

# Fusion of THz-TDS and NIRS Based Detection of Moisture Content for Cattle Feed

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Huang J, Luo B, Cao Y, Li B, Qian M, Jia N and Zhao W (2022) Fusion of THz-TDS and NIRS Based Detection of Moisture Content for Cattle Feed. Front. Phys. 10:833278. doi: 10.3389/fphy.2022.833278 As an essential index to evaluate feed quality, feed moisture content which is too high or too low will impose an adverse impact on feed nutritional value. Therefore, the quantitative analysis of feed moisture content is significant. In this paper, the detection of feed moisture content based on terahertz (THz) and near-infrared (NIR) spectroscopy and data fusion technology of THz and NIR (THz-NIR) was investigated. First, feed samples with different water content (29.46%-49.46%) were prepared, and THz (50-3000 µm) and NIR (900-1700 nm) spectral data of samples was collected and preprocessed, and the feed samples were divided into correction set and verification set by 2:1. Second, the spectral data was fused through the head-to-tail splicing, and the feed moisture content prediction model was established combined with partial least squares regression (PLSR). Third, competitive adaptive reweighting sampling (CARS) was applied to extract spectral characteristic variables for feature layer fusion, and the feed moisture content prediction model in feature level was constructed combined with PLSR. Finally, the evaluation parameters validation set correlation coefficient (Rp), the root mean square error of prediction (RMSEP), and the residual predictive deviation (RPD) were employed to evaluate the prediction effect of the model. The results indicated that THz, NIR spectra, and data fusion technology could quickly and effectively predict feed moisture content. Among them, the characteristic layer spectral data fusion model achieved the optimal prediction effect while Rp, RMSEP, and RPD reached 0.9933, 0.0069, and 8.7386 respectively. In conclusion, compared with the prediction model established by single THz and NIR spectrum, THz-NIR spectrum data fusion could more accurately predict feed moisture content and provide certain theoretical and technical support for inspirations and methods for quantitative analysis of feed moisture content of livestock and poultry.

Keywords: terahertz, near-infrared, spectral fusion, detection technology, moisture content

# **1 INTRODUCTION**

Moisture content is an essential index to evaluate feed quality, which is closely related to the calculation of various nutritional indexes[1]. On the one hand, the dry matter content could be obtained by detecting the moisture content. On the other hand, it is convenient to analyze other nutrients, which is of vital guiding significance to preventing the mildew and deterioration of the nutrients during the process of feed processing, transportation, and storage. According to GB/T

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6435-2014 (China Standard), the standard method for feed moisture content is the dry method, which has high reliability but high energy consumption and low efficiency[2]. Modern detection of feed moisture methods includes Karl Fischer, moisture detector, and spectral technology. The spectral technology has the advantages of rapid detection, extensive applicability, and high sensitivity. Therefore, terahertz timedomain spectroscopy (THz-TDS), near-infrared (NIR) spectroscopy, and other spectral detection technologies have been developed rapidly.

THz-TDS acting as an emerging technology has the characteristic of fringerprint and sensitive to moisture content, and it can be applied to sense the moisture content of food and agricultural products. And they are applied to food production, safety inspection, materials science, military communications, biological medicine, and agricultural inspection products<sup>[3–6]</sup>. However, the cost is still high and difficult to assess real samples. Most samples are made into tablets. Compared with THz-TDS, NIRS is relatively mature and detection of real samples without any process for practical application. The feed assessment may carried out at an online or *in situ* mode.

Nowadays, limited studies have been conducted to detect feed moisture content utilizing spectral technology. In terms of quantitative analysis of moisture content of agricultural products, Zhang et al. collected NIR spectroscopy data of corn DDGS and combined it with partial least squares (PLS) to construct a quantitative analysis model of corn DDGS moisture content [7]. Zhang et al. applied Fourier transform infrared spectrometer to collect spectral data of corn samples and established a prediction model of moisture content of single corn seed based on random forest (RF)[8]. Lu et al. collected the NIR spectroscopy data of rice and established the PLS model of rice moisture content[9]. Wu et al. scanned the terahertz (THz) timedomain spectra of corn seed samples through attenuated total reflection (ATR) attachment and constructed a nonlinear model for efficient quantitative analysis of corn seed moisture by utilizing a support vector machine based on RBF kernel function and grid search method [10].

Some scholars have employed spectral data fusion technology to improve the accuracy of rapid detection. Generally, data fusion includes data-level fusion, feature-level fusion, and decision-level fusion[11-13]. Due to its ability to analyze complex system samples, data fusion technology is extensively applied to numerous fields. Li et al. investigated the feasibility of X-ray fluorescence (XRF), NIR, and mid-infrared (MIR) spectra data fusion to detect metal elements in the soil[14]. Among them, XRF-MIR spectral data fusion exhibited the optimal prediction effect ( $R^2 = 0.98$ ). The results demonstrated that XRF-MIR spectral data fusion could improve detection accuracy. Li et al. investigated the effective components of the deltamethrin formula utilizing spectral data fusion strategy[15]. Compared with feature-level fusion and single spectrum, data-level fusion possesses a better prediction ability (RMSEP = 0.0645%,  $R^2$  = 0.9978). This study provides a feasible method for pesticide quality control and field monitoring. Chen et al. fused ultraviolet (UV) and NIR spectrum data to build a quantitative prediction model of chemical oxygen demand

(COD) concentration[16]. The results indicated that the feature level fusion model displayed the most accurate prediction performance ( $R^2 = 0.9947$ , RMSEP = 0.976), implying that the spectral data fusion could reflect more chemical information of water samples and provide certain technical support for on-line monitoring of COD concentration in water. However, the fusion of THz and NIR spectral data (THz-NIR) has not been investigated.

In this paper, THz-NIR spectroscopy and two kinds of spectral data fusion were applied as the detection methods of feed moisture content. The main research contents are presented in **Figure 1**. First, the samples were prepared and their terahertz and near-infrared spectra were collected. Afterward, derivative Savitzky-Golay (SG) smoothing and normalization were applied to preprocess the original spectral data. Competitive adaptive reweighted sampling (CARS) was used to extract characteristic variables from spectral data. Data level fusion (LLDF) and feature level fusion (MLDF) were applied to fuse the preprocessed spectral data. Finally, based on the PLSR algorithm, a feed water content prediction model was established.

## **2 MATERIALS AND METHODS**

## 2.1 Instruments and Materials

In this experiment, the THz time-domain spectrometer (TERAK15, Menlo systems company, Germany) was utilized for THz spectrum measurement. The handheld NIR instrument (BIO JHWGPY, independently developed by the Intelligent Equipment Technology Research Center of Beijing Academy of Agricultural and Forestry Sciences) was utilized for NIR spectrum measurement. Manual tablet press (Specac GS15011, United Kingdom) was employed for tablet pressing. Precision electronic balance (FA2004N, Shanghai Jinghai Instrument Co., Ltd., China) was used for weighing. The planetary mill (XQM-0.4L, Changsha Tianchuang Powder Technology Co., Ltd., China) was utilized for grinding. Electric blast drying oven (XMA-2000, Shanghai Jinmao Industrial Technology Co., Ltd., China) was applied to drying. The feed particle size was screened by a standard inspection sieve (60 and 100 mesh, Xiaojin Standard Sieve Factory, Shangyu City, Zhejiang Province, China).

The feed applied in this experiment was provided by a professional breeding cooperative in Beijing while Polyethylene powder (CAS 9002-88-4, particle size  $40-48 \mu$ m) was purchased from Sigma Aldrich (Shanghai) Trading Co., Ltd. (United States).

## 2.2 Sample Preparation

The total sample preparation process proceeds as follows. First, the feed sample was fully ground. Second, the samples were screened until the particle size range was 0.154–0.280 mm. Third, 108 samples were humidified to different gradient moisture contents (29.46%–49.46%) and stored in sealed bags for subsequent use. Fourth, each sample was divided into three groups, i.e., 5 g, 5 g, and 100 mg weighed using a precision electronic balance for chemical value determination, THz spectrum (tableting required), and NIR spectrum collection





TABLE 1 | Statistical information of moisture content of samples.

Number of Samples	Minimum/%	Maximum/%	Average/%	Standard deviation/%	
108	29.46	49.46	40.70	5.735	



FIGURE 3 | THz spectrum acquisition.

respectively. Finally, the samples were mixed with polyethylene in equal amounts and pressed into flakes (4.0t external force and 4 min pressing time). The compressed samples had a diameter of 13 mm and a thickness of 1–2 mm. Sample manipulation is presented in **Figure 2**.

## 2.3 Data Acquisition

## 2.3.1 Determination of Chemical Moisture Content

According to GB/T 6435-2014 (China) determination of moisture in feed, the chemical value was obtained through the drying method.<sup>2</sup> The statistical information of the chemical value of moisture content of 108 samples is presented in **Table 1**.

## 2.3.2 THz Spectrum Data Acquisition

The THz spectrum data acquisition experiment was conducted in the transmission mode. Nitrogen needed to be added for drying to keep the relative humidity of the test environment below 3%. 108 tablet pressing samples were scanned and collected 3 times respectively. Each sample was taken out and reloaded each time. The spectrum and absorption coefficient of the sample was calculated via the built-in software TeraMat\_v10.vi (Menlo systems company, Germany). THz spectrum acquisition is presented in **Figure 3**.

## 2.3.3 NIR Spectrum Data Acquisition

The NIR spectrometer number of scans is 32 times, the wavelength range is 900–1700 nm, and the working mode is diffuse reflection scanning. 108 samples were scanned and each sample was measured 3 times. Reload the sample for each measurement. The reflectance is determined by the instrument's software Nirscan Nano GUI\_boxed-shortcut



FIGURE 4 | NIR spectrum acquisition.



(Beijing Academy of Agricultural and Forestry Sciences, China). NIR spectrum acquisition is presented in **Figure 4**.

# 2.4 Spectral Data Processing and Fusion Method

In this experiment, MATLAB 2016a software (The MathWorks, America) was utilized for data processing while Origin 2018 software (OriginLab, America) was for drawing. First, derivative and SG smoothing was applied to preprocess the spectral data, thereby eliminating the spectral baseline drift and noise interference. Afterward, the spectral data was normalized to eliminate the influence caused by the different orders of magnitude between the two spectral data during fusion[17]. The sample set partitioning based on joint x-y distance (SPXY) was applied to divide the samples into correction set and verification set by 2:1 [18]. Finally, the spectral characteristic variables were selected by CARS algorithm.

In this experiment, to improve the effect of the feed moisture content prediction, a feed moisture content prediction model based on THz and NIR spectral data fusion was proposed.



Figure 5 shows two different data fusion methods based on the THz-NIR spectrum.

# 2.5 Model Establishment and Evaluation

In this study, PLSR was applied to establish a prediction model of feed moisture content. PLSR could realize multiple linear regression and principal component analysis simultaneously under one algorithm system. During the modeling process, PLSR considered the mutual influence of decomposition of the independent variable and dependent variable. Therefore, the use of PLSR for model construction could ensure the correlation between independent and dependent variables, thereby improving the predictive performance of the model.

To evaluate the performance of the prediction model, the root mean square error estimated by calibration (RMSEC), prediction (RMSEP), and correlation coefficient of calibration (Rc), prediction (Rp), and residual predictive deviation (RPD) were employed as evaluation indicators. A good model should have high Rc, Rp, and RPD values and low RMSEC and RMSEP values.

# **3 RESULTS AND DISCUSSION**

## 3.1 Spectra Analysis

The THz and NIR spectra of 108 feed samples are presented in **Figure 6**. The abscissa is the frequency while the ordinate is the THz absorption in **Figure 6A**, and each spectrum has 1,023 values. As presented in **Figure 6A**, the absorption value increases first and then decreases with no obvious absorption peak. With the increase of frequency, the spectral lines begin to fluctuate, hence it is difficult to analyze the regular changes of the spectrum. To reflect the spectral characteristics of absorption, preprocessing is needed to eliminate noises and improve the spectral signal-to-noise ratio. The abscissa is the wavelength while the ordinate is NIR reflectance in **Figure 6B**, and each spectrum of the sample is smooth within the range of 900-1,700 nm with weak absorption peaks near 1,200 nm and 1,425 nm.

# 3.2 Data Level Fusion Analysis

The number of principal factors is closely related to the prediction accuracy of the model. If it is too small, the essential information

of water content might not be reflected in the model, thus resulting in lower prediction accuracy. If it is too large, the noise of the model will become larger during the modeling process. In the present study, the result of the correction set is suitable, but the prediction accuracy of the model is poor due to the inclusion of more information in the prediction set. Therefore, it is essential to apply a reasonable number of principal factors to the modeling. Nowadays, the most extensively applied method to determine the number of principal factors is Prediction Residual Error Sum of Squares (PRESS). After the spectral data is preprocessed, the optimal number of factors is selected by comparing the sum of squares of prediction residuals obtained by interactive verification. The results are presented in **Figure 7**.

As presented in **Figure 7**, when the number of principal factors of THz, NIR, and THz-NIR is 20, 18, and 17 respectively, the sum of squares of prediction residuals obtained from interactive verification is the lowest. Therefore, the respective optimal number of principal factors is selected for the construction of the model. The comparison of the results of PLSR model establishment is presented in **Table 2**.

It could be seen from Table 2 that RMSEC and RMSEP of the single spectrum prediction model are quite different. The prediction results of both THz and NIR full spectrum models are not accurate. The Rc of THz and NIR full spectrum models is 0.996 and 0.998 respectively while the RMSEC of them is sufficiently low, which is 0.005 and 0.002 respectively. However, the prediction accuracy of the single spectrum data model is not high with Rp being 0.977 and 0.959 respectively, and the difference between single spectrum prediction model RMSEC and RMSEP is large, implying that the prediction accuracy is not high enough and the model is unstable. Compared with the single spectral model, the Rc and Rp of the THz-NIR data layer fusion model reach 0.988 and 0.984 respectively, and its RMSEC and RMSEP being 0.009 and 0.010 respectively are relatively low, between which the difference is small. The prediction accuracy of the THz-NIR data-level fusion model is high and the model is relatively stable, implying that the prediction accuracy of the data-level



### TABLE 2 | Results of PLS model establishment.

Model classification	Number of factors	Rc	RMSEC	Rp	RMSEP	RPD
NIR full spectrum	18	0.998	0.002	0.959	0.015	3.548
THz-NIR(LLDF)	17	0.988	0.009	0.984	0.010	5.558



fusion model is remarkably improved compared with the single spectral prediction model. Its prediction accuracy is verified by the verification set experiment, as presented in **Figures 8A,B**, in **Figure 8C**, the overall samples of models a and b are evenly distributed and concentrated near the centerline, which indicates that the predicted value of the model approaches the real value and the model is also relatively stable.

## 3.3 Feature Level Fusion Analysis

Based on the importance level of each wavelength, CARS selects n wavelength subsets from N Monte Carlo (MC) samples iteratively and competitively. In each sampling, a fixed proportion of samples is randomly selected to establish the calibration model. Afterward, based on the regression coefficient, two steps of forced wavelength selection based on exponentially decreasing function (EDF) and competitive wavelength selection based on adaptive reweighting sampling (ARS) are conducted to select the key wavelength. Finally, cross-validation (CV) is applied to select the subset with the smallest CV root mean square error (RMSECV). The flow chart of the CARS algorithm is presented in **Figure 9**.

Through 50 MC iterations sampling, 80% of the samples in the correction set are randomly selected each time to establish the PLSR model. ARS is applied to screen the wavelength variables, and the lowest subset of RMSECV of the model is selected by a 10-fold interactive test. The process of selecting the optimal variables for THz spectrum and NIR spectrum data is presented in **Figures 10**, **11** respectively.

Figure 10 presents the trend of the number of sampling variables (Figure 10A), RMSECV value (Figure 10B), and regression coefficient path of each variable (Figure 10C) with the increase of sampling times. As the number of runs increases, the number of optimized wavelength variables gradually decreases (Figure 10A). The number of sampling variables decreases rapidly at the first stage of EDF while at the second stage of EDF, it decreases very slowly, which indicates that the proposed two-stage selection, i.e., fast selection and fine





selection, is realized in CARS. During the process of 1–24 sampling, the RMSECV value continuously decreases, implying that the variables removed during the screening process are not related to the water content. After 24

samplings, the RMSECV value shows an upward trend, which implies that the essential variables related to the water content are removed, thus resulting in the rise of the RMSECV value (Figure 10B). As presented in Figure 10C, when the number of

## **TABLE 3** | Comparison of model evaluation indexes.

Model classification	Rc	RMSEC	Rp	RMSEP	RPD
THz characteristic variable model	0.989	0.008	0.986	0.010	6.020
NIR characteristic variable model	0.994	0.007	0.982	0.010	5.431
THz-NIR(MLDF)	0.994	0.006	0.993	0.007	8.739



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samples is small, the absolute value of the regression coefficient of each wavelength is small. With the increase of the number of samples, the coefficients of some wavelengths become larger while those of other wavelengths become smaller. In particular, when the corresponding wavelengths are eliminated by CARS, the coefficient will drop to zero because they are not selected. Therefore, the larger the absolute coefficient, the greater the possibility of survival of the corresponding wavelength. The selection mechanism of CARS resembles "the survival of the fittest" in Darwin's theory of evolution. Each wavelength could be regarded as an individual, and all the other wavelengths are naturally regarded as its "environment". Based on this, the CARS algorithm uses adaptive reweighted sampling technology to realize the most suitable individual selection process. In general, in Figure 10, when the number of samples reaches 24, the RMSECV value reaches the minimum and the corresponding subset of spectral variables is the optimal (the position corresponding to the dotted line in Figure 10C), which contains 55 spectral variables. In Figure 11, as the number of runs increases, the number of optimized wavelength variables gradually decreases (Figure 11A). When the number of samples is 15, the RMSECV value reaches the minimum (Figure 11B),

and the corresponding subset of spectral variables is the optimal (the position corresponding to the dotted line in **Figure 11C**), which contains 53 spectral variables. After the CARS wavelength optimization, the number of variables screened by THz is 55 frequency points, as presented in **Figure 12A**. The number of variables screened by NIR is 53 wavelength points, as shown in **Figure 12B**.

Among them, the spectral variable of the THz spectrum optimized by CARS is only 5.4% of the full spectrum, implying that CARS wavelength optimization could simplify the model. The THz and NIR characteristic variables optimized by CARS are fused as the independent variables while the real value of feed moisture content is the dependent variable of the model. The feed moisture content prediction model is established by PLSR. The Rc and RMSEC of the correction set are 0.994 and 0.006 respectively while the Rp and RMSEP of the verification set are 0.993 and 0.007 respectively. In comparison, the PLSR model (short for THz characteristic variable model and NIR characteristic variable model) is established with the respective characteristic variables of THz and NIR optimized by CARS as independent variables and the real value of feed moisture content as the



dependent variable. The comparison of model evaluation indexes of the correction set and the prediction set is presented in **Table 3**.

As indicated in **Table 3**, the Rp, RMSEP, and RPD of THz characteristic variable model established through CARS characteristic variable optimization are 0.986, 0.010, and 6.020 respectively while the RP, RMSEP, and RPD of THz full spectrum prediction model are 0.977, 0.012 and 4.693 respectively. The RPD values of the full spectrum model and characteristic variable model exceed 3, implying that both of them could better quantitatively predict feed moisture content.

However, the THz characteristic variable model uses only 5.4% of the full spectrum variables to achieve better prediction results than the full spectrum model, and the difference between RMSEC and RMSEP is smaller, implying that the THz characteristic variable model is more stable than the full spectrum model. After the optimization of CARS characteristic variables, the values of Rp, RMSEP, and RPD of the NIR characteristic variable model are also higher than those of the NIR full spectrum model. This demonstrates that the full spectrum model contains a large amount of redundant information, which will exert a negative impact on the prediction ability of the feed moisture content model, and the CARS characteristic variable optimization will select the characteristic variables related to feed moisture to optimize the model. The Rp, RMSEP, and RPD scores of the THz-NIR feature level data model reach 0.993, 0.007, and 8.739. The prediction effect is not only better than the model established using single spectral feature data, but also has higher prediction accuracy and stability than the data-level fusion model. The Rp, RMSEP, and RPD of the feature layer fusion model are 0.96%, 49.28%, and 36.40% higher than those of the data layer fusion model. This indicates that the THz-NIR model based on feature level data fusion could achieve the optimal prediction effect in the detection of feed moisture content in this experiment. The prediction results of the model established by the preferred characteristic variables of the CARS algorithm are presented in Figures 13A,B, in Figure 13C, the overall samples in models a and b are evenly distributed and concentrated near the centerline, implying that the predicted value of the model approaches the measured value, and the model is relatively stable.

## **4 CONCLUSION**

In this paper, the moisture content of the feed was quantitatively analyzed based on THz and NIR spectroscopy. On this basis, the prediction effects of single spectral modeling (THz and NIR) and two fusion strategy modeling (LLDF and MLDF) were analyzed step by step. The characteristic variables were selected by the CARS algorithm, and the prediction model was established by PLSR. The major conclusions are as follows.

- The prediction model of feed moisture content was established by THz and NIR spectroscopy combined with PLSR, and the prediction effect of THz and NIR spectroscopy on feed moisture content was analyzed. The results indicate that the Rp, RMSEP, and RPD of the THz optimal prediction model are 0.986, 0.010, and 6.020 respectively, and the Rp, RMSEP, and RPD of the NIR optimal prediction model are 0.982, 0.010, and 5.431 respectively. It is demonstrated that THz and NIR spectroscopy could quickly and effectively predict feed moisture content.
- 2) CARS optimal selection of characteristic variables could improve the prediction ability of the model. Compared with the full spectrum model, the Rp, RMSEP, and RPD of THz spectral characteristic variables prediction model increase by 0.88%, 25.77%, and 22.05% respectively, and

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those of the NIR spectral characteristic variable prediction model increase by 2.35%, 53.61%, and 34.67% respectively.

- 3) THz and NIR spectral data was fused by data level fusion technology, and the feed moisture content prediction model was established. The prediction effects of THz, NIR, and data layer fusion technology on feed moisture content were analyzed and compared. The results indicate that the Rp, RMSEP, and RPD of the data level fusion prediction model are 0.984, 0.010, and 5.558 respectively, and the prediction ability is better than THz and NIR full spectrum prediction models.
- 4) THz and NIR spectral characteristic variables were fused by feature level fusion technology, and the feed moisture content prediction model was constructed. The prediction effects of THz, NIR, and feature level fusion technology on feed moisture content were analyzed and compared. The results indicate that the Rp, RMSEP, and RPD of the feature-level fusion prediction model are 0.993, 0.007, and 8.739 respectively. The prediction effect is better than not only the THz and NIR feature variable prediction model but also the data-level fusion prediction model.

The results indicate that feature-level data fusion is the most effective method to establish a quantitative analysis model of feed moisture content. In general, the spectral data fusion combined with the CARS algorithm to select characteristic variables is a feasible and effective quantitative analysis method for feed moisture content. This method provides the theoretical basis and technical support for the quantitative analysis of feed moisture content, which could be used as a reference for the establishment of new methods for online or *in situ* practical detection applications.

## DATA AVAILABILITY STATEMENT

The raw data supporting the conclusion of this article will be made available by the authors, without undue reservation.

# AUTHOR CONTRIBUTIONS

All authors listed have made a substantial, direct, and intellectual contribution to the work and approved it for publication.

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