

GREY RELATIONAL ANALYSIS OF MECHANICAL PROPERTIES AND MAJOR CHEMICAL COMPONENTS OF WHEAT GRAINS

小麦籽粒力学特性及其与主要化学成分灰色关联度研究

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ABSTRACT

To reduce mechanical damage to wheat grains during planting, harvesting, transportation, storage, and processing, the mechanical properties of ten wheat varieties were investigated. The grain compression process was simulated and analyzed using ANSYS software. Moisture content was selected as a single factor to evaluate its effect on grain mechanical properties. In addition, the chemical composition of the grains, including moisture, starch, protein, fat, and fiber content, was analyzed, and grey relational analysis was conducted to evaluate the relationship between mechanical properties and chemical components. The results showed that the crushing load ranged from 68.09 to 170.51 N, the elastic modulus from 23.88 to 158.46 MPa, and the hardness from 30.60 to 57.86 N/mm. The average moisture, starch, protein, fat, and fiber contents were 13.26%, 56.72%, 12.94%, 2.54%, and 3.81%, respectively. The grey relational analysis indicated that fiber and protein exhibited the strongest correlations with the mechanical properties of wheat grains. The correlation values between crushing load and chemical components ranged from 0.5994 to 0.6888, those for elastic modulus ranged from 0.5877 to 0.7127, and those for hardness ranged from 0.5964 to 0.7192. These findings provide a theoretical basis for the design and optimization of agricultural machinery for wheat harvesting, handling, drying, and processing, as well as for wheat breeding.

摘要

为了降低小麦籽粒在种植、收获、运输、储藏及加工过程中的机械破碎与损伤，对 10 个品种的小麦籽粒进行了力学特性研究。通过 ANSYS 软件，对籽粒压缩过程进行了仿真分析。选取含水率作为单因素变量，研究籽粒力学特性与含水率的变化规律。同时，对籽粒含水率、粗淀粉、粗蛋白、粗脂肪和粗纤维等化学组分含量进行了研究分析，获取小麦籽粒力学特性与其主要化学组分灰色关联度特性。试验结果表明，籽粒破碎负载范围为 68.09~170.51N，弹性模量范围为 23.88~158.46MPa，硬度范围为 30.60~57.86N/mm。其含水率、粗淀粉、粗蛋白、粗脂肪和粗纤维含量平均值分别为 13.26%、56.72%、12.94%、2.54%、3.81%。籽粒破碎负载与各化学组分的关联度分别为 0.6066、0.6128、0.6690、0.5994、0.6888；籽粒弹性模量与各化学组分的关联度分别为 0.6215、0.6119、0.6557、0.5877、0.7127；籽粒硬度与各化学组分的关联度分别为 0.7192、0.5964、0.6755、0.6522、0.6960。该研究结果可为小麦收获、运输、干燥及加工等农机具的设计和作物品种选育提供参考和依据。

INTRODUCTION

Wheat is a kind of cereal crop widely planted around the world. Its total output is second only to corn and ranks second in the world (Qiu et al., 2019). As one of the three major cereals, it is rich in starch, fat, protein and vitamins (Kaliniewicz et al., 2023). Wheat is subjected to loads during harvesting, transportation, drying and storage, which causes internal stress in the wheat grains and the grains to rupture or permanently deform (Zhang et al., 2023). All that will in turn affects its utilization rate, character and seed germination rate (Kenghe et al., 2012; Ficco et al., 2020; Fu et al., 2022). Therefore, it is great significance to study the mechanical properties of wheat grains.

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Scholars at home and abroad had done a lot of work on the mechanical properties of grains and had obtained many useful results. *Lü et al. (2013)* studied the effect of the chemical composition of roots on their mechanical properties. The experimental results showed that root tension was positively correlated with cellulose content, hemicellulose content, and total cellulose content, and negatively correlated with lignin content and the ratio of lignin to cellulose content. The tensile strength of roots was negatively correlated with cellulose content, hemicellulose content, and total cellulose content, and positively correlated with lignin content and the ratio of lignin to cellulose content. The effect of root chemical composition on tensile strength and tensile strength varied for different tree species.

Zhang et al. (2017) conducted chemical composition, penetrometer indentation, shear, and compression tests on various soybean seeds, measuring the content of crude protein, crude fat, crude starch, and crude fiber, as well as the range of seed hardness, damage strength, and ultimate shear force. The results of grey relational analysis showed that the mechanical indicators most closely related to chemical component content were hardness and contact stiffness. The content of crude protein and crude fat had the greatest impact on hardness and contact stiffness, followed by crude cellulose and crude starch content. The research results could provide new methods and basis for quality prediction and variety identification.

Kaliniewicz et al. (2022) studied the morphology and mechanical properties of seven wheat grains and their correlation. The experimental results indicated that the morphological and mechanical properties of grain and the correlations between these traits were investigated in seven Polish genotypes of durum wheat. Hardness index (HI) values (81–89) were relatively similar. The highest HI values were noted in grains with a thickness of 2.90–2.95 mm. Grain structure was damaged within a deformation range of around 18–21%. Rupture force, rupture energy and HI values increased with a rise in grain vitreousness. Rupture force was lowest in grains with vitreousness of 70–75%.

Zhang et al. (2025) conducted a comparison between naturally dehydrated corn (CK) and corn treated with desiccants (SY) and analyzed the moisture content of various plant organs, grain starch composition, and puncture resistance characteristics across three grain regions during maturation. In both treatments, decreasing grain moisture content led to the development of a thicker and denser internal cuticle layer, which increased the yield load and elastic modulus in the lateral and apical grain regions. When grain moisture content dropped below 25%, the SY group exhibited significantly higher yield load and elastic modulus than the CK group.

Although scholars at home and abroad have done a lot of research on the mechanical characteristics of rice, corn and soybean, the research objects and mechanical indicators were scattered, and the selection of factors affecting the mechanical indicators was relatively simple. The research studied on the correlation between mechanical indexes and chemical components of different wheat varieties were relatively little. In this study, a universal testing machine was used to perform puncture and compression tests on wheat grains to determine their mechanical properties. Using ANSYS software, the finite element simulation of the grain compression process was performed. At the same time, relevant experiments were performed on chemical components of wheat grains, and the correlation between the mechanical indexes of wheat grains and chemical components was studied and analyzed. The research results could provide reference and basis for the design of agricultural machinery and crop breeding such as wheat harvesting, transportation, drying and processing.

MATERIALS AND METHODS

Experimental materials

In order to ensure the scientific validity and versatility of the test results, the wheat samples was collected from multiple varieties across different regions of the country. In order to reduce the random error, the wheat varieties used in the test require full grains, no damage and no pests. The relevant physical characteristics of various wheat varieties are shown in Table 1.

Table 1

Related physical parameters of each wheat variety tested

Variety no.	Variety name	Planting area	1000 grain weight / g	Length / mm	Width / mm	Height / mm
1	Zhou Mai 18	Zhoukou City, Henan Province	48.2	6.93±0.35	3.56±0.16	3.27±0.21
2	Yang Mai 16	Yancheng City, Jiangsu Province	40.0	6.93±0.48	3.34±0.27	3.02±0.23
3	Yan Nong 19	Yantai City, Shandong Province	42.3	6.49±0.43	3.27±0.35	2.94±0.19

Variety no.	Variety name	Planting area	1000 grain weight / g	Length / mm	Width / mm	Height / mm
4	Ji Mai 22	Zaozhuang City, Shandong Province	45.5	6.65±0.47	3.37±0.22	3.02±0.21
5	Liao Chun 23	Shenyang City, Liaoning Province	36.8	6.38±0.45	3.05±0.30	2.74±0.19
6	Liang Xing 77	Heze City, Shandong Province	47.4	6.39±0.36	3.38±0.32	3.16±0.32
7	Yu Mai 68	Shangqiu City, Henan Province	50.1	6.98±0.47	3.65±0.18	3.35±0.19
8	Chuan Mai 602	Bazhong City, Sichuan Province	46.7	7.26±0.51	3.57±0.22	3.10±0.29
9	Jin Mai 101	Changzhi City, Shanxi Province	44.8	6.51±0.55	3.54±0.25	3.11±0.28
10	Yun Mai 69	Kunming City, Yunnan Province	43.2	6.39±0.48	3.47±0.35	2.74±0.21

Test equipment for mechanical property

The mechanical property tests were conducted using an Instron 3340 series single-column universal testing machine (maximum load: 1000 N; force resolution: 0.001 N; displacement resolution: 0.001 mm), along with a vernier caliper and a digital camera.

Chemical composition analysis equipment and drugs

The equipment used in the chemical composition measurement test includes K9860 automatic Kjeldahl nitrogen analyzer, SHZ-D circulating water vacuum pump, DHG-9240A electric heating blast drying box, ME204 electronic balance, HH-8 electric heating thermostatic water bath, SHA-CA type water bath constant temperature oscillator, etc. Chemical reagents mainly include potassium iodide, anhydrous ethanol, petroleum ether, ether, toluene, hydrochloric acid, sodium hydroxide, copper sulfate, potassium sodium tartrate, potassium ferrocyanide, methyl red, glucose, etc.

Analysis method of mechanical properties

The mechanical properties of wheat grains measured by experiments were mainly divided into crushing load and hardness. The crushing load data was obtained through a compression test. The compression test indenter was a flat indenter. Since the wheat grains were similar to an ellipsoid, the lower indenter was provided with a sample placement groove to prevent the grain from sliding during the compression process (Dai *et al.*, 2016). During the test, the wheat sample was placed in the groove of the fixed lower indenter. The upper indenter was loaded vertically at a speed of 1 mm / min. When the static crushing load displayed on the operation interface reached the peak, the loading was stopped and the crushing load was read by the test system operation interface. According to Hertzian contact theory and related derivations (Jiang *et al.*, 2020) the elastic modulus was calculated using Eq. (1). Each test was repeated five times, and the average value was used.

$$E = \frac{3F(1 - \mu^2 \sqrt{HK^3(B^2 + L^2)})}{\pi D^{3/2} BL} \quad (1)$$

where:

E is the elastic modulus of wheat grains, MPa; F is the external load applied, N;

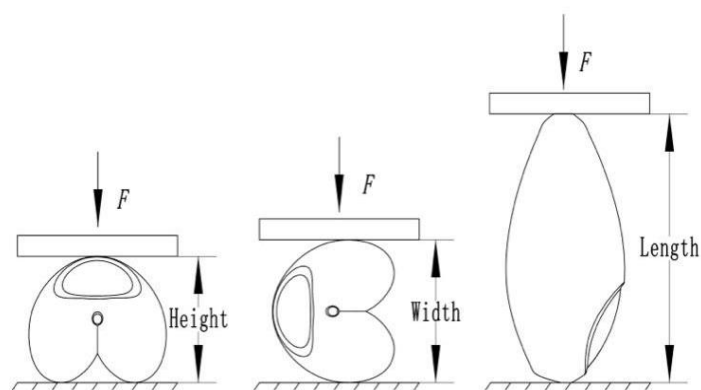
μ is the Poisson's ratio of the material. The Poisson's ratio of most agricultural materials is in the range of 0.2 to 0.5. The Poisson's ratio of wheat grains is 0.4 (Dai *et al.*, 2016; Ren *et al.*, 2025);

L , B , and H are the length, width and height of the wheat grains, respectively, mm;

K is a constant, and its value depends on the angle between the principal curvature radius of the contact point and the normal plane of the principal curvature;

D is the amount of deformation in the grain compression process, mm.

According to the different placement methods of wheat grains during the experiment, compression tests were divided into M-type compression, B-type compression, and D-type compression, as shown in Fig.1.



a. M-type compression b. B-type compression c. D-type compression

Fig. 1 - Compressed form of wheat grain

Grain hardness was determined using a puncture test. This method employs a universal testing machine to record the load-deformation curve during needle penetration into the wheat grain, and the hardness is calculated from the slope of the curve. The steel needle used in the test had a diameter of 1.2 mm, a length of 70 mm, and a tip angle of 22.6° (Ibrahim et al., 2018; Li et al., 2025). The indentation depth was set to 0.4 mm, and the loading speed was 1 mm/min. Each test was repeated three times.

Chemical component content analysis method

The chemical composition of wheat grains tested mainly included moisture, crude starch, crude protein, crude fat and crude fiber (Zheng et al., 2017). Each chemical index of each variety was measured 5 times and the average value was calculated. The specific measurement methods of each index are shown below.

The moisture content was determined using the 105 °C oven-drying method. The calculation is given in Eq. (2).

$$W_1 = \frac{m_1 - m_2}{m_1 - m_3} \times 100 \quad (2)$$

where:

W_1 is the moisture content, %; m_1 is the total mass of the sample and the weighing bottle before drying, g; m_2 is the total mass of the sample and the weighing bottle after drying, g; m_3 is the mass of the empty weighing bottle, g.

The crude starch mass fraction was determined using the method shown in Eq. (3).

$$W_2 = \frac{(m_4 - m_5) \times 0.9}{m_6 \times 1000} \times 100 \quad (3)$$

where:

W_2 is the crude starch mass fraction, %; m_4 is the glucose content in the sample, mg; m_5 is the reagent blank value, mg; m_6 is the mass of the sample, g; 0.9 is the conversion factor from glucose to starch.

The crude protein mass fraction was determined using the Kjeldahl method. The calculation is given in Eq. (4).

$$W_3 = \frac{(V_1 - V_2) \times c \times 0.014}{\frac{m_7}{100} \times 10} \times N \times 100 \quad (4)$$

where:

W_3 is the crude protein mass fraction, %; V_1 is the volume of standard hydrochloric acid solution consumed during sample titration, ml; V_2 is the volume of hydrochloric acid solution consumed during blank titration, ml; c is the concentration of the hydrochloric acid standard solution, mol/L; m_7 is the mass of the sample, g; N is the nitrogen-to-protein conversion factor, typically taken as 6.25 for food materials (Zhang et al., 2017).

The crude fat mass fraction was determined using the method shown in Eq. (5).

$$W_4 = \frac{m_8 - m_9}{m_{10}} \times 100 \quad (5)$$

where: W_4 is the crude fat mass fraction, %; m_8 is the mass of the receiving bottle and fat after drying to constant weight, g; m_9 is the mass of the empty receiving bottle, g; m_{10} is the mass of the sample, g.

The crude fiber mass fraction was determined using the method shown in Eq. (6).

$$W_5 = \frac{A_1 - A_2}{m_{11} \times (100 - S)} \times 100 \quad (6)$$

where: W_5 is the crude fiber mass fraction, %; A_1 is the mass of the crucible, crude fiber, and residue, g; A_2 is the mass of the crucible and residue after ashing, g; m_{11} is the mass of the air-dried sample, g; S is the moisture content of the sample, %.

Correlation analysis method of mechanical properties and chemical components of wheat

According to the needs of the gray system theory, the mechanical index and the chemical composition are considered as a whole, in which the mechanical characteristic index is set as a reference sequence, and the chemical composition index is set as a comparison series to construct a gray system (Guo et al., 2012; Zhang et al., 2017). Due to inconsistencies in the units of different indicators, the data were standardized prior to grey relational analysis using Eq. (7) to eliminate dimensional effects.

$$X'_i(k) = \frac{X_i(k) - \bar{X}_i}{S_i} \quad (7)$$

where:

$X'_i(k)$ is the normalized value of the i -th indicator for the k -th sample, $X_i(k)$ is the original value of the i -th indicator for the k -th sample, \bar{X}_i is the mean value of the i -th indicator, S_i is the standard deviation of the i -th indicator.

The absolute difference between the reference sequence and each comparison sequence was calculated using Eq. (8).

$$\Delta_i(k) = |X'_0(k) - X'_i(k)| \quad (8)$$

where: $\Delta_i(k)$ is the absolute difference between the i -th indicator of the k -th sample and the corresponding reference sequence, $X'_0(k)$ is the normalized value of the reference sequence for the k -th sample and $X'_i(k)$ is the normalized value of the i -th indicator for the k -th sample.

In grey system theory, the grey relational coefficient between the reference sequence and the comparison sequence reflects the degree of similarity between each indicator and the reference value. The larger the coefficient, the closer the indicator is to the reference sequence. The grey relational coefficient is calculated using Eq. (9).

$$\zeta_i(k) = \frac{\min_i \min_k \Delta_i(k) + \rho \max_i \max_k \Delta_i(k)}{\Delta_i(k) + \rho \max_i \max_k \Delta_i(k)} \quad (9)$$

where: $\zeta_i(k)$ is the grey relational coefficient between the i -th comparison sequence and the reference sequence at the k -th sample, ρ is the distinguishing coefficient, with a value in the range of 0 to 1, typically taken as 0.5.

The grey relational grade reflects the overall closeness between each comparison sequence and the reference sequence, and is calculated using Eq. (10). A larger relational grade indicates a stronger relationship between the comparison sequence and the reference sequence. The indicators are ranked according to the magnitude of the grey relational grade.

$$r_i = \frac{1}{N} \sum_{k=1}^N \zeta_i(k) \quad (10)$$

where: r_i is the grey relational grade of the i -th comparison sequence, N is the number of samples.

Finite Element Analysis of Mechanical Properties of Wheat Grain

Finite element analysis was performed using ANSYS software to investigate the mechanical behavior of wheat grains during compression. First, a finite element model of the wheat grain was established, followed by the application of appropriate boundary conditions and loading for the simulation.

Construction of wheat grain geometric model

The geometric model of the wheat grain was constructed based on its physical dimensions. The wheat cultivar Ji Mai 22 was selected, with a grain length of 6.65 mm, width of 3.37 mm, and thickness of 3.02 mm.

Material properties definition and meshing of wheat grain

In the simulation compression test of wheat grains, the setting of the elastic modulus of wheat grains under three compression forms referred to the results of the mechanical performance bench test of wheat grains. The Poisson's ratio was set to 0.4 and the density was 1270 kg/m^3 (Ren et al., 2025). The mesh of the model was selected from the solid three-dimensional 20-node solid structural unit (Peng et al., 2018; Qiao et al., 2022).

Constraints and loads

The three compression modes used in the simulation are shown in Fig. 2. The bottom surfaces were defined as fixed constraint boundaries, while the opposite surface was defined as the loading surface.

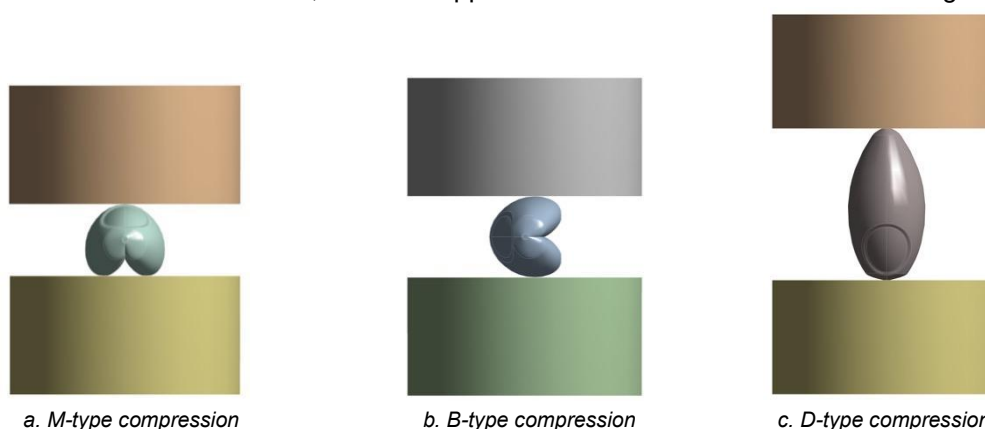


Fig. 2 - Compressed form of wheat grain in the simulation test

First, the compression displacement of the upper platen was set according to the data measured in the preliminary compression test. The reaction force exerted by wheat grains on the upper platen was measured and compared with the grain crushing load obtained from the actual compression test, so as to determine the accuracy of model construction and parameter setting, as well as the feasibility of the compression process simulation (Moya-Ignacio et al., 2024). Then, simulation tests under the same load were carried out for three compression modes, and the deformation nephograms and stress distribution nephograms of wheat grains were obtained.

RESULTS AND DISCUSSION

Analysis of test results of mechanical properties of wheat grain

During the compression test, the load-displacement curve was recorded in real time using a universal testing machine. Based on this curve, the crushing load and deformation of the wheat grains were determined, and the elastic modulus was calculated using Eq. (1). After the puncture test, the associated software automatically calculated the slope of the load-displacement curve to determine the hardness of the wheat grains. The test results are presented in Table 2.

Table 2

Mechanical properties of wheat grains

Variety	Crushing load / N			Elastic Modulus / MPa			Hardness / (N/mm)
	M-type	B-type	D-type	M-type	B-type	D-type	
Zhou Mai 18	98.65 ±8.04	124.88 ±15.48	135.66 ±11.94	50.58 ±7.76	73.02 ±15.20	117.93 ±8.91	48.31 ±7.30
Yang Mai 16	68.11 ±16.08	85.79 ±15.26	108.56 ±8.10	32.37 ±6.22	46.60 ±8.58	106.82 ±12.28	37.25 ±7.77
Yan Nong 19	90.41 ±17.42	109.65 ±18.43	138.03 ±6.73	40.47 ±6.67	63.72 ±14.29	146.42 ±12.34	52.15 ±8.55
Ji Mai 22	115.98	135.78	170.51	65.13	93.70	158.46	40.17

Variety	Crushing load / N			Elastic Modulus / MPa			Hardness / (N/mm)
	M-type	B-type	D-type	M-type	B-type	D-type	
	±7.76	±15.09	±29.16	±4.39	±8.01	±18.29	±5.21
Liao Chun 23	95.35 ±7.79	99.34 ±6.19	105.12 ±6.71	49.50 ±18.10	64.13 ±14.89	139.40 ±18.00	50.49 ±7.01
Liang Xing 77	84.17 ±12.31	90.61 ±16.79	95.72 ±6.92	55.77 ±13.09	81.16 ±18.36	122.07 ±17.81	57.86 ±6.51
Yu Mai 68	92.10 ±7.91	107.51 ±16.67	115.74 ±11.16	26.66 ±7.83	36.85 ±2.35	104.05 ±14.26	30.60 ±5.64
Chuan Mai 602	83.68 ±11.39	90.26 ±19.43	108.76 ±8.86	23.88 ±3.14	52.58 ±14.65	125.85 ±12.03	44.77 ±6.98
Jin Mai 101	86.92 ±18.73	97.83 ±16.27	116.46 ±8.13	35.22 ±9.11	61.61 ±12.79	116.52 ±13.47	44.19 ±4.97
Yun Mai 69	68.09 ±9.33	97.87 ±16.34	117.78 ±13.19	25.12 ±4.75	58.74 ±11.10	134.08 ±17.94	40.64 ±8.62

As shown in Table 2, the crushing load range of wheat grain under the three compression modes was from 68.09 to 170.51 N. Under M-type, B-type and D-type compression, the average crushing load was 88.35N, 103.95N, 121.23 N, respectively. The elastic modulus range of wheat grains under the three compression modes was from 23.88 to 158.46 MPa. Under M-type, B-type and D-type compression forms, the average elastic modulus was 40.47 MPa, 63.21 MPa, 127.16 MPa, respectively. This showed that wheat grains were anisotropic in terms of internal structure, material composition, and mechanical properties. The range of grain hardness was from 30.60 to 57.86 N/mm and the average value was 44.64 N/mm, which showed that there was a significant difference in grain hardness among different wheat varieties.

The variance analysis was performed on the mechanical properties of different wheat varieties. The test results are shown in Table 3. The influence of crop variety factors on the mechanical properties of wheat grains was extremely significant, which indicated that there were significant differences in the relevant mechanical properties of different wheat varieties. The factors of compression form had significant effects on crushing load and elastic modulus, indicating that there were significant differences in relevant mechanical indicators under different compression forms.

Table 3

Analysis of variance of mechanical parameters of wheat grain

Source of variation	Variable	Sum of squares	df	Mean square	F value	P value
Variety	M-type crushing load	8991.29	9	999.03	6.53	<0.01
	B-type crushing load	11433.512	9	1270.39	4.99	<0.01
	D-type crushing load	21051.10	9	2339.01	14.27	<0.01
	M-type elastic modulus	9103.50	9	1011.50	12.06	<0.01
	B-type elastic modulus	12277.93	9	1364.21	8.32	<0.01
	D-type elastic modulus	13612.37	9	1512.49	6.845	<0.01
	Hardness	2834.499	9	314.944	6.60	<0.01
Compression mode	Crushing load	27061.97	2	13530.99	30.91	<0.01
	Elastic modulus	202027.67	2	101013.84	276.30	<0.01

Analysis of chemical composition of wheat grains

The chemical composition of wheat grains for each variety was determined using Eqs. (2)–(6), and the results are presented in Table 4. The moisture content ranged from 11.27% to 17.27%, with an average value of 13.26%. The starch content ranged from 51.05% to 60.91% (average 56.72%), protein from 10.47% to 14.33% (average 12.94%), fat from 2.19% to 2.97% (average 2.54%), and fiber from 1.90% to 5.07% (average 3.81%). These results indicate that significant differences exist in the chemical composition among different wheat varieties.

Table 4

Contents of chemical components in wheat grain

Variety	Moisture content (%)	Crude starch (%)	Crude protein (%)	Crude fat (%)	Crude fiber (%)
Zhou Mai 18	11.74±0.02	51.05±1.36	13.89±0.10	2.35±0.15	3.77±0.21
Yang Mai 16	14.07±0.01	58.56±1.35	11.64±0.14	2.73±0.15	5.07±0.11
Yan Nong 19	11.27±0.01	52.38±1.61	11.46±0.08	2.95±0.06	4.56±0.23
Ji Mai 22	11.55±0.01	59.27±1.36	13.80±0.08	2.27±0.14	4.82±0.40
Liao Chun 23	15.06±0.02	55.05±1.59	12.82±0.01	2.23±0.01	4.17±0.21
Liang Xing 77	11.96±0.16	57.76±1.32	13.09±0.03	2.19±0.01	4.19±0.27
Yu Mai 68	17.27±0.02	59.50±1.50	13.88±0.13	2.92±0.03	3.44±0.17
Chuan Mai 602	13.59±0.01	54.77±1.02	14.02±0.17	2.63±0.05	3.11±0.06
Jin Mai 101	13.57±0.02	57.93±1.70	14.33±0.06	2.23±0.07	3.11±0.07
Yun Mai 69	12.18±0.03	60.91±1.21	10.47±0.02	2.85±0.07	1.90±0.10

The analysis of variance of chemical composition parameters of different wheat varieties were performed and the test results are shown in Table 5. The effect of crop variety factors on the content of chemical components in wheat grains was extremely significant, indicating that the chemical components of different varieties of wheat had significant differences.

Table 5

Analysis of variance of chemical composition of wheat grains

Source of variation	Variable	Sum of squares	df	Mean square	F value	P value
Variety	Moisture content (%)	161.00	9	17.89	6645.25	<0.01
	Crude starch (%)	476.51	9	52.95	26.44	<0.01
	Crude protein (%)	78.44	9	8.72	918.75	<0.01
	Crude fat (%)	4.361	9	0.49	59.46	<0.01
	Crude fiber (%)	40.99	9	4.55	104.24	<0.01

Mechanical-chemical correlation analysis of wheat grains

The mechanical properties and chemical composition of wheat grains were standardized using Eq. (7), and the normalized results are presented in Table 6. Each mechanical indicator was defined as a reference sequence, while each chemical composition indicator was defined as a comparison sequence. The normalized data were then processed using Eqs. (8)–(10) to calculate the grey relational coefficients and grey relational grades, and to determine the ranking of the relationships between mechanical properties and chemical components. The results are shown in Table 7.

Table 6

Standardized values of mechanical and chemical indicators of wheat grains

Variety no.	Standardized data											
	X1'	X2'	X3'	X4'	X5'	X6'	X7'	X8'	X9'	X10'	X11'	X12'
1	0.7290	1.3128	0.6670	0.7108	0.5939	-0.5307	0.4621	-0.7854	-1.7419	0.7206	-0.5936	-0.0461
2	-1.4316	-1.1393	-0.5860	-0.5695	-1.0057	-1.1695	-0.9316	0.4461	0.5661	-0.9861	0.6126	1.3150
3	0.1460	0.3574	0.7766	-4.99E-16	0.0308	1.1074	0.9460	-1.0338	-1.3332	-1.1226	1.3745	0.7810
4	1.9550	1.9965	2.2783	1.7338	1.8459	1.7997	-0.5637	-0.8858	0.7843	0.6523	-0.8475	1.0532
5	0.4955	-0.2893	-0.7450	0.6349	0.0556	0.7038	0.7368	0.9693	-0.5126	-0.0910	-0.9745	0.3727
6	-0.2954	-0.8369	-1.1797	1.0757	1.0867	-0.2927	1.6655	-0.6691	0.3202	0.1138	-1.1015	0.3937
7	0.2656	0.2232	-0.2540	-0.9709	-1.5959	-1.3288	-1.7696	2.1373	0.8550	0.7130	1.2157	-0.3916
8	-0.3301	-0.8589	-0.5767	-1.1664	-0.6436	-0.0753	0.0160	0.1924	-0.5987	0.8192	0.2952	-0.7371
9	-0.1009	-0.3840	-0.2207	-0.3691	-0.0969	-0.6118	-0.0571	0.1818	0.3725	1.0543	-0.9745	-0.7371
10	-1.4330	-0.3815	-0.1597	-1.0792	-0.2707	0.3979	-0.5044	-0.5528	1.2883	-1.8736	0.9935	-2.0039

Note: X₁' - X₃' represent the crushing load under M-, B-, and D-type compression, respectively, X₄' - X₆' represent the elastic modulus under M-, B-, and D-type compression, respectively, X₇' represents hardness, X₈' represents moisture content, X₉' represents crude starch content, X₁₀' represents crude protein content, X₁₁' represents crude fat content, X₁₂' represents crude fiber content.

Table 7

Grey relational grades and ranking between chemical composition and mechanical properties of wheat grains

Mechanical property		Chemical composition				
		Moisture	Starch	Protein	Fat	Fiber
M-type crushing load	Correlation	0.5985	0.5776	0.6958	0.5242	0.6789
	Order	3	4	1	5	2
B-type crushing load	Correlation	0.6366	0.6465	0.6938	0.6291	0.7020
	Order	4	3	2	5	1
D-type crushing load	Correlation	0.5848	0.6144	0.6174	0.6450	0.6855
	Order	5	4	3	2	1
M-type elastic modulus	Correlation	0.5769	0.5673	0.6395	0.5036	0.7028
	Order	3	4	2	5	1
B-type elastic modulus	Correlation	0.6194	0.6498	0.6975	0.5642	0.7087
	Order	4	3	2	5	1
D-type elastic modulus	Correlation	0.6683	0.6186	0.6301	0.6954	0.7268
	Order	3	5	4	2	1
Hardness	Correlation	0.7192	0.5964	0.6755	0.6522	0.6960
	Order	1	5	3	4	2

The grey relational analysis results (Table 7) indicate that the correlation between chemical composition and crushing load varies with compression mode. For M-type compression, the correlation ranking (from highest to lowest) is: protein > fiber > moisture > starch > fat, with values ranging from 0.6958 to 0.5242. For B-type compression, the ranking is: fiber > protein > starch > moisture > fat (0.7020–0.6291). For D-type compression, the order is: fiber > fat > protein > starch > moisture (0.6855–0.5848). Considering the average correlation across the three compression modes, the overall ranking of chemical components influencing crushing load is: fiber > protein > starch > moisture > fat, with corresponding correlation values of 0.6888, 0.6690, 0.6128, 0.6066, and 0.5994, respectively. For the elastic modulus, similar trends were observed. Under M-type compression, the correlation ranking is: fiber > protein > starch > moisture > fat (0.7028–0.5036). Under B-type compression, the same order is obtained, with values ranging from 0.7087 to 0.5642. For D-type compression, the ranking is: fiber > fat > moisture > protein > starch, with values ranging from 0.7268 to 0.6186.

Based on the average correlation values across the three compression modes, the correlation between chemical composition and elastic modulus (from highest to lowest) is: fiber > protein > moisture > starch > fat, with corresponding values of 0.7127, 0.6557, 0.6215, 0.6119, and 0.5877, respectively. For grain hardness, the correlation ranking is: moisture > fiber > protein > fat > starch, with correlation values of 0.7192, 0.6960, 0.6755, 0.6522, and 0.5964, respectively.

Overall, considering the relationships between crushing load, elastic modulus, hardness, and chemical composition, fiber and protein exhibit the strongest correlations with the mechanical properties of wheat grains. Therefore, these two components can be used as key indicators to indirectly evaluate the mechanical properties of wheat grains.

As shown in Table 7, moisture content exhibits a strong correlation with the mechanical properties of wheat grains. Compared with other chemical components, moisture content can be readily adjusted, making it a key factor for further investigation. Therefore, the effect of moisture content on the mechanical properties of wheat grains was studied. Considering that the optimal moisture content for wheat harvesting and subsequent processing typically ranges from 11% to 17%, five moisture levels (10%, 12%, 14%, 16%, and 18%) were selected in this study. The moisture content was adjusted using two methods: drying (forward adjustment) and rehydration (reverse adjustment). In the drying process, wheat grains were naturally ventilated, and the moisture content was monitored using a handheld moisture meter until the target level was reached. In the rehydration process, the amount of water added was calculated using Eq. (11) based on the principle of constant mass.

$$w = \frac{M(Q_2 - Q_1)}{1 - Q_2} \quad (11)$$

where: w is the amount of water added, ml; M represents the mass of the sample, kg; Q_1 represents the initial moisture content, %; Q_2 represents the target moisture content, %. The wheat variety Ji Mai 22 was selected, and the moisture content was adjusted to the specified levels using the above methods. Mechanical tests were then conducted under M-type compression, with a loading speed of 1 mm/min.

The test results are shown in Fig. 3.

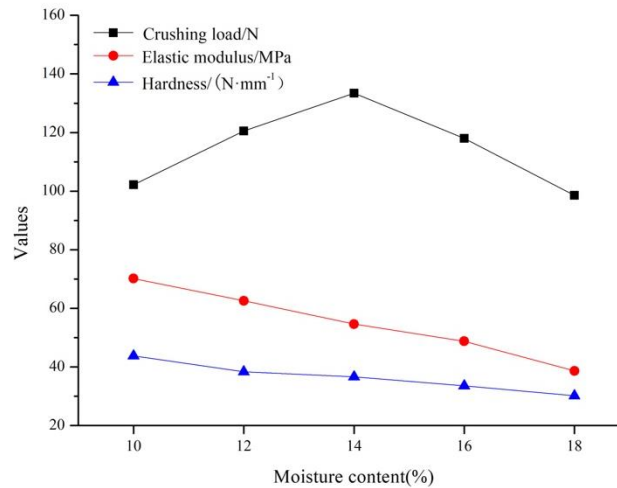


Fig. 3 - Variation of mechanical properties of wheat grains with moisture content

The results indicate that the crushing load of wheat grains initially increases and then decreases with increasing moisture content, while the elastic modulus and hardness decrease continuously as moisture content increases. This behavior is attributed to changes in the internal structure and mechanical strength of the grains with moisture content. At higher moisture levels, the internal tissues of the wheat grains become softer, resulting in lower mechanical strength and reduced resistance to deformation and fracture. Consequently, grains are more prone to deformation and breakage under compression. As the moisture content decreases, the internal structure becomes more compact and rigid, leading to increased mechanical strength and higher resistance to deformation. Therefore, the crushing load increases initially with decreasing moisture content. However, when the moisture content decreases further, the internal bonding within the grains weakens and brittleness increases, making the grains more susceptible to fracture under load. As a result, the crushing load decreases at low moisture levels. In addition, as moisture content increases, the softening of the outer layer and internal tissues leads to greater deformation under the same load. According to Eq. (1), this results in a decrease in elastic modulus. Similarly, the softening effect reduces the resistance to puncture, leading to a decrease in grain hardness with increasing moisture content.

Analysis of Simulation Results of Wheat Grain Compression Process

The internal stress distribution and deformation of wheat grains under compressive loading are important for understanding the grain breakage mechanism and mechanical damage. Based on the experimental results, the elastic modulus values under M-, B-, and D-type compression were 65.13 MPa, 93.70 MPa, and 158.46 MPa, respectively, at a moisture content of 11.55%. The corresponding deformation at the point of grain failure was 0.436 mm, 0.472 mm, and 1.312 mm, respectively. By applying the corresponding displacement to the upper platen in the simulation, the reaction forces exerted by the grains on the platen were obtained, as shown in Table 8. The relative errors between the simulated and experimental values for the three compression modes were 11.00%, 9.01%, and 12.50%, respectively. These results indicate that the finite element model provides a reasonable prediction of the grain compression behavior, confirming the feasibility of using the finite element method to simulate the wheat grain compression process.

Table 8

Compression mode	Interaction force between wheat grain and upper platen		
	Interaction force between grain and upper plate		
	Simulation value / N	Experimental value / N	Relative error / %
M-type compression	128.52	115.78	11.00
B-type compression	148.01	135.78	9.01
D-type compression	191.82	170.51	12.50

The relative errors may be attributed to the following factors: ①The viscoelastic behavior of the material was simplified as an isotropic linear elastic model; ②discrepancies exist between the measured grain geometry and the actual grain shape; ③differences between the actual loading position in the mechanical tests and that used in the simulation; ④deviations between the assigned material properties in the simulation (e.g., Poisson's ratio and elastic modulus) and those of the real material (Yang *et al.*, 2021).

To further investigate the internal stress distribution and deformation behavior of wheat grains during compression, finite element simulations were conducted under three compression modes with the same applied load. The load was set to 80 N, and the deformation contours and equivalent stress contours of the grains were obtained, as shown in Figs. 4–6.

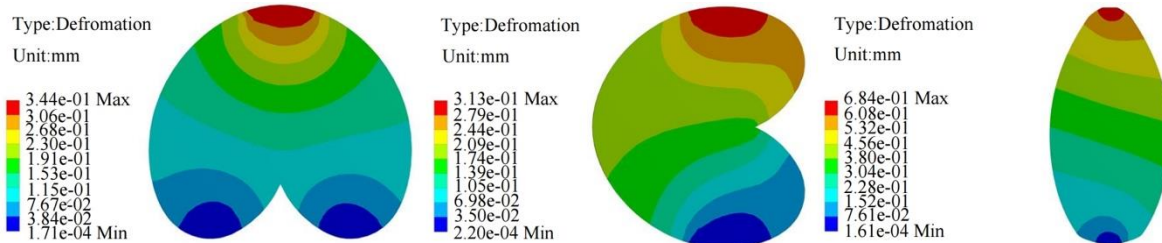


Fig. 4 - Cloud diagram of internal grain deformation

As shown in Fig. 4, the deformation range under M-type compression is 0.00017–0.34442 mm, while for B-type compression it is 0.00022–0.31348 mm, and for D-type compression it is 0.00016–0.68387 mm. In all three compression modes, the maximum deformation occurs at the contact region between the grain and the upper platen, whereas the minimum deformation occurs at the contact surface with the lower platen. The internal deformation gradually decreases from the loading point to the support region. Among the three modes, D-type compression exhibits the largest maximum deformation, which is attributed to its smaller contact (bearing) area compared with the other two modes. Although the contact area in B-type compression is similar to that in M-type compression, the higher elastic modulus in B-type compression results in smaller deformation than in M-type compression.

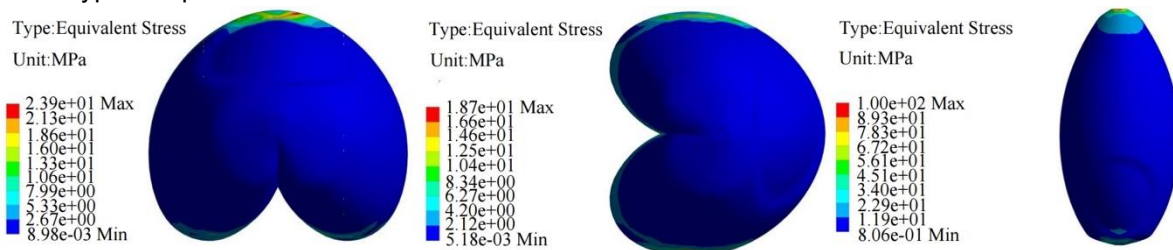


Fig. 5 - Cloud diagram of epidermal equivalent stress of grain

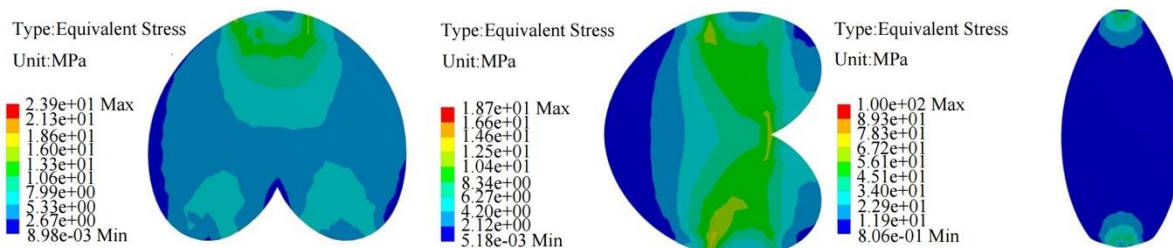


Fig. 6 - Equivalent stress distribution in wheat grain under compression

As shown in Figs. 5 and 6, the equivalent stress ranges for the three compression modes are as follows: 0.0089836~23.949 MPa for M-type compression, 0.051808~18.708 MPa for B-type compression, and 0.80631 ~ 100.38 MPa for D-type compression.

In all three compression modes, the maximum equivalent stress occurs on the outer surface of the grain, primarily near the upper loading point and the lower support point, while the regions of minimum equivalent stress are more dispersed. Among the three modes, D-type compression exhibits the highest maximum equivalent stress, whereas B-type compression shows the lowest. In B-type compression, the maximum equivalent stress is concentrated near the ventral groove (crease) of the grain, indicating that this region is more prone to fracture under this loading condition.

CONCLUSIONS

1) Mechanical properties of wheat grains were experimentally investigated. The results showed that the crushing load ranged from 68.09 to 170.51 N, the elastic modulus ranged from 23.88 to 158.46 MPa, and the hardness ranged from 30.60 to 57.86 N/mm. Significant differences were observed among wheat varieties and compression modes. Analysis of variance confirmed that both factors had a significant effect on the mechanical properties, indicating that wheat grains exhibit anisotropic mechanical behavior.

2) The chemical composition of wheat grains was analyzed. The moisture content ranged from 11.27% to 17.27% (average 13.26%), starch from 51.05% to 60.91% (average 56.72%), protein from 10.47% to 14.33% (average 12.94%), fat from 2.19% to 2.97% (average 2.54%), and fiber from 1.90% to 5.07% (average 3.81%). Significant differences in chemical composition were observed among different wheat varieties.

3) Grey relational analysis showed that fiber and protein have the strongest correlation with the mechanical properties of wheat grains. For crushing load, the correlation ranking is: fiber > protein > starch > moisture > fat (0.6888–0.5994). For elastic modulus, the ranking is: fiber > protein > moisture > starch > fat (0.7127–0.5877). For hardness, the ranking is: moisture > fiber > protein > fat > starch (0.7192–0.5964). In addition, the results of single-factor tests indicate that crushing load first increases and then decreases with increasing moisture content, while elastic modulus and hardness decrease continuously.

4) Finite element simulations of the wheat grain compression process were conducted and validated against experimental data, with relative errors of 11.00%, 9.01%, and 12.50% for the three compression modes. The results confirm the reliability of the simulation approach. Under identical loading conditions, D-type compression exhibited the largest deformation and equivalent stress, while B-type compression showed the smallest values.

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