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Predicting the moisture content of Daqu with hyperspectral imaging

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Abstract: Daqu, a Chinese liquor fermentation starter, contains all kinds of microorganisms and enzymes for Chinese liquor fermentation. The moisture content of Daqu significantly influence on the reproduction of microorganisms in Daqu. This work presents for the first time that determination of moisture content of Daqu with hyperspectral imaging. The characteristic spectrum of water is extracted based on comparative experiments with varying moisture content. The molds based on the full bands and feature bands were established by the support vector regression (SVR) method, which is used to predict moisture content of Daqu during fermentation process. The performance of the model based on the feature bands ($R^2 = 0.9870$, root mean square error (RMSE) = 0.0091) is comparable to the full bands and the dimensions of the spectral information were significantly reduced. This work presents a novel, rapid and nondestructive approach for detecting the moisture content in Daqu and lays a foundation for the application of hyperspectral imaging.

Keywords: Daqu; feature band; hyperspectral imaging; moisture content.

1 Introduction

Moisture content in food processing is the basis for the selection of food processing process and the determination of technological parameters [1]. It is also an important index to control the final food quality [2–4]. Specially, the moisture content of Daqu during fermentation process is of key importance [5], the reproductive rate of microorganisms will change depending on the moisture content [6]. As moisture content generally varies throughout the production process, the traditional detection method (the gravimetric oven method) is time-consuming, and cumbersome. Several detection methods reported in literature such as nuclear magnetic resonance, microwave, capacitance, near-infrared spectroscopy, and hyperspectral imaging (HSI) have been used for rapid detection of moisture content in food [7, 8]. Among them, HSI has attracted much attention from researchers due to its fast measurements, high accuracy, and non-destructive and non-toxic properties. HSI is an emerging platform that combines traditional spectral and imaging techniques to obtain spectral and spatial information from samples [9]. Hyperspectral technology is widely used in geology and minerals, atmospheric sciences, oceans, agriculture, industrial production, and other fields [10–12]. Due to HSI information with the large spectral information, large frequency band, and high redundancy, the information processing of HSI is difficult. Dimensional reduction has become an obstacle in HSI applications and information processing [13]. To solve the problems of processing high-dimensional data, researchers developed feature extraction methods used to reduce the dimensionality [14]. Wei [7] selected 12 and 11 feature bands for the front side and back side, respectively of tea using the random frog (RF) and successive projection algorithm (SPA) algorithm; Sun [15] used four feature selection algorithms to extract the most effective wavelengths of the tea. Zhou [16] used the partial least squares regression (PLSR) algorithm to extract characteristic wavelengths of lettuce leaves. However, the water feature bands extracted by different data processing methods are inconsistent [16, 17]. Identifying find the characteristic bands of water is of great significance for the application of HSI [18]. In this work, according to the interaction mechanisms of electromagnetic wave and water molecular vibrations [19], experiments with different

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moisture contents were designed to define characteristic wavelengths, the continuum removal (CR) algorithm and the first order derivative spectroscopy (FODS) used to handle the raw spectra. The three characteristic wavelengths and three waveform variation characteristic wavelengths of water were extracted. The support vector regression (SVR) was adopted to establish the prediction models based on full bands and feature bands to predict the moisture content of Daqu during the fermentation process. A model based on feature bands compared to full band where R^2 values of 0.9826 and 0.9925 as well as root mean square errors (RMSE) of 1.14 and 0.65% were attained for calibration and prediction, respectively. The current study presents a novel efficient and rapid method to select feature bands and lays a foundation for the application of HSI.

2 Materials and methods

The main flowchart of the research process used in the current study is illustrated in Figure 1, which includes the selection of feature bands by experiment and application to predict the moisture in Daqu [20].

2.1 Selection of characteristics spectral of water

To investigate the spectral differences with and without water, quartz sand was used as the experimental control. Comparison of the spectral reflectance curves of quartz sand powder with and without water, and the effect of moisture on the spectral information was investigated.

Table 1: Hyperspectral experiments of the quartz sand/water mixture.

Groups	Experimental name	Collection instructions
1	Quartz sand powder	In a circular petri dish, add 55 g white quartz sand powder
2	Quartz sand/water mixture	In group 1, 12 ml of water was added to the petri dish

Table 2: Hyperspectral experiments of moisture content in dough.

Groups	Experimental name	Collection time
1	Dough 1	18:15
2	Dough 2	18:30
3	Dough 3	18:45
4	Dough 4	19:00

The hyperspectral experiment of the quartz sand/water mixture is shown in Table 1.

The dough is used to study the change of the hyperspectral curves with different water content. In brief, a certain amount of flour and water are mixed evenly and kneaded it into a dough. Continuous kneading was performed to reduce moisture in the dough, and hyperspectral data was collected every 15 min. The scheme of the hyperspectral experiment of moisture content in dough is shown in Table 2.

2.2 Daqu sample preparation

Daqu is prepared by solid-state fermentation from wheat, barley and/or peas with ingredient formulation, grinding and mixing, shaping,

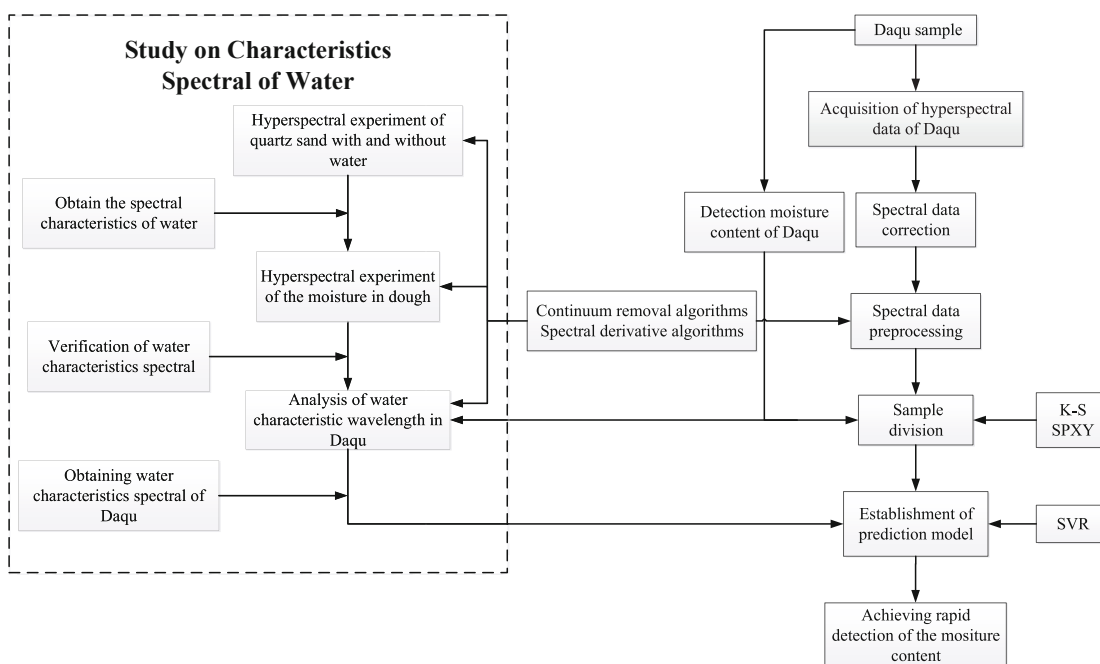


Figure 1: Schematic diagram of hyperspectral image analysis.

incubation, and maturation [21]. Daqu Samples were collected from a winery in Yibin, Sichuan province, from April 17 to May 15, 2018. And 160 samples were collected in total.

2.3 Hyperspectral image acquisition

A pushbroom HSI system was used for acquisition of the hyperspectral image of each sample, with 224 spectral bands in the range of 900–1700 nm with a resolution of 3.5 nm [22]. The main components of this system include an electronically controlled conveyor belt (Finland), two 150 W halogen lamps (Finland) as the illumination unit, a bracket used to support camera and light source, a hyperspectral camera with lens (FX17, Specim, Finland), and a system control software (Lumos-scanner, Finland) was used for setting the optimal parameters (e.g., exposure time, conveyor speed) for imaging [23].

During hyperspectral image acquisition, the samples in the petri dish were placed flat on a black baseplate for scanning. The movement speed of the conveyor belt was set to be 16.57 mm/s in order to match the scanning of the camera, the exposure time was adjusted to 4.02 ms, the vertical distance between samples and lens was 29 cm, and the object distance was set to 15 cm to obtain clear hyperspectral images.

2.4 The measurement of moisture content in Daqu

Drying under 101–105 °C temperature, the moisture content of Daqu samples were calculated by weighing. The equipment includes an electronic balance with a precision of 0.1 mg which was used to determine the weight, and an electric oven with a precision for plus or minus 2 °C was utilized to accelerate moisture evaporation, and a weighing flask with size of 50 × 30 mm, and a dryer with desiccant [24].

Experimental procedures are described as follows: step 1: drying the clean weighing bottle under 101–105 °C in the electric heating oven for 1 h while tilting the bottle cap on the bottle edge, covering the cap and placing the bottle in the dryer for 0.5 h, weighing the samples lastly, after then repeat the above procedures until the weight difference should not be more than 0.002 g, finally the result is the bottle's constant weight. Step 2: 4–5 g samples of Daqu are obtained in bottle with a precision of 0.0001 g. Drying under 101–105 °C in the electric heating oven for 3 h while opening the bottle cap, after the drying is completed, covering the cap and putting the bottle in the dryer for 0.5 h, after then repeat the above procedures until the weight is no longer changed. The moisture content of the Daqu was calculated by the following formula [25],

$$X = \frac{m_2 - m}{m_1 - m} \times 100 \quad (1)$$

In this formula, X is the moisture content of Daqu in g/100 g, m is the weight of the bottle in g, m_1 and m_2 denote the current and dry weights of the Daqu in g, respectively. After the above treatment, 160 moisture content values were obtained.

2.5 Data analysis

2.5.1 Hyperspectral calibration and average spectra: To eliminate the impacts of variations on illumination intensity, the detector sensitivity and the transmission properties of the optics were corrected by radiometric calibration utilizing dark and white reference images [26], all the raw images were calibrated using the following equation:

$$R(\lambda) = \frac{(I[\lambda] - D[\lambda])}{(W[\lambda] - D[\lambda])} \quad (2)$$

where R is the corrected image, I is the raw hyperspectral image, D is the dark reference image acquired by covering the camera completely (about 0% reflectance), and W is the white reference (teflon white cuboid panel with 99% reflectance, 200 × 25 × 10 mm).

When the average spectrum of each Daqu was extracted, the hyperspectral image data was opened and then selecting the region of interest (ROI) (80 × 80 pixels) manually to extract the relevant spectra, and the average reflectance spectrum of Daqu was obtained through calibration [27]. The first 10 and the last 10 bands were removed due to the high noise, and a total of 204 bands were taken into account in subsequent studies.

2.5.2 Spectral pretreatment: The CR algorithm is a common spectral analysis method, which is used to normalize reflectance spectra [28]. It can effectively highlight the absorption and reflection characteristics of spectral curves and compare individual absorption features from a common baseline. It is advantageous to compare the eigenvalues with other spectral curves so as to extract the key wavelengths for classification and recognition [29, 30]. The CR algorithm effect of the Daqu average spectral reflectance curve is shown in Figure 2, where the blue curve represents the original Daqu spectral reflectance curve, the black dotted line indicates the envelope of the Daqu spectral reflectance curve and the pink curve indicates the spectral reflectance curve after the envelope is removed. Compared with the original Daqu spectral reflectance curve, the spectral characteristic absorption peak of the curve after correction by CR is well-defined.

First order derivative spectroscopy uses first derivatives of the absorbance or reflectance with respect to wavelength for qualitative and quantitative analysis. Spectral derivation can eliminate spectral overlapping translation, enhance spectral characteristics, improve spectral resolution and highlight the changes of the spectra based on slope waveform[31]. The effects of spectral derivation are shown in Figure 3, where Figure 3(a) is the average spectral reflectance curve of Daqu, and Figure 3(b) is the first derivative average spectral reflectance curve of Daqu.

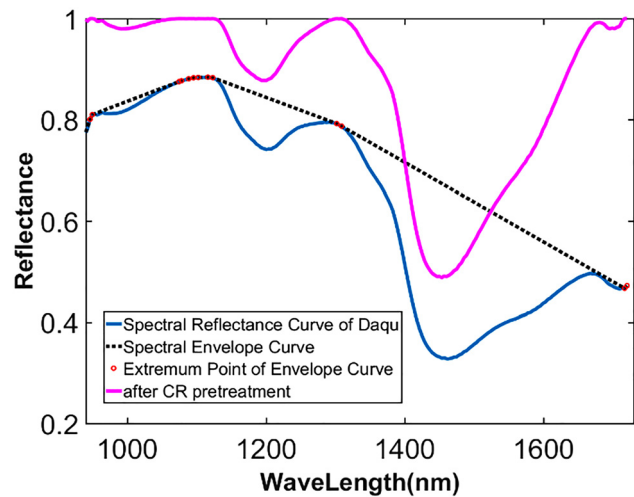


Figure 2: The average spectral reflectance curve of Daqu after CR treatment.

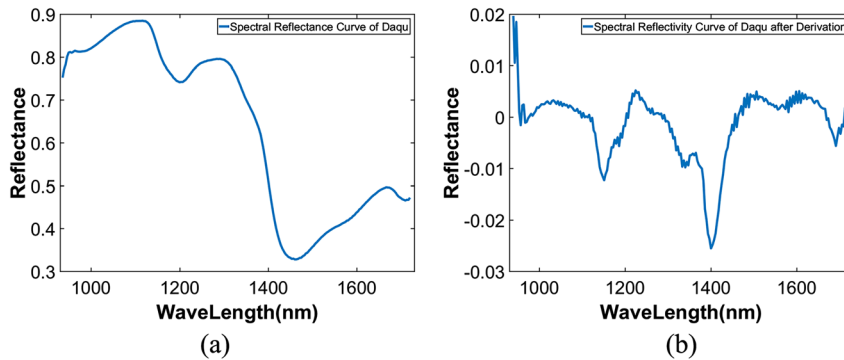


Figure 3: The spectral curve of Daqu (a) and after FORDS treatment (b).

2.5.3 Sample division method: Generally, all the samples were divided into a calibration set and a prediction set [7], Kennard–Stone (KS) algorithm and sample set partitioning based on joint x – y distance (SPXY) algorithm were adopted to select a calibration set with 120 samples and a prediction set with 40 samples for analysis in this work [32].

2.6 Model establishment and evaluation

Support vector regression is a classical modeling method with excellent generalization capability and high prediction accuracy, it uses mapping relationships to transform the data with non-linear relationship in low-dimensional space into high-dimensional space, so that a linear function can be constructed to describe the relationship between these data. In general, it can transform non-linear data into linear, data with regression [33].

After the regression models were established, the evaluation indices primarily included the determination coefficient and cross-validation RMSE, which were used to evaluate and compare the performances of the models.

The equation for the determination coefficients of the set (R^2) is:

$$R^2 = \frac{\sum_{i=1}^n (y_i - y_{i\text{actual}})^2}{\sum_{i=1}^n (y_i - y_{\text{mean}})^2} \quad (3)$$

The equation for the RMSE of the sets:

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^n (y_i - y_{i\text{actual}})^2}{n - 1}} \quad (4)$$

In the above equation, n is the number of the set. For RMSE, the closer the value is to 0, the better it is. For R^2 , the closer the value is to 1, the better it is [34].

3 Results and discussion

3.1 Experiments to determine the characteristic water spectrum

The acquisition spectrum range of FX17 series hyperspectral cameras used in this paper is 940–1730 nm, which is in the range of near infrared spectroscopy. This camera was chosen as it collects spectral reflectance information of

the sample. Water has strong light transmission and absorption characteristics, and quartz sand, a carrier material, was used to determine the characteristic water spectrum for its stability. When water is added to quartz sands, the changes in spectral characteristics of water can be clearly observed. The spectral enhancement algorithm is used to determine the characteristic water bands [35]. The dough shaping method is similar to the Daqu shaping method. By analyzing the spectral reflectance curves of dough with different moisture content, the relationship between the spectral reflectance of the characteristic bands, which were found in the quartz sand/water experiments, and the moisture content gradient of dough was studied. Thus, the reliability of the water spectral characteristics was verified.

3.2 Hyperspectral experiments of the quartz sand/water mixture

To explore the spectral differences of substances with and without water, quartz sand was used as the control medium. The spectral reflectance curves of pure quartz sand powder and quartz sand with water were compared, and the effects of water on the spectral information were studied.

After the hyperspectral data acquisition was acquired, the ROI were divided (Figure 4). Figure 4(a) shows the spectral image of quartz sand powder and ROI, while Figure 4(b) shows the spectral image and ROI of quartz sand with added water.

After the division of ROI was completed, the average spectral reflectance data were extracted, and the ROI average spectral reflectance curves of quartz sand powder with and without water are shown in Figure 5. It was found that the spectral reflectance curves of quartz sand powder with and without water are quite different. Owing to the strong absorption of water, the overall spectral reflectance of water-added quartz sand is lower than that of quartz sand powder. In addition, there are reflection troughs at

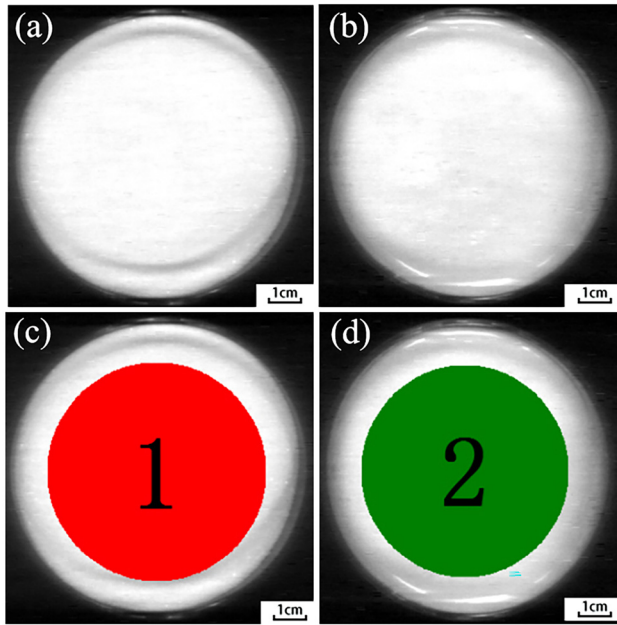


Figure 4: Hyperspectral image of quartz sand (a), quartz sand/water mixture (b), and after the ROI division (c) and (d), respectively.

980, 1200 and 1440 nm bands, and reflection peaks at 1090 and 1270 nm bands. To highlight the spectral characteristics, the spectral enhancement is carried out by using the CR algorithm and first order spectral derivative algorithm. The effects after spectral enhancement are shown in Figure 6. Figure 6(a) is the spectral reflectance after treatment by the CR algorithm, and Figure 6(b) is the spectral reflectance after first order spectral derivation treatment. From Figure 6(a), it can be seen that there are obvious characteristic absorption peaks at 980, 1200, and 1440 nm. An obvious characteristic reflection peak is found at 1270 nm, but there was not a characteristic water band near 1090 nm due to spectral crossover. As shown in Figure 6(b), the spectral derivative represents the slope of the reflectance, which can eliminate the influence of the overall absorbance of water and explains the change of the spectral waveform. Compared with quartz sand powder, the abrupt change of the characteristic waveform of quartz sand mixed with water primarily occurs in the bands near 950, 1140, and 1330 nm.

3.3 Hyperspectral experiments of moisture content in dough

Since only adhered to the surface of quartz sand and did not absorb into the bulk of the quartz sand, hyperspectral

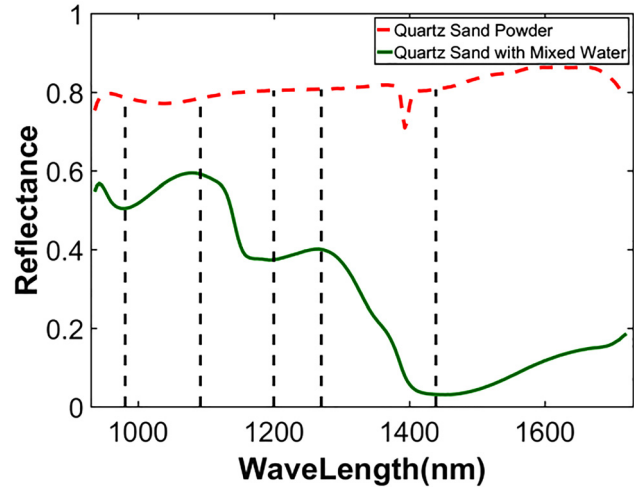


Figure 5: The spectral reflectance curve of quartz sand powder ROI and quartz sand/water ROI.

experiments of moisture in dough were carried out to study the hyperspectral curves of water with varying moisture contents. When preparing the experimental samples, a certain amount of flour and water were evenly mixed and kneaded into dough. Continuous kneading was performed to reduce moisture in dough, and the data were collected every 15 min. The changes of spectral curve were studied when the water content changed, and the water dispersion gradient was used to carry out comparative experiments.

The hyperspectral data of the collected dough were divided into ROI, and the ROI was shown in Figure 7. After ROI was partitioned, the average spectral reflectance of dough ROI was extracted, and the reflectance curves of dough at different time points were obtained as shown in Figure 8. To highlight the spectral characteristics, the spectral curves after pretreatments by the CR algorithm and spectral derivative algorithm are shown in Figure 9(a, b), respectively.

As shown in Figures 8 and 9, there is no characteristic reflectance change in water at the 1090 nm. At 980, 1200, 1270, and 1440 nm bands, the spectral reflectance increases with a decrease of water content, which satisfies the general understanding of water because of its strong absorption characteristics. According to the principles of spectral molecular oscillation, near infrared spectroscopy is caused by the combination frequency or double frequency vibration of molecules after absorbing electromagnetic waves. The O–H bond of water absorbs light energy to form a reflection spectrum, so the absorption peaks at 980, 1200, and 1440 nm are the spectral characteristics of water, while 1270 nm is not. From the local magnification in Figure 9(b), it can be seen that the reflectivity of the derivative spectrum increases with a decrease of water content at the bands of

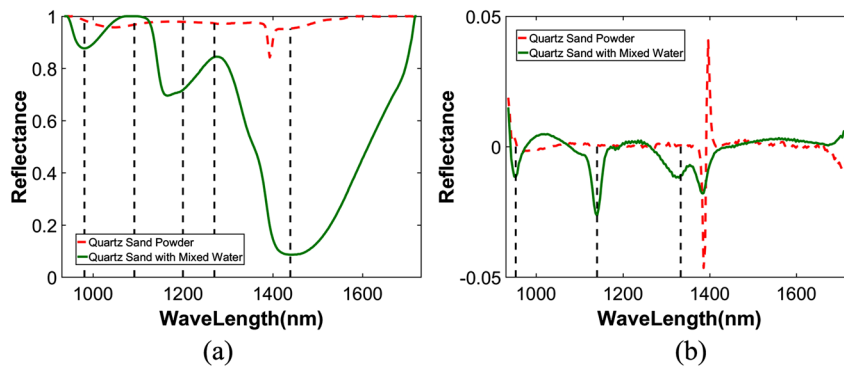


Figure 6: The spectral reflectance curve of quartz sand powder and quartz sand/water ROI after CR treatment (a), and after FORDS treatment (b).

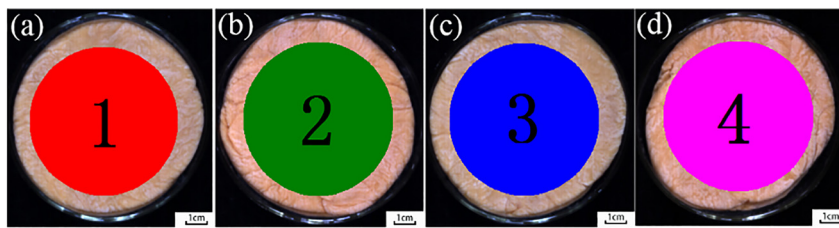


Figure 7: Hyperspectral image of dough after ROI division with different knead time, 0 min (a), 15 min (b), 30 min (c) and 45 min (d).

950, 1140, and 1330 nm, which also satisfies the variation law of water characteristics.

3.4 Analysis of characteristic water wavelength in Daqu

According to the water experiments of quartz sand and dough, the water spectral characteristics exist in the 980, 1200, 1270, and 1440 nm bands. For these four bands, the variation of spectral reflectance and corresponding water content of Daqu were investigated. According to the data

collected from Daqu in a distillery, the change of average moisture content in Daqu during fermentation is shown in Figure 10. Daqu fermentation consists of three stages, which are the pre-turning stage in 0–5 days, post-turning stage at 6–10 days and another post-turning stage at 15–30 days. As can be seen from Figure 10, during the fermentation process of Daqu, the moisture content first decreased and then plateaued. In the pre-and post-warping stages, the water content decreased rapidly, and the change of water content was relatively smooth after the second warping. According to the three fermentation stages of Daqu, the spectral reflectance curves of the 2nd, 6th, 10th, 18th and 26th days at the 3rd point of No. 1 Qufang were superimposed and analyzed. The relationship between the moisture content and spectral reflectance curve of Daqu was studied (Figure 11).

It can be found that the overall spectral reflectance curve of Daqu increases with a decrease of water content. Due to the interference of the overall absorption characteristics of water, the CR algorithm is used to enhance the spectrum and highlight the characteristic water bands. The spectral derivative algorithm is used to eliminate the interference caused by the overall absorbance of water and highlight the changes of the characteristic waveform. The spectral curves after correction by the CR and spectral derivation algorithm are shown in Figure 12(a, b), respectively. As shown in Figure 12(a), there is no variation of water characteristics in the 1270 nm band, so there may be no water characteristics in the vicinity of the 1270 nm band. The spectral reflectance values of the bands around 980, 1200 and 1440 nm change regularly according to the water content, so it can be inferred that the spectral characteristic

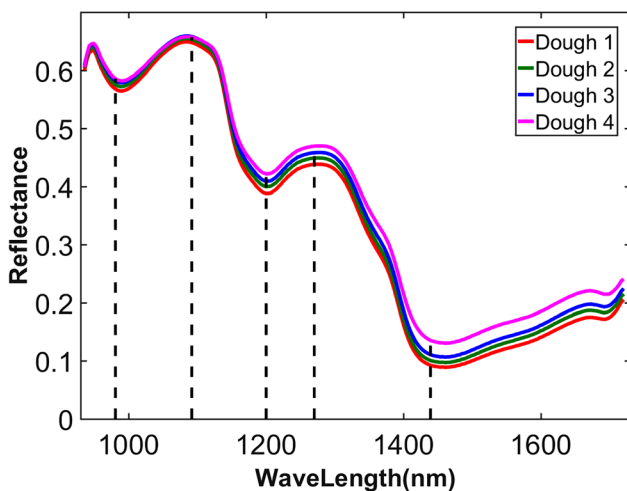


Figure 8: The spectral reflectance curve of dough with varying moisture content.

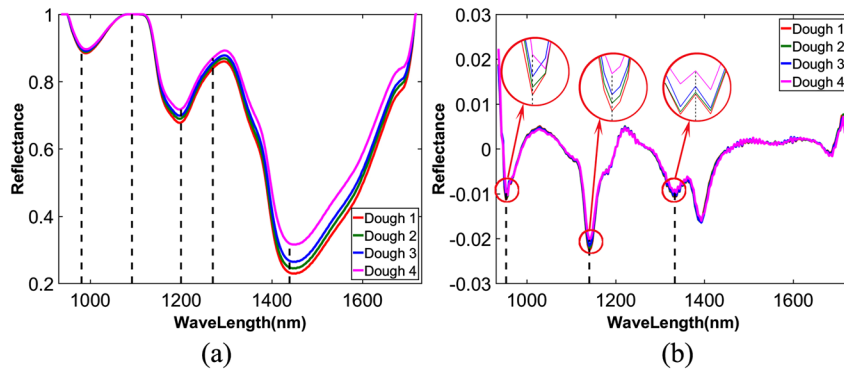


Figure 9: The spectral reflectance curve of dough after the CR treatment (a) and FORDS treatment (b).

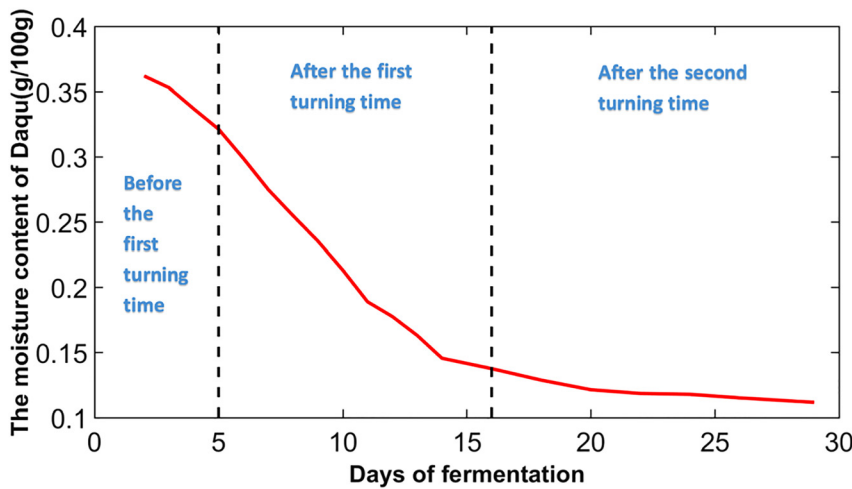


Figure 10: Variation trend of moisture content of Daqu fermentation process.

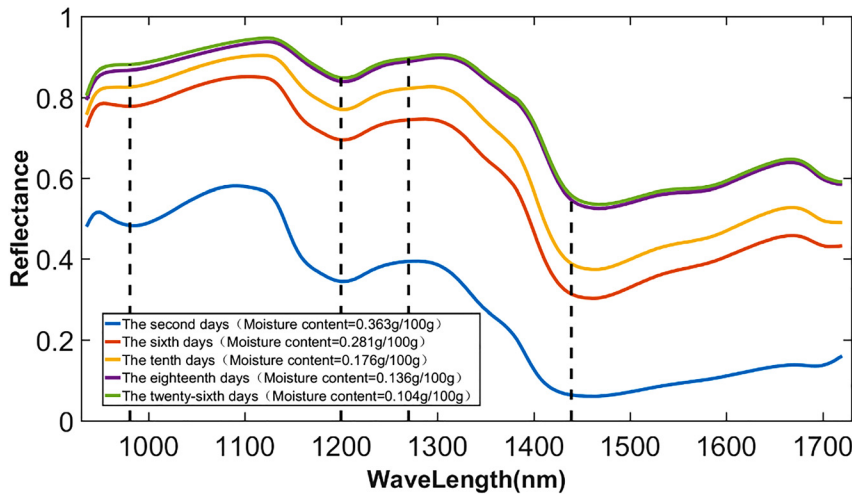


Figure 11: The spectral reflection curves of Daqu with different fermentation days.

wavelength of Daqu water is primarily around 980, 1200, and 1440 nm. Figure 12(b) shows that the spectral reflectance near the 950, 1140, and 1330 nm bands increases with a decrease in water content after eliminating the influence of the overall absorbance of water. Therefore, it can be speculated that the characteristic waveforms of water can be reflected at the 950, 1140, and 1330 nm bands.

3.5 Establishment of the moisture content in Daqu prediction model

Through designed experiments, it was found that the water characteristic bands were primarily distributed at the 980, 1200, and 1440 nm, and the characteristic bands which affected the characteristic water waveform were primarily

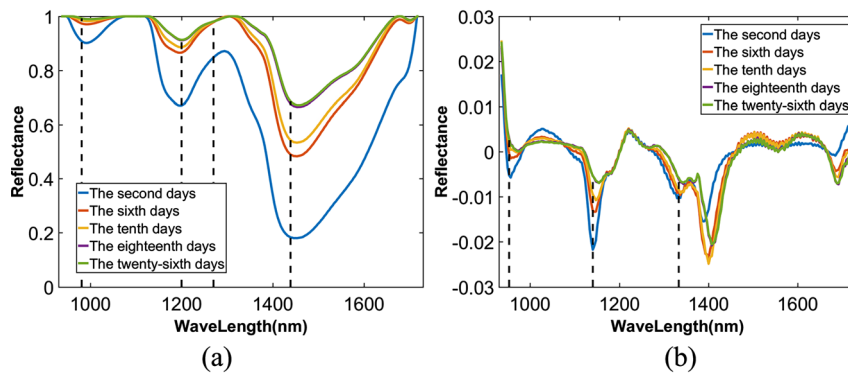


Figure 12: The spectral reflection curves of Daqu after the CR treatment (a) and FORDS treatment (b).

Table 3: Performance of the models based on full spectrum bands.

Models	Bands	Pretreatment	Classification of sample datasets	Calibration set		Prediction set	
				R^2	RMSE	R^2	RMSE
SVR	Full spectrum band	None	KS	0.9945	0.0064	0.9830	0.0094
			SPXY	0.9908	0.0083	0.9968	0.0041
		Derivation	KS	0.9922	0.0076	0.9972	0.0042
			SPXY	0.9914	0.0079	0.9979	0.0033

distributed at the 950, 1140, and 1330 nm. The spectral characteristic band is inputted as the independent variable, and the moisture index is outputted as the dependent variable. The KS and SPXY were used to divide the sample set, and the optimal prediction model was found by comparing the unprocessed and spectral derivative data. The determinant coefficient (R^2) and RMSE are used to evaluate the fitting effect of the model. The whole spectrum and characteristic spectrum were compared to verify the reliability of the characteristic spectrum band.

3.6 Analysis of the full spectrum model

The 224 bands in the 940–1730 nm spectral range were used as independent variables to establish the prediction

model. The 120 Daqu samples were selected as calibration set by the sample set partition method, and the remaining 40 samples were used as the prediction set. The statistical results of full spectral modeling are shown in Table 3.

As can be seen from Table 3, the prediction effect of the spectral derivation model is generally better than that of the unprocessed model. The model based on spectral derivative pretreatment and KS algorithm for dividing the sample set performed best where R^2 values of 0.9922 and 0.9972 as well as RMSEs of 0.76 and 0.33% were attained for calibration and prediction, respectively. The fitting effects of calibration set and prediction set is shown in Figure 13(a, b), respectively.

Although the prediction effect of the full spectrum modeling is very ideal, the input feature dimension is large,

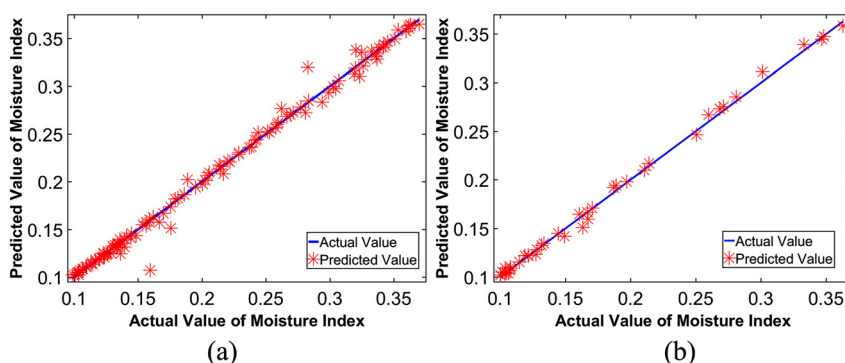


Figure 13: The performance of the best model based on the full bands, measured vs. predicted plot for calibration (a) and prediction (b).

the training efficiency of the model calculation is low, and there are bands unrelated to water characteristics. Therefore, the model of based on the characteristic spectral bands of water were established and compared with the full-band model.

3.7 Analysis of the characteristic spectrum model

The spectral characteristic bands obtained from the design experiments are used as independent variables for predictive modeling. The 120 samples also were selected as the calibration set and 40 samples were used as the prediction set. The performance of the model based on the characteristic spectrum is shown in Table 4.

As can be seen from Table 4, the model based on spectral derivative pretreatment and KS algorithm for dividing the sample set performed best where R^2 values of 0.9844 and 0.9870 as well as RMSE of 1.07 and 0.91% were attained for calibration and prediction, respectively. The fitting effects of the training set and test set are shown in Figure 14(a, b), respectively.

Compared with the full spectrum modeling, three feature bands can greatly reduce the data dimension and increase the algorithm speed, while the modeling and prediction effects are also very good. The spectral derivation pretreatment method is generally better than the untreated method in modeling. Spectral derivation can eliminate the overall absorption characteristics of liquid, highlight the waveform change of the reflectance curve, and reduce some interference. One of the advantage of HSI is that it can visualize the distribution of predicted values (spatial domain) in the food matrix in a pixel-wise manner [9]. The characteristic spectrum model was used for producing visualization maps where the moisture content of Daqu were presented, As shown in Figure 15, the pixels color of the image with higher moisture contents was displayed in dark red, while the image with lower contents was shown in dark blue. With the decrease of moisture content of Daqu, the color of the image will change to blue. There is a stripping effect on images, it is mainly caused by the small number of training data samples. Visualizing distribution map of Daqu offered a more intuitive and comprehensive assessment of moisture contents at each pixel, and the HSI spectroscopy

Table 4: Performance of the models based on feature bands.

Models	Bands	Pretreatment	Classification of sample datasets	Calibration set		Prediction set	
				R^2	RMSE	R^2	RMSE
SVR	980.58 nm	None	KS	0.9884	0.0092	0.9849	0.0103
	1199.87 nm		SPXY	0.9843	0.0108	0.9883	0.0079
	1439.07 nm	Derivation	KS	0.9844	0.0107	0.9870	0.0091
	952.89 nm						
	1140.47 nm						
	1326.18 nm						

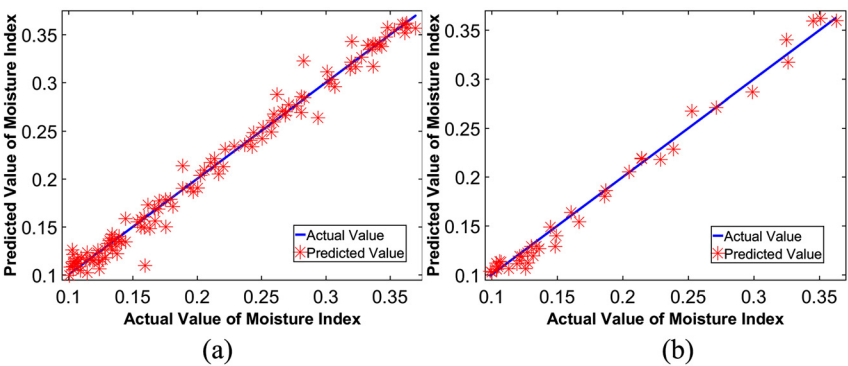


Figure 14: The performance of the best model based on the feature bands, measured vs. predicted plot for calibration (a) and prediction (b).

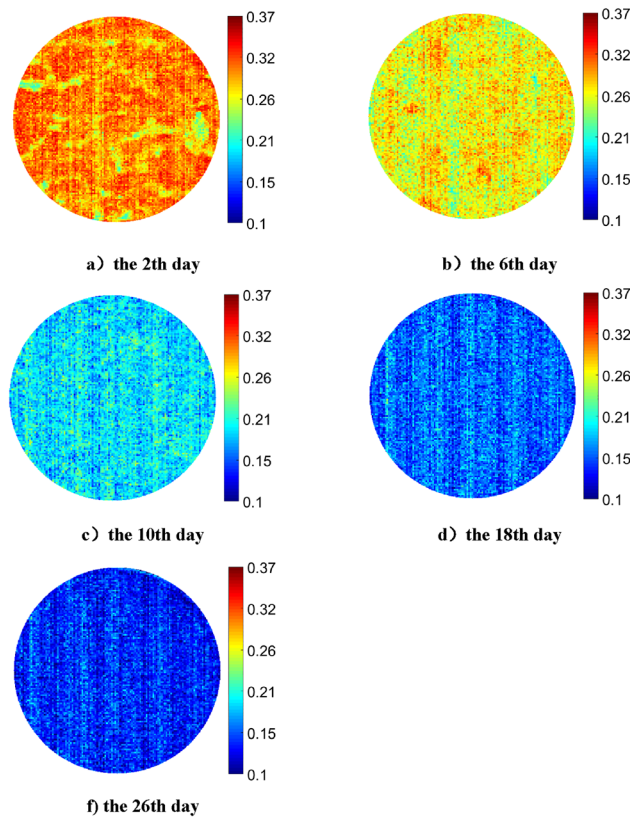


Figure 15: Visualization of Daqu moisture content in different periods.

provides a reliable tool compared with the visual inspection for in-line systems.

4 Conclusions

In this paper, the characteristic spectral bands of water were found by the quartz sand and dough water gradient contrast experiments. The CR algorithm was used to enhance the spectrum. In the near infrared band of 940–1730 nm, the characteristic water spectrum was found near 980, 1200, and 1440 nm. To eliminate the overall absorption characteristics of liquids, the spectral derivative algorithm was used to find the characteristic distributions near 950, 1140, and 1330 nm, which affect the spectral waveforms. The full spectral band and characteristic spectral band reflectance values were used as feature inputs, and the moisture index was used as spectral feature outputs. The prediction model was established by the SVR algorithm to realize fast detection. Through the comparison of full spectrum and characteristic spectrum modeling, it was found that although the modeling effect of characteristic spectrum is slightly lower than that of full

spectrum, the input characteristic dimension is reduced from 224 to three bands, and the operation speed of the optimization modeling is high. Above all, this study provides a novel and fast moisture content detection method based on HSI.

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Conflict of interest statement: The authors declare no competing financial interest.

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