ANALYSIS AND CALIBRATION OF PARAMETERS OF BUCKWHEAT GRAIN BASED ON THE STACKING EXPERIMENT
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基于堆积试验的荞麦籽粒离散元参数分析及标定

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ABSTRACT
The stacking test based on response surface method (RSM) was carried out to calibrate the simulation parameters of buckwheat grain by discrete element method (DEM). The static friction coefficient of buckwheat-buckwheat and that of buckwheat-steel are significant factors affecting the repose angle. A quadratic polynomial model for the repose angle and the 2 significant parameters was established and optimized. The optimal combination was obtained: buckwheat-buckwheat static friction coefficient of 0.482, buckwheat-steel static friction coefficient of 0.446. It was found that there was no significant difference between the results of the simulation test and physical test (P>0.05), indicating that the parameter calibration method based on RSM is feasible. The calibrated parameters can provide reference to the simulation of buckwheat production process and machineries design.

ABSTRACT
为了确定离散元模拟所需的荞麦籽粒参数，本文基于堆积试验进行了荞麦籽粒休止角的测量与模拟试验。以得到的休止为响应值，采用响应面法对仿真参数进行了标定。在 Plackett-Berman 试验中，荞麦-荞麦和荞麦-钢板的静摩擦系数是影响休止角的重要因素。根据最陡爬坡试验和中心组合设计的结果，建立了休止角和 2 个显著参数的二次多项式模型，并进行了优化。通过求解优化后的回归方程，得到最佳参数组合：荞麦-荞麦静摩擦系数为 0.482，荞麦-钢静摩擦系数为 0.446。在最佳组合下进行了验证实验。结果表明，验证试验结果与测量试验结果无显著性差异（P>0.05），说明基于响应面法的参数标定方法是可行的。标定参数的优化组合可为荞麦生产过程的离散元模拟仿真及机具设计提供参考。

INTRODUCTION
Coarse cereals having rich nutrition and high economic benefits are grains of an important variety which improve dietary structure and promote nutritional health, as well as important cash crops for improving the income of farmers in old and rural areas. Buckwheat plays an important role in the kingdom as one of the main varieties of coarse cereals. However, buckwheat is a kind of crop with Infinite inflorescence. Its maturity is extremely inconsistent, and the moisture content of the stem in the harvest period is very high, which makes it easily breakable. Therefore, mechanical harvesting faces some difficulties, such as high impurity content, high loss rate and high damage rate, which seriously restrict the development of buckwheat industry.

With the development of computer technology, the discrete element method (DEM) is being used increasingly in agricultural equipment research *(Li Z. et al., 2011; Qiu B. et al., 2012; Li H. et al., 2011; Ma Z. et al., 2017; Zhang T. et al., 2016; Boac J. et al., 2014; Sarnavi H. et al., 2013)*. A comprehensive and systematic simulation study on buckwheat would be helpful to the application of the DEM in the research and development of agricultural equipment for buckwheat production.

It is well known that many parameters are required in DEM simulation, of which the static friction coefficient, rolling friction coefficient and collision recovery coefficient are the basic contact parameters. At present, there are two methods to obtain the parameters: direct measurement and indirect calibration. When the direct measurement method is adopted, the measured values vary widely due to the influence of humidity, material and shape, which create some difficulties in the research and application.

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Therefore, many scholars use computation based "virtual calibration" method to study the parameters. *Yuan C. et al., (2020),* calibrated the simulation parameters of the fermented sheep manure by the skateboard test, and obtained optimal parameters of three kinds of fermented sheep organic manure with different moisture contents. In the collapse experiment, *Liu Y. et al., (2019),* calibrated the static friction coefficient and rolling friction coefficient of rice grains. *Grima A. et al., (2011),* calibrated and verified the rolling friction coefficients required by dry and wet particles in the DEM simulation. Based on the response surface method (RSM), *Santos K. et al., (2015),* measured the dynamic repose angle of dried cherry fruits using a rotary drum device, and calibrated some parameters required in the DEM simulation. *Yu Q. et al., (2020),* determined the optimal contact parameters between Panax notoginseng seeds, and verified the seed metering test.

The stacking test is favored by some scholars because of its convenient and simple operation, and many measurable parameters *(Jia F. et al., 2014; Grima A. et al., 2011)*. However, such studies either adopt a trial and error method or lack a standardized parameter calibration method. So, some scholars have proposed standardized methods for parameter calibration by the DEM based on the RSM *(Liu F. et al., 2016; Wang Y. et al., 2016)*. In this study, taking buckwheat grain as the research object and the repose angle obtained by cylinder lifting as the response value, the simulation parameters were calibrated by the Plackett-Burman (PB) test, steepest climb test and central composite test, and the simulation and real test values were compared and verified. The calibrated parameters of buckwheat grain can provide a reference to the analysis and research on the DEM simulation of production process for buckwheat, such as sowing, threshing and cleaning. It can also help in developing equipment for buckwheat production and realizing production mechanization.

MATERIALS AND METHODS

The buckwheat variety used in the experiment was Heifeng No.1, which was collected from the experimental field. The moisture content of the grain was 13.68% and its density was 698kg/m^3. The real repose angle of buckwheat grains was first measured by the cylinder lifting device, and then the simulation of cylinder lifting was carried out by EDEM 2.7. Taking the obtained repose angle of buckwheat grains as the response value, the simulated parameters of buckwheat grain were calibrated by the PB test, the steepest climb test and center combination test. All tests were designed by Design Expert 10.0. After that, the calibrated optimal parameters were used in simulating the verification test, and drawing conclusions.

Entity measurement test of repose angle

A cylinder lifting test device was used in this research. The three-dimensional design drawing of the device was shown in Fig.1.

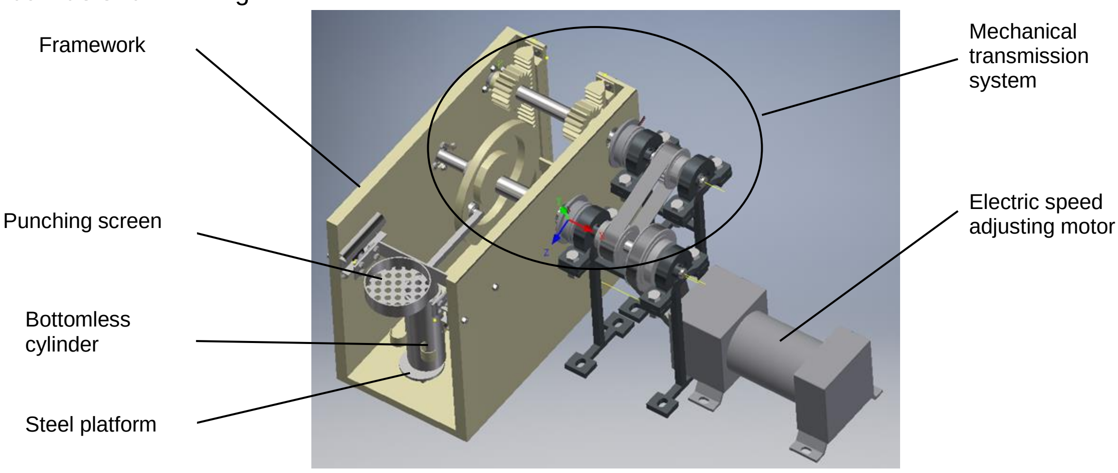


Fig. 1 - The three-dimensional design drawing of test device

A bottomless Q235 steel cylinder was used in the test. The surface roughness of the inner wall of the cylinder was made close to that of the cleaning screen of buckwheat combine harvester, which is about 50μm. The size of the cylinder was determined according to the particle size of buckwheat. The shape of the buckwheat grain is tri-pyramid with a maximum grain size of 7.60mm. Hence, the inner diameter of the cylinder was determined to be 35mm and its height to be 110mm, which conformed to the requirements proposed by *Jia F. et al., (2014)*, that the diameter should be about 4-5 times of the maximum grain size, and the ratio of height to diameter is about 3:1.

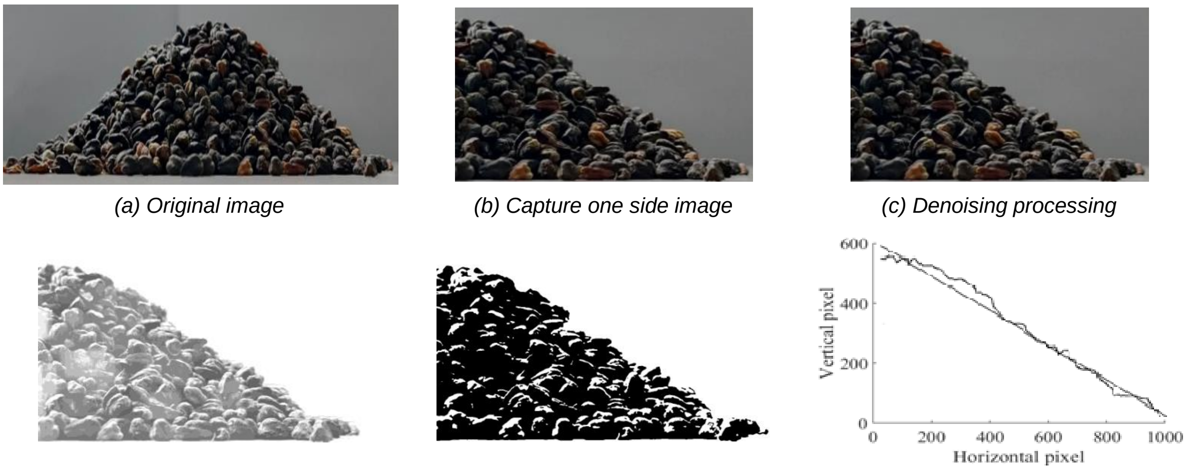
At the time of taking measurement, the cylinder was attached to a fixed horizontal circular steel platform, and filled with buckwheat grains by particle accumulating method *(Sun Q. et al., 2009)*. Then the cylinder was lifted by a driving mechanism at a constant speed of 0.05 m/s, and then a pile with pyramidal grains was formed on the circular platform as shown in Fig.2 *(Li Q. et al., 2010)*. When the artesian surface of the heap became relatively static, the angle between the artesian surface and the horizontal plane was measured, which was the repose angle. The test was repeated for 5 times.

Fig. 2 - Experiment of buckwheat grain cylinder lifting

In order to improve the measurement accuracy and to avoid human error as far as possible, Image J and MATLAB software were used in this paper to process the images collected under the above experimental conditions. The procedure is shown in Fig. 3. The slope of the fitted line was determined by counting pixels in both horizontal and vertical directions, and the repose angle was obtained by calculating the inverse tangent of the slope of the line as shown in Formula (1).

$$\theta = \frac{tan^{-1}|k| \times 180^{\circ}}{\pi} \tag{1}$$

where: θ is the repose angle and k is the slope of the fitted line.



(a) Original image *(b) Capture one side image* *(c) Denoising processing*

(d) Gray processing *(e) Threshold segmentation* *(f) Linear fitting*

Fig. 3 - Image processing procedure of repose angle of buckwheat grain

After the cylinder lifting test, image process and data analysis, the results of 5 entity tests were obtained. The mean repose angle and standard deviation of buckwheat granules are 30.148° and 0.518°, respectively.

Contact model and parameters

In the simulation, the Hertz-Mindlin (no slip) contact model was adopted. The normal force (N) and tangential force (T) of buckwheat-buckwheat particles and buckwheat particles-geometric bodies are determined by formulas (2) and (5), respectively, *(Sun Q. et al., 2009)*.

The normal force (N) between particles:

$$N = \frac{4}{3}E^{*}(R^{*})^{1/2}\delta_n^{3/2} \tag{2}$$

where:

δ_n represents the normal overlapping of particle 1 and particle 2; E^* is equivalent elastic modulus; and R^* is the equivalent particle radius. R^*, E^* are calculated by formulas (3) and (4), respectively.

$$\frac{1}{R^*} = \frac{1}{R_1} + \frac{1}{R_2} \tag{3}$$

$$\frac{1}{E^*} = \frac{1-\nu_1^2}{E_1} + \frac{1-\nu_2^2}{E_2} \tag{4}$$

where: R_1, E_1, ν_1; R_2, E_2, ν_2 are the radius, elastic modulus and Poisson's ratio of particle 1 and particle 2, respectively.

The tangential force (T) between particles:

$$T = -S_t \delta_t \; ; \; S_t = 8G^* \sqrt{R^* \delta_n} \tag{5}$$

where: δ_t is the tangential overlap; and S_t is the tangential stiffness. G^* is the equivalent shear modulus, which is calculated by formula (6).

$$G^* = \frac{2-\nu_1}{G_1} + \frac{2-\nu_2}{G_2} \tag{6}$$

where: G_1 and G_2 are the shear modulus of the two particles, which are determined from the relations of the corresponding elastic modulus and Poisson's ratios as expressed by formula (7).

$$G_1 = \frac{E_1}{2(1+\nu_1)}; \; G_2 = \frac{E_2}{2(1+\nu_2)} \tag{7}$$

Buckwheat grains are complex and diverse, and some parameters are dispersed. According to the reported results of agricultural material and DEM simulation, Table 1 describes the parameters and range *(Hou H., 2019; Sun J., 2019; Keppler I. et al., 2012)*.

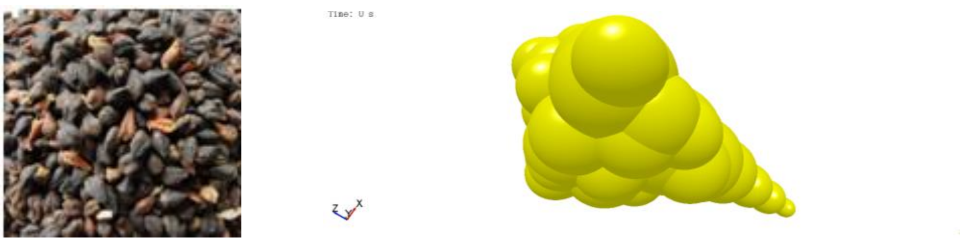
Table 1

Parameters and value required in DEM simulation

Parameters	Value
Poisson's ratio of buckwheat	0.16~0.42
Buckwheat shear modulus /MPa	6.81~61.84
Buckwheat density /(kg/m^3)	698
Poisson's ratio of steel plate	0.30
Steel plate shear modulus / MPa	70000
Steel plate density /(kg/m^3)	7800
Buckwheat-buckwheat restitution coefficient	0.10~0.26
Buckwheat- steel plate restitution coefficient	0.20~0.80
Buckwheat-buckwheat coefficient of static friction	0.32~0.60
Buckwheat- steel plate coefficient of static friction	0.18~0.58
Buckwheat-buckwheat coefficient of rolling friction	0.03~0.08
Buckwheat-steel plate coefficient of rolling friction	0.02~0.09

Development of discrete element model

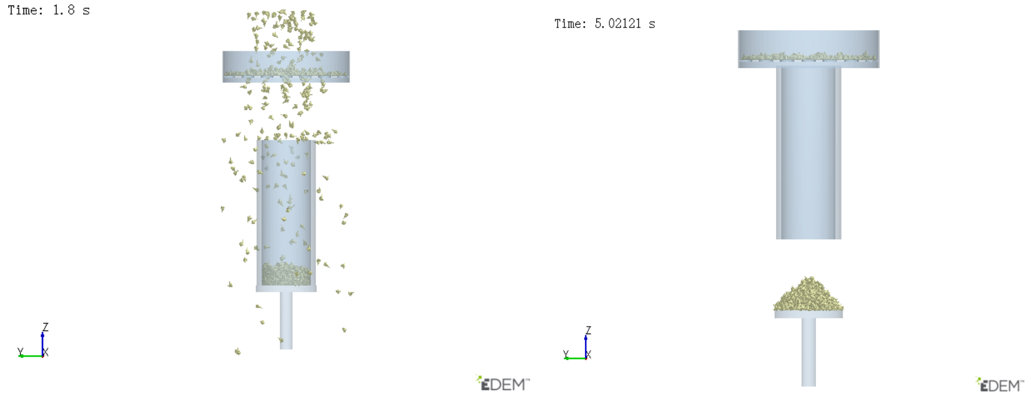
The buckwheat grain used in this test is almost of a tri-pyramid shape. Its structure is shown in Fig. 4 (a). According to the measured tri-axial dimensions (the average height of 5.90mm, and the three bottom edges of 3.94mm, 3.92mm and 3.93mm respectively), the contour of buckwheat grain was established in AutoCAD, which was imported into EDEM 2.7 during the setting of the parameters of simulated materials. Nine overlapping spherical particles were manually filled in the CAD contour to get buckwheat particles. While filling, the radius and spherical coordinate of each spherical particle need to be specified to clarify the position relationship between spherical particles. The model of buckwheat grain is shown in Fig. 4 (b).



(a) *(b)*

Fig. 4 - Buckwheat grain and DEM model

The model of a bottomless steel cylinder and a horizontal steel plane of the same size as the solid test was imported into the EDEM 2.7, and the size of buckwheat grain was dynamically generated according to the standard normal state, whose mean value was 1, and standard deviation was 0.05. The generating rate was 3000 per second, and which poured into the cylinder at a vertical velocity of 0.5 m/s. When the cylinder was filled with buckwheat grains, the calculation area was reset. The cylinder was set to move vertically upward at a speed of 0.05 m/s. In this experiment, 25% of the Rayleigh time was used. The simulation time was 5.5s. The simulation process is shown in Fig. 5. After the completion of the simulation, the size of the simulation interface was made the same, and the image of repose angle was obtained by the screenshot processing. The measuring method for repose angle is the same as that of entity measurement test.



(a) (b)

Fig. 5 - The simulation process

Plackett - Burman test

Many parameters will be used in the DEM simulation. If all of them are calibrated, it is difficult to achieve. Therefore, the PB test was performed to screen out the parameters having significant influence on the repose angle. Out of the parameters related to the buckwheat grains used in the DEM simulation, 8 were selected as parametric variables and 3 were kept in reserve as dummy variables for error analysis. In this paper, a PB table with N=12 was used. The repose angle was taken as the response value, and 2 levels of each variable were taken as high (+1) and low (-1). Table 2 shows the factors and levels for simulation.

Table 2

Factors and levels of Plackett-Burman experiment

Factors		Levels	
Symbol	**Parameters**	**Low level (-1)**	**High level (+1)**
A	Poisson's ratio of buckwheat	0.16	0.42
B	Buckwheat shear modulus / MPa	6.81	61.84
C	Buckwheat-buckwheat restitution coefficient	0.10	0.26
D	Buckwheat-steel plate restitution coefficient	0.20	0.80
E	Buckwheat-buckwheat coefficient of static friction	0.32	0.60
F	Buckwheat-steel plate coefficient of static friction	0.18	0.58
G	Buckwheat-buckwheat coefficient of rolling friction	0.03	0.08
H	Buckwheat-steel plate coefficient of rolling friction	0.02	0.09
I_1, I_2, I_3	Virtual parameters	—	—

The steepest climb test

According to the results of the PB test, it is difficult to establish an effective response surface fitting equation. The best region of each significant factor can be approached quickly and economically by the steepest climb test. In this test, the direction of the climb path was determined according to the positive and negative effects of the significant factors in the PB test. The step size was determined by the t-value of effect.

The central combination test

After approximating the optimal response area by the steepest climb test, the response surface analysis was carried out by the central combination test. Five levels of significant factors and the average level of the non-significant factors were selected. Meanwhile, 5 central points were used in the design. According to the test results, the regression equation was obtained by fitting the response surface model, and the best combination of simulation parameters of buckwheat grain closest to the actual angle of repose was predicted.

RESULTS

Results of Plackett - Burman test

The design and results are shown in Table 3, and Table 4 shows the results of ANOVA. The static friction coefficient of buckwheat-steel plate and that of buckwheat-buckwheat had significant influence on the repose angle (P<0.1), while the influence of other factors was not significant (P>0.1). Therefore, only the two significant factors were selected for the steepest climb test.

Table 3

Design and results of Plackett-Burman test

No.	Factors											Repose angle θl (deg)
	A	*B*	I_1	*C*	*D*	I_2	*E*	*F*	I_3	*G*	*H*	
1	1	-1	1	1	1	-1	-1	-1	1	-1	1	9.265
2	-1	1	1	-1	1	1	1	-1	-1	-1	1	15.329
3	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	9.110
4	1	1	-1	-1	-1	1	-1	1	1	-1	1	22.968
5	1	-1	1	1	-1	1	1	1	-1	-1	-1	24.444
6	-1	1	1	1	-1	-1	-1	1	-1	1	1	27.597
7	-1	-1	1	-1	1	1	-1	1	1	1	-1	21.647
8	1	1	1	-1	-1	-1	1	-1	1	1	-1	9.902
9	-1	-1	-1	1	-1	1	1	-1	1	1	1	14.425
10	1	1	-1	1	1	1	-1	-1	-1	1	-1	12.150
11	1	-1	-1	-1	1	-1	1	1	-1	1	1	29.954
12	-1	1	-1	1	1	-1	1	1	1	-1	-1	30.784

Table 4

Analysis of significance of parameters in Plackett-Burman test

Parameters	Sum of squares	*F* value	*P* value	Significance
A	8.69	1.25	0.3445	5
B	8.14	1.17	0.3578	6
C	7.93	1.14	0.3632	7
D	9.51	1.37	0.3260	4
E	40.70	5.87	0.0939*	2
F	633.84	91.44	0.0024**	1
G	1.19	0.17	0.7067	8
H	11.02	1.59	0.2964	3

Note: "" and "**" represent significant levels of 0.1 and 0.01, respectively.*

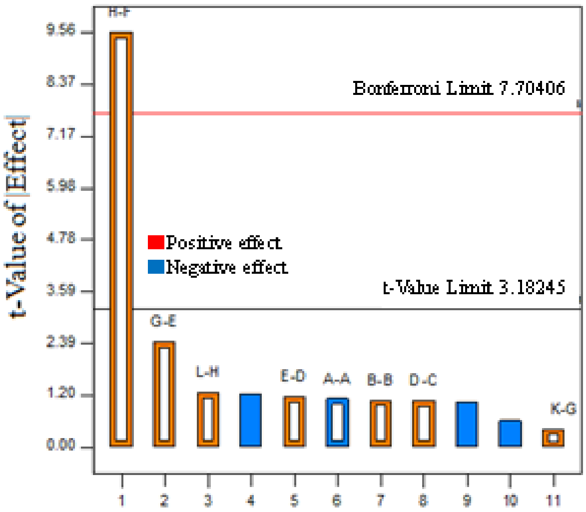


Fig .6 - Pareto chart of Plackett-Burman experiment

The Pareto chart (Fig. 6) shows that the static friction coefficient of buckwheat-steel and that of buckwheat-buckwheat had positive effects on the repose angle. Hence, the two factors became the rising path in the steepest climb test.

Results of the steepest climb test

Table 5 shows the design and results of the steepest climb test. With increasing static friction coefficient of buckwheat-steel plate and that of buckwheat-buckwheat, the relative error of the repose angles between the simulation and solid tests first decreased and then increased. The No.4 had the smallest error, indicating that the optimal area of each factor was near test 4. Therefore, the static friction coefficient of buckwheat-buckwheat and that of buckwheat-steel plate were taken as 0.48 and 0.45, respectively, which were selected as the center points for subsequent response surface tests.

Table 5

Design and results of steepest ascent test

No.	Buckwheat-buckwheat static friction coefficient (*E*)	Buckwheat- steel static friction coefficient (*F*)	Repose angle *θ*/ (deg)	Relative error /%
1	0.30	0.15	9.348	68.99
2	0.36	0.25	19.389	35.69
3	0.42	0.35	28.097	6.80
4	0.48	0.45	29.766	1.26
5	0.54	0.55	31.601	4.82
6	0.60	0.65	33.085	9.74

Results of the central composite design

According to the result above, the center combination test of 2 factors with 5 levels was designed. Table 6 shows the design and results. A quadratic polynomial fitting was performed, and the regression model between the repose angle and significant parameters was developed as follows:

$$\theta = 59.714 - 107.570E - 43.457F + 121.167EF + 70.678E^2 - 3.890F^2 \quad (8)$$

Table 6

Results of the central composite design

No.	Buckwheat-buckwheat static friction coefficient (*E*)	Buckwheat- steel static friction coefficient (*F*)	Repose angle *θ*/（deg）
1	1（0.54）	-1（0.35）	29.176
2	0（0.48）	0（0.45）	30.913
3	-1（0.42）	-1	28.643
4	0	0	30.481
5	0	0	30.271
6	0	1.414（0.591421）	31.554
7	0	0	29.619
8	-1.414（0.395147）	0	29.757
9	0	-1.414（0.308579）	29.002
10	1.414（0.564853）	0	31.972
11	0	0	29.685
12	-1	1（0.55）	29.865
13	1	1	33.306

Table 7

ANOVA of the steepest ascent test

Source of variation	Freedom	Mean square	*F* value	*P* value
Model	5	3.79	14.17	0.0015*
E	1	6.31	23.06	0.0018*
F	1	10.04	37.52	0.0005*
EF	1	2.11	7.90	0.0261*
E^2	1	0.45	1.68	0.2357
F^2	1	0.011	0.039	0.8484
Residual	7	0.27		
Lack of fit	3	0.23	0.76	0.5740
Pure error	4	0.30		
Sum	12			
R^2=0.9101，R^2_{Agj}=0.8459；C.V.=1.71%；Adeq precision=13.128				

*Note: * shows the term is significant(P<0.05).*

The Analysis of variance (ANOVA) of this model is shown in Table 7. The *P*-value of the model was 0.0015 (*P*<0.01), which indicated that the independent and dependent variables in this model were highly correlated. The fitting degree of the model equation was good. The static friction coefficient of buckwheat-buckwheat, and that of buckwheat-steel plate, and the interaction between them had a significant influence on the repose angle of buckwheat grain. While the loss fitting term, which was 0.5740 (*P*>0.05), had no significant effect. The precision of the regression equation was 13.128, the correlation coefficient was 0.9101, and the correlation coefficient of calibration was 0.8459, which indicated that the model was highly reliable and the predicted value was correlated with the measured value.

In order to further optimize the model equation, on the premise of ensuring good significance and high correlation coefficient of the model, non-significant factors were eliminated, and then the optimized regression equation was obtained as follows:

$$\theta = 60.799 - 108.921E - 46.958F + 121.167EF + 72.086E^2 \tag{9}$$

The ANOVA was performed for the optimized model (Table 8), and the fitting model (*P*=0.0003) was significantly improved after the optimization. The coefficient of variance was reduced to 1.60%, and the test reliability was further increased. The correlation coefficient was 0.9096, and the correction adjustment coefficient was 0.8644, both were close to 1, which indicated that the model had a high degree of fitting. The precision was increased to 15.219, about 16% higher than that before optimization.

Table 8

ANOVA of the modified model of central composite design experiment

Source of variation	Freedom	Mean square	*F* value	*P* value
Model	4	6.13	36.10	0.0003*
E	1	6.31	37.17	0.0008*
F	1	6.06	35.66	0.0002*
EF	1	6.02	35.46	0.0172*
E^2	1	0.48	2.02	0.1926
Residual	8	0.24		
Lack of fit	4	0.17	0.58	0.6970
Pure error	4	0.30		
Sum	12			
R^2=0.9096, R^2_{Agj}=0.8644; C.V.=1.60%; Adeq precision=15.219				

Note: shows the term is significant (P<0.05).*

Interactive effect of regression model

Table 8 shows the Interactive term (*EF*) between the static friction coefficient of buckwheat-buckwheat and that of buckwheat-steel had a significant influence on the repose angle (*P*<0.05).

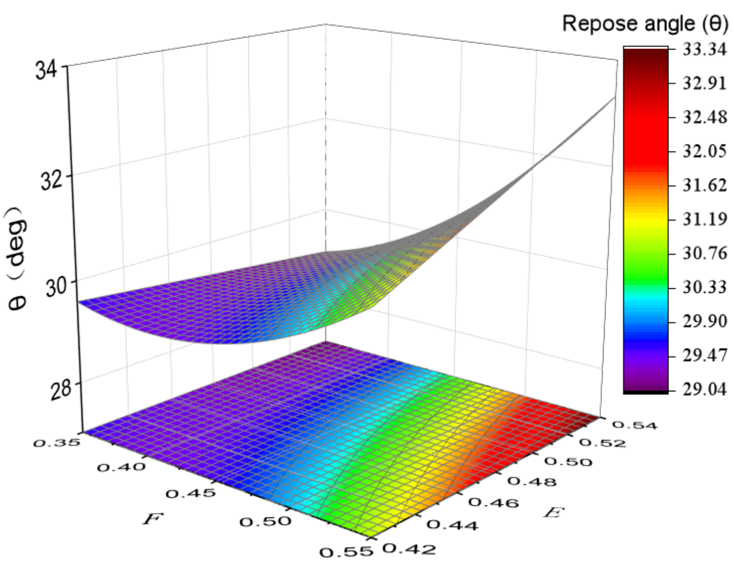


Fig. 7 - Response surface of interaction

As seen in the Fig.7, the repose angle increased with the static friction coefficient of buckwheat-steel and buckwheat-buckwheat. And the increasing rate with the static friction coefficient of buckwheat-steel was larger than that with the static friction coefficient of buckwheat-buckwheat. When either of the two parameters was taken as the larger value, the increasing trend of the repose angle with the increase of the other parameter is greater than that with the former parameter being smaller.

Determination of optimal parameter combination and test verification

Making the measured repose angle of buckwheat grain as the starting point of the optimized regression model, the optimal parameter combination close to the target value was obtained: the static friction coefficients of buckwheat-buckwheat and buckwheat-steel plate are 0.482 and 0.446, respectively.

Fig. 8- Verification of the repose angle by DEM simulation

In order to verify the accuracy and effectiveness of the optimal parameters obtained by the RSM, the calibrated simulation parameters were used in verification test (Fig.8). In the test, the Poisson's ratio was 0.29, and the elastic modulus was 34.325 MPa. The static friction coefficient of buckwheat-buckwheat was 0.482, and that of buckwheat- steel was 0.446. The rolling friction coefficient of buckwheat-buckwheat was 0.055, and that of buckwheat- steel was 0.055. The recovery coefficient of buckwheat-buckwheat was 0.180, and that of buckwheat-steel was 0.500. The experiment was repeated for 3 times, in which the repose angles were 30.121°, 31.574° and 29.283°, respectively, with an average value of 30.321°. The T test was carried out on the results, where *P* value is 0.7685 ($P>0.05$), indicating that there was no significant difference between the simulation value and the measured value, indicating that the agreement was good.

CONCLUSIONS

(1) The static friction coefficient of buckwheat-buckwheat and that of buckwheat-steel had significant influences on the repose angle of buckwheat grain. And the Poisson's ratio, shear modulus, recovery coefficient and rolling friction coefficient had no significant influence on the repose angle.

(2) A quadratic polynomial model for the repose angle and the 2 significant parameters was established and optimized. Furthermore, the 2 significant parameters and their interaction had significant effects on the repose angle of buckwheat grain.

(3) The optimal combination of the parameters of buckwheat grain obtained by calibration were as follows: the Poisson's ratio of 0.29, elastic modulus of 34.325MPa. The buckwheat-buckwheat static friction coefficient of 0.482, rolling friction coefficient of 0.055, and recovery coefficient of 0.180. The recovery coefficient was 0.500, static friction coefficient was 0.446, and rolling friction coefficient was 0.055 between buckwheat grain and steel plate. There was no significant difference between the repose angle of buckwheat grain obtained from the verification test and solid test ($P>0.05$), indicating that the model can be used to predict the repose angle of buckwheat grain. The response surface method was feasible to calibrate the discrete element parameters of buckwheat grain based on the stacking test, which could improve the accuracy of the DEM simulation.

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