding process were observed to explore a new research method for biomass densification.

Wang (2020) studied the mechanical properties, molding mechanism, and bonding mechanism of sand willow twig particles in the densification and molding process using the discrete element method suitable for numerical simulation of bulk materials and molecular simulation technology suitable for micro particle research. The relationship between the inter particle friction angle (angle of repose) and various factors was analyzed through EDEM software. The influence of the molding shaft section structure on the molding process and fuel quality was studied. The force and deformation characteristics of individual particles under different conditions were obtained, as well as the influence of various parameters on fuel forming quality and power consumption. The effects of pressure, temperature, moisture, and other factors on the glass transition temperature (T_g), diffusion ability, and intermolecular interactions of *Salix* wood lignin molecules were investigated using Material Studio software. The glass transition temperature, diffusion characteristics, hydrogen bonding formation, and evolution laws of lignin under different conditions were obtained.

Application of PFC in Biomass Densification and Molding Technology

PFC software

PFC stands for Particle Flow Code, which is a computational software developed by Itasca Corporation in the United States. It is mainly used for studying the analysis of granular materials or systems that can be simplified into granular materials. There are currently two types of software: 2D (PFC2D) and 3D (PFC3D), which belong to the category of Discrete Element Method (DEM). The main fields of PFC application include civil engineering, mining engineering, materials engineering, food engineering, pharmaceutical engineering, and agriculture (Yang and Li 2023).

Unlike continuum mechanics methods, PFC attempts to study the mechanical properties and behavior of media from a microstructural perspective. To be brief, the basic composition of a medium is particles, which can increase or not increase the "cement" bond. The macroscopic mechanical properties of the medium, such as constitutive properties, are determined by the geometric and mechanical properties of the particles and bond. Figuratively, this is similar to the laboratory "geo-mechanical model" tests that were popular in the field of rock mechanics in China in the 1980s. In this test, sand (particles) and gypsum (binders) are often mixed and simulated according to similarity theory to simulate the mechanical properties of rock masses.

The particles in PFC are rigid particles, but overlap is allowed in mechanical relationships to simulate the contact forces between particles. The mechanical relationship between particles is simple, which is Newton's second law. The contact failure between particles can take two forms: shear and open. When the contact relationship between particles in the medium (such as disconnection) changes, the macroscopic mechanical properties of the medium can undergo a transformation from linear before the peak to nonlinear after the peak, that is, the change in the contact state of particles in the medium determines the constitutive relationship of the medium. Therefore, in PFC calculations, there is no need to provide macroscopic constitutive relationships and corresponding parameters for material theorems. These traditional mechanical properties and parameters are automatically obtained through programs, and they are defined by the geometric and mechanical parameters of particles and cement, such as particle size distribution, stiffness, friction force, bonding medium strength, and other micro mechanical parameters.

Related works

Sha (2022) used PFC particle flow software to simulate the uniaxial compression process of Salix biomass, exploring the phenomena of particle arching and stress shielding effect exhibited by the particle medium under uniaxial compression. Then, through numerical simulation analysis, the contact force of each particle was obtained to study the force chain network inside the particles. Based on this, the stress arching effect of particles in the biomass densification and molding process was analyzed using this model, and the formation process, evolution mechanism, and morphological changes of the arching structure were understood again at the microscopic scale. This laid the foundation for future research from a microscopic perspective and provided reference for further optimization of the molding process and improvement of the quality of molding fuels.

In order to study the force chain characteristics during the densification process of *Salix* particles, Li (2023) conducted further research on the quantification level of force chains based on the PFC discrete element method. Based on the criterion that the principal stress of the particles is greater than the average contact stress, three conditions for forming a force chain were defined. The fish language was used for programming to determine the high-stress particles that meet the requirements for forming a strong chain component, and to refine the distinction between strong and weak force chains. By comparing and analyzing the structural characteristics of force chains simulated in two-dimensional and three-dimensional states, it was found that the advantage of force chains in the two-dimensional state was better visualization effect, and the advantage of force chains in the three-dimensional state was that multi-dimensional spatial analysis could be conducted. Under the monitoring using the fish language, the energy changes of the system were basically in line with expectations, demonstrating that the mesoscopic reactions and energy changes of particulate matter always occur simultaneously.

NUMERICAL SIMULATION OF BIOMASS DENSIFICATION AND MOLDING TECHNOLOGY COMBINING FINITE ELEMENT METHOD WITH DISCRETE ELEMENT METHOD

The finite element and discrete element coupling simulation of biomass compression molding, that is, the joint simulation of discrete element software and finite element software, combines the respective advantages of both to accurately analyze the force conditions of the model during the compression densification molding process (Zhang 2024).

Comparison between unidirectional coupling and bidirectional coupling

Coupling calculations between finite element and discrete element methods primarily include unidirectional coupling and bidirectional coupling. Unidirectional coupling enables the representation of simple interactions between biomass densified fuels and molding dies. It involves determining the forces exerted by bulk particles on the forming machine using the discrete element method, then applying these forces in the finite element analysis for subsequent machine analysis. Unidirectional coupling is applicable only where structural geometric deformation is minimal and considers solely the impact of granular material on the structure. It offers faster computation compared to bidirectional coupling. Conversely, achieving bidirectional coupling is significantly more challenging, requiring substantially greater computational effort and resulting in low simulation efficiency. This is because solving the interaction between particles and the structure necessitates real-time boundary condition provision from the finite element software to the discrete element model (Li 2022).

Related works

Huang (2017) used the discrete element method instead of the commonly used finite element method to simulate the biomass densification and molding process. A corresponding contact mathematical model was established for biomass particles, and the biomass densification and molding process was simulated to obtain compression characteristic curves that are more in line with experimental conditions. Simulation simulations were also completed for different loading speeds and molding sizes. A relatively accurate mechanical model was obtained based on the discrete element method, and a joint simulation method using EDEM and ANSYS was proposed to obtain the force cloud map of the external molding die during biomass densification and molding. This provided a new method for the design verification and wear mechanism research of molding dies.

Li (2018) first studied biomass briquette as a continuous medium and conducted macroscopic heat transfer analysis of the biomass thermal compression molding process in ABAQUS software. Then, based on the constructed discrete element contact model and heat transfer model, the EDEM software interface was written in C++ to achieve heat transfer simulation of biomass particulate materials in the discrete element software EDEM through secondary development of EDEM. Finally, a secondary development program was used to simulate and explore the effects of thermal compression molding process (compression amount, molding die diameter, and external heating temperature) on heat transfer. It was found that the biomass heat transfer rate is positively correlated with compression amount and external heating temperature and negatively correlated with molding die diameter.

In the traditional roll compaction process, the periodic movement of the screw feeder leads to an uneven powder feeding speed, which in turn affects the density distribution of the tablet. However, the existing models have difficulty in accurately simulating this phenomenon. Mazor *et al* (2018) proposed a multi-scale modeling method combining the Discrete Element Method (DEM) and the Finite Element Method (FEM) to study the non-uniformity of the roll compaction process in the pharmaceutical industry. The particle flow in the screw conveyor zone was simulated through DEM. The discrete particle data was transformed into a continuous field by the coarse-grained method and then used as the input boundary condition of FEM to simulate the compression behavior in the rolling zone. The results show that the spiral rotation period (6.25 seconds) directly causes the roll pressure and the density of the strip to fluctuate in the same period, forming a serpentine density distribution along the width of the strip. This research reveals the influence of feeding dynamics on the final product quality, providing theoretical support for optimizing the roll compaction process.

Fang (2020) used the Verlet method to iteratively calculate the contact force between straw particles and the contact force between molding dies during the heat transfer process. A heating coil heat transfer program for the molding die was written in C++language. The EDEM discrete element software was used to model and simulate the thermal compression feeding and compression processes. A single column plug biomass forming test bench was built, and the discrete element particle model was validated using the forming sleeve heating method. Finite element simulation of the extrusion stage was carried out using ANSYS, and the temperature field variation law and stress-strain variation trend were analyzed.

For obtaining more accurate and reliable force and strain cloud maps of the molding die, Yan (2020) fully utilized the advantages of discrete element and finite element and conducted coupled simulation of discrete element and finite element. The force and position information calculated using the discrete element method were used as inputs for finite element analysis to analyze the external force and deformation of the molding die, solving the problem of traditional finite element analysis being unable to predict accurate load distribution. The conclusion was that the force and deformation of the molding die gradually increased from top to bottom along the central axis.

Guo (2022) imported the extrusion force data obtained from discrete element method into finite element method for static strength analysis of the core component ring die. The coupling of discrete element and finite element method could obtain more accurate stress distribution. Using extrusion force as the loading condition, the prestressing mode and harmonic response analysis of the ring die forming machine were carried out, and the first six natural frequencies and amplitude frequency response curves in X, Y, and Z directions were obtained. The results indicated that the forming machine was prone to resonance at frequencies of 226, 310, and 366 Hz, corresponding to the first, third, and fifth natural frequencies of modal analysis. This excitation should be avoided during operation.

DISCUSSION

Over the past years, scholars throughout the world have taken ANSYS and ABAQUS as the dominant platforms for biomass densification modelling, integrating the Drucker–Prager model and its Cap extension to construct a complete analysis chain from "temperature–stress–densification" to "die fatigue". The work of Gao (2004) and others demonstrates that when crushed straw is idealized as a continuum, the finite-element method can, within a few hours, yield the stress concentration factor of die holes, the optimal length-to-diameter ratio, and the allowable heating temperature range, delivering a directly usable dimension–load–life curve for industrial ring-die design. Nevertheless, the continuum assumption inherently masks particle geometry, gradation, and local force-chain information, preventing the simulation from explaining the experimentally observed tri-modal failure pattern of "spring-back, cracking, and surface spalling". Moreover, although the Drucker–Prager Cap model captures the coupling between volumetric compression and shear, it is incapable of reproducing the viscous flow of molten lignin or the rearrangement of particles. In short, FEM is highly efficient for macroscopic process optimization, but it possesses an inherent blind spot in microscopic mechanism elucidation.

The emergence of EDEM and PFC has, for the first time, enabled researchers to visualize force-chain arches, stress shielding, and particle rotation trajectories within the forming chamber. Li *et al.* (2015) and others employed a soft-sphere model to back-calculate contact stiffness and found that when the particle size distribution index is about 1.8, energy consumption is minimized and inter-particle locking is most stable. Sha (2022) reproduced arching behavior under uniaxial compression *via* PFC and showed that the contact force at arch feet can reach 3.4 times the average value, serving as the primary locus for crack initiation. These findings provide a mechanical basis for optimizing the inlet cone angle of dies and controlling spring-back. However, DEM reliability is critically dependent on the calibration of contact parameters (stiffness, friction, and bond strength), which are still obtained by reverse trial-and-error against macroscopic stress–strain curves, due to the absence of *in-situ* measurement techniques. Furthermore, particle shapes are reduced to spheres or clumps, ignoring the anisotropy of straw fibers, consequently, the predicted orientation of force chains deviates from XCT observations. Therefore, while DEM excels at revealing the "displacement–force chain–porosity" physical picture, it remains distant from true quantitative prediction.

Confronted with the dual dilemma that FEM cannot describe particle motion and DEM struggles to deliver a full-field die stress, scholars have begun to explore coupling frameworks. Huang (2017) proposed a one-way mapping workflow in which EDEM calculates contact loads and ANSYS performs die-strength verification, reducing the prediction error of maximum wear depth from 35% to 8%. Li (2018) embedded a heat-transfer module in EDEM and implemented bidirectional iteration with ABAQUS's thermal–displacement coupled field, incorporating the temperature-lag effect of particles into die thermal-fatigue assessment for the first time. Going further, Mazor *et al* (2018) transformed DEM data into FEM boundary conditions through coarse-grained methods, which were used to simulate the roll compaction process, providing a new idea for optimizing the roll compaction process parameters and improving product uniformity. Yan (2020) and Guo (2022) treated the time-varying boundary forces from DEM as dynamic loads in FEM, achieving a synchronous "particle–die" solution and successfully capturing two coupled resonance peaks at 226 and 310 Hz, providing direct guidance for vibration-avoidance design of forming machines. Nevertheless, current couplings remain at the level of "force–displacement" transfer, without addressing chemo-thermo-mechanical processes, such as lignin glass transition and moisture evaporation. Moreover, the computational complexity increases exponentially with the number of particles, and the example of millions of particles and 100,000 grids requires hundreds of cores in parallel, which limits its applicability in online optimization. Future efforts must focus on a unified framework for "mesoscopic constitutive laws, heat transfer, and chemical reactions", heterogeneous parallel algorithms, and closed-loop experimental validation to bridge the multi-scale chain from particle to equipment.

CONCLUSIONS

1. The crushed biomass material consists of a great many biomass particles, and the mechanical behavior of the biomass particle system formed can be analyzed based on the theory of particle mechanics. The commonly used theoretical framework for the macroscopic behavior of particulate matter systems is based on the stress-strain constitutive relationship of volume microelements. The situation can be analyzed using elastic-plastic theory, fluid mechanics, *etc*., treating the material as a continuous medium material. However, details, such as particle geometry, particle size distribution characteristics, and particle physical properties, cannot be carefully considered at present. For performing numerical calculations, it is necessary to use some phenomenological parameters to modify the constitutive model of the particle system. Although this is beneficial for numerical calculations, it is not conducive to revealing the inherent physical mechanisms of particle system motion.
2. The discrete element method has undergone decades of development, with significant advancements in various related theories and increasingly mature algorithms. However, due to the inherent lack of theoretical rigor in the discrete element method, the three major elements of motion, force, and deformation are assumed. Under these assumptions, simulation results may deviate significantly from reality. Therefore, how to reasonably determine the relevant parameters in the discrete element and how to reflect the position and role of real joints in biomass densification and molding technology as much as possible requires theoretical improvement.
3. For meeting the trend of research from discontinuous media to continuous media, the coupling of discrete element method and continuous media method is an inevitable trend. The coupling of algorithms can fully leverage their respective strengths and greatly expand the application scope of numerical methods.

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Article submitted: August 1, 2025; Peer review completed: November 22, 2025; Revised version received: November 27, 2025; Accepted: November 30, 2025; Published: January 9, 2026.
DOI: 10.15376/biores.21.1.Ning