Evaluation of Blend Uniformity and Terminal Point during Continuous Mixing in Water for Modified Double-Base Propellant Components Using a Near-Infrared Method

Ben Liu, Lei Xiao, Zongkai Wu, Duo Li, Yubing Hu, Guangpu Zhang, Fengqi Zhao, Xiuduo Song,* Wei Jiang, and Gazi Hao*

ABSTRACT: A near-infrared (NIR) spectrometer was used to test the double-base absorbent powder sample and to quantitatively analyze the contents of each component as well as their dispersion uniformity to establish a rapid quantitative test method for blending uniformity of modified double-base (MDB) propellant components. First, the quantitative calibration models of hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) were constructed based on sample testing, and the RDX model’s correlation coefficient was 0.9929. Then, during the blending process, NIR spectra were continually collected. For the original spectra of samples, the blend uniformity was assessed using the coefficient of moving block standard deviation (MBSD). After 160 min, the sample’s MBSD value had reached a steady state of less than 0.003, indicating that the sample’s components were distributed uniformly. The findings reveal that NIR spectroscopy can be used to verify the blending uniformity of MDB propellant components.

1. INTRODUCTION
A typical modified double-base (MDB) propellant, which consists of nitrocellulose (NC), nitroglycerin (NG), aluminum powder, hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX), and water, has higher energy, is easy to transport, is safe to use, has a long life, and is used to power missiles and tactical rockets. Multiple procedures such as absorption (mixing), calendering (plasticizing), compression, and extension processes must be performed during the industrial manufacture of MDB propellants. The first and most important process in propellant manufacturing is the mixing procedure. Mixing refers to the process of suspending NC in a dispersion medium using a specific dispersion method such that the components of the MDB propellant are uniformly and properly measured blended and securely integrated. The mixing effect of the propellant components is critical in determining the theoretical performance of the propellants. We currently rely on experienced operators to subjectively assess whether the propellant components have been mixed uniformly in the manufacturing process based on their experience and determine the process of the manufacturing process based on the judgment results. However, the most significant disadvantage of subjective judgment is that it cannot accurately reflect the uniformity of propellant component mixing, and there is likely to be a large error, resulting in differences in the absorption effect of propellant components, which is reflected in the finished propellant having difficulty in maintaining the stability of the propellant performance.

To ensure the absorption quality of the propellant, the uniformity of the propellant components is often checked during the manufacturing process using classic wet chemical...
methods. Specifically, high-performance liquid chromatography (HPLC),8 gas chromatography, ultraviolet–visible (UV–vis) spectrophotometry, and dissolution-weighing methods were used to analyze the content of RDX, NC, and NG, the propellant’s primary components, one by one, to determine their deviation in content. However, this off-line testing method also has a number of disadvantages: (1) the sampling process not only interrupts production but also poses safety risks; (2) it is time-consuming and environmentally polluting; (3) it can only determine the overall uniformity of a large number of macroscopic propellant components and cannot be used to determine the microscopic uniformity of the propellant components; (4) it is unable to ensure continuous and automated production of solid propellants and to meet the requirements of “real-time, safe and environmentally friendly” production quality control methods.9

As a result, researchers have been seeking a rapid, online, and accurate method for the determination of the absorption uniformity of propellant components to assess the absorption effect and guide the propellant quality and stability control. The United State Food and Drug Administration released a draft application of process analysis technology in 2004 and recommended the use of near-infrared (NIR) spectroscopy as a fast, safe, and environmentally friendly online detection technology for quality control of food and drug production processes in order to improve the production line’s real-time correction capability and thus ensure product quality.10 Thus, the ability of NIR spectroscopy analysis technology to detect the content of major propellant components and the mixing uniformity online will provide key technical support for ensuring the quality of solid propellants produced continuously and automatically with high reliability and reproducibility. Modern NIR analysis approaches combined with chemometric methods can extract information from the NIR spectra of various components and construct quantitative analytical models with reliable and consistent performance, which can readily quantify multiple components without degrading the drug.11 Additionally, because NIR light has high transmission capabilities in standard optical fiber materials and can be transmitted over long distances via optical fibers, NIR analysis technology has been widely used in many fields such as food,12 pharmaceuticals,13 cereals,14 tobacco,15 chemicals,16,17 and the military industry18,19 and developed rapidly in recent years. In the civil sector, NIR is commonly used to determine the homogeneity of pharmaceuticals. Ma et al. used the near-infrared chemical imaging (NIR-CI) method to study the homogeneity in the distribution of chlorpheniramine maleate (CPM) tablets. A method called “distributional homogeneity index (DHI)” was used to evaluate the uniformity of distribution of six different brands of CPM.20 Wahl et al. used the NIR-CI technique to evaluate the consistency of caffeine within and between tablets using both standard deviation (SD) and DHI methods.21 For the military application, Zou et al. presented an NIR method for in-process detection of the absorbent powder homogeneity. The absorbent powders’ NIR spectra were acquired using a micro-NIR spectrometer under stirring circumstances, and the spectra deviation was quantified using the moving block of SD moving block standard deviation (MBSD) method. Additionally, HPLC is used to confirm the accuracy of the NIR analysis on the obtained data. NIR analysis has been shown to be effective, environmentally friendly, and safe.22 It demonstrates the viability of using the NIR method to determine the homogeneity of MDB propellant components.

While the MBSD algorithm is capable of reflecting the system changes throughout the mixing process in real time, the preceding study has the following two limitations: (1) the study processed deviation on three consecutive spectral lines across the entire spectral band range, and the characteristic peaks of the main propellant components were obscured by the absorption peaks of a large amount of water, making it difficult to fully reflect the mixing uniformity change process of RDX, NC, and other propellant components; (2) the study concluded that the terminal point of absorption is ∼131 s, which is very different from the actual situation of propellant plants producing propellant components generally in more than 2 h.22 It is difficult to accurately represent the actual state of the absorption process, and the result reached is insufficient to justify practical implementation. As a result, it is required to choose the characteristic peaks of the propellant’s major components and combine them with the overall spectral characteristics to conduct a comprehensive analysis and determine the propellant component mixing uniformity and absorption endpoint. Furthermore, to recreate the absorption process more accurately, the absorption process’s mixing time should be increased to acquire the SD over a lengthy period of time. Nonetheless, the MBSD algorithm used in this paper serves as a good reference for our study of the blend homogeneity of and calculation of the absorption endpoint.

This paper will use the MBSD algorithm, reflecting the typical characteristics of the spectrum to achieve online detection of the mixing endpoint of typical MDB propellant components in order to improve and optimize the MBSD algorithm for the online determination of the absorption endpoint of typical MDB propellant components.

Figure 1. Overall design idea for the evaluation of blend uniformity and terminal point for MDB propellant components.
2. MATERIALS AND METHODS

2.1. Overall Design Idea. The general design concept for evaluating the blend uniformity and terminal point of MDB propellant components during continuous mixing in water using an NIR method is shown in Figure 1.

The process can be summarized as follows: (1) preparing a representative sample of MDB propellant components; (2) configuring an NIR detection device to evaluate the characteristic spectra of the sample; (3) detecting the spectra of various MDB propellant components, then selecting their characteristic spectra, and further evaluating the feasibility of online NIR detection for blend uniformity and terminal point of MDB propellant components; and (4) establishing a correlation between the blend uniformity and terminal point of MDB propellant components and the results collected by an NIR spectrometer’s characteristic spectrum collection.

2.2. Sample Preparation. The typical propellant components were used, including a 1:1 mixture (weight ratio) of RDX and NC/NG, with the NC being plasticized with an equivalent proportion of NG in advance. Because the content of minor components such as stabilizers and catalysts in the MDB propellant is typically less than 5%, they were not considered in this typical formula. These propellant components are obtained directly from an explosive manufacturer, and they all have high sensitivity and risk, requiring extra caution during the experiment.

2.3. Construction of the Test Equipment. Figure 2 shows the self-built equipment used to determine the blend uniformity and terminal point of MDB propellant components. The device operates in the following way: the propellant components were introduced and were continuously mixed in the jacketed beaker. A constant-temperature water bath was used to maintain the sample's temperature. Then, utilizing Thermo Antaris II NIR spectroscopy, a specially designed fiber optic probe was placed into the suspension to get the sample’s NIR spectrum. Simultaneously, computer software was used to record and process the sample’s spectral information. Finally, by analyzing these spectral data, a wealth of important information can be gleaned.

2.4. Characteristic Spectrum Selection of MDB Propellant Components. The selection of the characteristic spectrum is based on the premise that the spectrum of a certain region of the propellant components represents only that region and is unaffected by the spectrum of other components, particularly water. The NIR spectrum of each component (RDX, NC, NC + NG, H₂O, RDX + H₂O, NC + H₂O, NC + NG + H₂O, RDX + NC + NG + H₂O) is identified in this example with or without water (RDX + H₂O, NC + H₂O, NC + NG + H₂O, RDX + NC + NG + H₂O). All in situ NIR spectra were acquired with a resolution of 16 cm⁻¹ and averaged over 10 scans in the range from 4000 to 10 000 cm⁻¹. Each spectrum capture takes ~8 s.

2.5. Feasibility Blend Uniformity and Terminal Point of MDB Propellant Components. The oscillation of mass concentration of the suspension was used to determine if it is evenly mixed. When we determined that the blend uniformity and terminal point of MDB propellant components had been reached, we took a uniform distribution of at least one sample mass across time. In particular, as long as the propellant component’s concentration can be quantified quantitatively
using NIR spectroscopy, its blend homogeneity may be reflected.

Based on the result of Section 2.4, the characteristic components and spectrum of the MDB propellant would be chosen. The operation proceeded in the following way: using an electronic balance, 600 g of deionized water is weighed. The RDX mass fraction is adjusted to a range of 1–15.5% at 0.5% interval, and it is ensured that each sample has 600 g of water. We prepared a total of 30 samples. Mechanical stirring blades were added into the sample at a speed of 650 rpm to ensure uniform mixing of the RDX and H2O in the system. After continuous stirring, the optical fiber probe was placed directly into the sample, and the NIR spectrum of 30 samples was obtained successively. Among them, 23 samples served as the calibration set for developing a quantitative chemometrics model, while the remaining seven samples served as prediction sets for evaluating the model’s performance. Table 1 summarizes the samples used to develop a quantitative chemometrics model of the RDX concentration in water.

Following that, TQ Analyst software was used to do spectral preprocessing and multivariate regression. To eliminate random noise and false contribution caused by a baseline shift, all spectra were preprocessed using the first-derivative method. Subsequently, a quantitative model for RDX over the selected wavenumber ranges was created using a partial least squares (PLS) regression algorithm, which extracts the maximum information from signals effectively. The appropriate number of PLS variables was determined using leave-one-out cross-validation with the root-mean-square error as the minimal statistic (RMSECV, formula 1).

\[
RMSECV = \sqrt{\frac{\sum_{i=1}^{n} (\hat{y}_i - y_i^{\text{ref}})^2}{n - 1}}
\]  

where \(\hat{y}_i\) is the RDX content predicted by the NIR model, \(y_i^{\text{ref}}\) is that obtained by weighing, and \(n\) is the number of samples.

### 2.6. Evaluation of Blend Uniformity and Terminal Point

The construction between blend uniformity and terminal point as well as the RDX spectrum can be used to deduce the blend uniformity and terminal point of MDB propellant components. To illustrate the change in the uniformity of MDB propellant components, a simple approach called MBSD was used to demonstrate the difference between the spectra at different times. The MBSD method is straightforward and convenient as it avoids the lengthy operations associated with conventional methods and does not require pre-calibrated stoichiometry. The algorithm of MBSD is as follows

\[
S_i = \sqrt{\frac{\sum_{j=1}^{n} (A_j - \bar{A})^2}{n - 1}}, \quad S = \frac{\sum_{i=1}^{m} S_i}{m}
\]

where \(A_j\) denotes the absorbance of the \(j\)-th spectrum at the wavenumber value of \(i\), \(\bar{A}\) is the average absorbance value of the selected continuous \(n\) spectra at the wavenumber value of \(i\); \(m\) denotes the total number of selected wavenumbers, and \(S\) denotes the average of the SD of absorbance that corresponds to the selected \(m\) waves. It should be noted that if one of the number \(n\) of selected continuous spectra is greater, it is easy to ignore the partial discrepancies between the spectra. In this study, the value of \(n\) is 3, implying that three consecutive spectra are selected for calculation each time. The MBSD algorithm calculates a real-time difference between NIR spectra during the full mixing process of MDB propellant components. Taking into account the influence of accidental elements in the real mixing process, after the beginning of the mixing process, when the \(S\) values of multiple consecutive nodes are less than the threshold, they are evaluated as a blend uniformity and terminal point.

Further, microscopic pictures of the mixed MDB propellant components at different mixing times were taken to verify their homogeneity.

### 3. RESULTS AND DISCUSSION

#### 3.1. Spectral Analysis

Figure 3 shows the NIR \(\text{lg}(1/R)\) spectra of RDX, NC, NC + NG, and H2O. As shown in Figure 3, RDX has four main absorption bands: 4000–4730, 5750–6250, 6930–7510, and 8730–9020 cm\(^{-1}\). The spectra of 5750–6250 cm\(^{-1}\) are placed directly between the water absorption peaks of 5100 and 6880 cm\(^{-1}\), which are less influenced by water and are relatively strong in comparison to other bands. Because the spectra of 6930–7510 cm\(^{-1}\) are covered by the water absorption peak at 6880 cm\(^{-1}\), and 8730–9020 cm\(^{-1}\) is covered by the water absorption peak at 6880 and 8500 cm\(^{-1}\), respectively, water will interfere with these two spectral bands significantly. As a result, two spectral regions, 4000–4730 and 5750–6250 cm\(^{-1}\), are preferred as RDX modeling intervals.

Additionally, the NIR spectra of RDX + H2O, NC + H2O, NC + NG + H2O, and RDX + NC + NG + H2O were collected to validate the modeling intervals for RDX. As shown in Figure 4, when RDX, NC, NC + NG, and RDX + NC + NG are combined with water, their absorption strength is greatly increased. While both are affected by water’s strong peaks, the characteristic peaks of RDX in the 4000–4730 and 5750–6250 cm\(^{-1}\) spectral bands can be retained intact, and the characteristic absorption peaks of RDX + H2O, NC + H2O, NC + NG + H2O, and RDX + NC + NG + H2O.
peaks of NC have a considerable overlap with those of water. As a result, it can be determined that RDX is capable of being used for spectral modeling in the 4000−4730 and 5750−6250 cm\(^{-1}\) spectral regions.

Figure 5 shows the sample spectra collected using the 2.5 method. It was found that the absorbance of RDX + H\(_2\)O decreased with the increase of RDX content from 1 to 15.5%.

After automatic optimization by the system software, the decreased with the increase of RDX content from 1 to 15.5%. After automatic optimization by the system software, the additional chosen spectral modeling intervals were 4244.2−4557.4 and 6024.33−6106.74 cm\(^{-1}\), and the preprocessing method was the first-order derivative.

3.2. Feasibility Analysis. In this study, TQ Analyst software randomly chose 23 samples from 30 standard samples to serve as the calibration set, and the PLS method was used to create the quantitative calibration model for RDX. The remaining seven samples (with RDX concentrations of 1.5, 3.5, 5, 8.5, 10.5, 12, and 15%, respectively) were not used in the model construction but were used for the prediction validation.

Internal cross-validation refers to the process of extracting \(m\) samples (\(m < n\)). RMSECV was obtained by using the leave-one-out method.\(^{25}\) When the appropriate number of major factors is found, the matching RMSECV value is modest, indicating that the former model is stable and dependable. As shown in Figure 6, the optimal number of major factors for modeling the RDX content model is 9.

Table 2 contains the values for the relevant parameters used during the model construction process. \(R^2_c\) and RMSEC for the model’s internal correction were 0.9929 and 0.36, respectively, indicating that the model performed well in terms of internal correction,\(^{26}\) which is a result of the simplicity of the system.

Furthermore, the preprocessing using the first-order derivative method minimizes NIR light scattering by RDX particles, and the instrument’s random noise contributes to the good results.\(^{27}\) Figure 7 shows the results of an internal cross-test to determine the RDX content.

External validation is the process of validating a model using samples from the validation set that are unrelated to the calibration set. External validation not only indicates the model’s predictive ability but also checks that it is not over-fitted, which is important for complex systems. The fiber optic probe was immediately inserted into seven external validation samples in a continuous stirring state, and the absorbent powder samples’ NIR spectra were collected. The obtained spectra are then analyzed according to the predefined model, and the absorbent powder’s RDX concentration is shown directly on the computer interface. The entire process, from spectral collecting to model processing to acquire results, is straightforward and does not require any pretreatment of the sample, does not utilize chemical reagents, and produces no waste that contributes to environmental pollution. Figures 8 and 9 show the numerical connection between the predicted values of the RDX quantitative model and the actual values of the medium component content of the validation set samples. The quality of prediction was assessed in terms of RMSECV and \(R^2\).\(^{28}\) As shown in Figures 8 and 9, the results of the calibration model in predicting the RDX contents are well accepted.

In conclusion, in situ detection of RDX content was performed by constructing a two-component system consisting of RDX and swirling it continuously in water under continuous stirring conditions. The optimal spectral pre-treatment method and algorithm for modeling were optimized. By analyzing the impacts of significant amounts of water present and continuous stirring on the NIR spectra, the optimal spectral pretreatment method and modeling algorithm were optimized. Additionally, a more appropriate modeling interval was chosen for the model by analyzing the samples and the RDX NIR spectrograms. The constructed model may accurately reflect the current issue.

3.3. Blend Uniformity Analysis. The absorbent powder system was subjected to a total of three consecutive mixing stages of stationary−starting mixing−mixing homogeneously, and the absorbent powder’s NIR spectra were acquired in real time and are shown in Figure 10. In the illustration, there are two distinct spectral overlap bands, and the overlap area 1 corresponds to the spectrum of the material at rest. However, the NIR spectral similarity increased gradually and the spectra eventually overlapped at spectral interval 2, which were attributed to the improved homogeneity of the components within the absorbent powder system throughout the mixing process.

Obviously, it is highly difficult to distinguish subtle differences between the spectra through direct observation of the NIR spectra of the absorbent powder samples, which cannot adequately reflect changes in homogeneity during the mixing process. As a result, the NIR spectra of continually collected samples were analyzed using chemometric software. Conventional NIR spectroscopy determines the mixing endpoint by detecting whether the content of each component in different parts is consistent, which not only introduces interference from spectral band overlap and a large amount of liquid water but also necessitates the collection of massive representative samples to build a quantitative calibration model. Additionally, the model’s maintenance and updating at a later stage demands a significance of resources. Furthermore, because the mixing process is
influenced by incidental factors, the mixing terminal point is defined as the point at which several consecutive S values are smaller than a predefined threshold value\(^{29}\) (0.03 in this study) after the mixing process begins. The major logical procedures of the work flow devised in this study for analyzing the effect of absorbent powder mixing homogeneity that meet the requirements for online testing are summarized in Table 3.

The NIR spectra of the absorbent powder component configured in Section 2.5 were obtained for \(\sim 2.5\) h at a certain temperature. As shown in Figure 11, 290 spectral curves were obtained. The change pattern of the absorbent powder’s spectral curve shows a lot of fluctuation at first but progressively stabilizes at a given point with reduced fluctuation later, which shows the absorbent powder’s mixing homogeneity.

They recorded the average deviations of three consecutive spectral lines and archived values of close to 80—90. Figure 12 shows the mean deviation of the absorber for three consecutive spectral lines as a function of time. The mean deviation of the absorber’s three consecutive spectral lines showed a little variation, and it is obvious that the mean deviation of the absorber’s three consecutive spectral lines showed an overall decrease with time, indicating that the absorber’s mixing uniformity was improved. It can be observed that after \(\sim 80\) min of absorption, the percentage of the average deviation of the three consecutive absorber drug spectral lines less than 0.01 gradually increases, whereas there are few spectral deviations less than 0.01 before \(\sim 80\) min; after \(\sim 154\) min, the average deviation of the three consecutive absorber drug spectral lines is less than 0.03, whereas there are numerous deviations greater than 0.03 before \(\sim 154\) min. When the NG in the absorbent powder has a strong swelling effect on the NC, the NC consistency in the system becomes more stable, and the variability of the mixed system with RDX becomes relatively small. As a result, the average deviation of three consecutive absorber spectral lines shows an overall decreasing trend.

Replication tests were conducted to determine whether a necessary link could be made between this online test result and the uniformity of the absorbed samples. For the absorber fraction specified in Section 2.5, NIR spectra were collected for \(\sim 2.8\) h. As shown in Figure 13, 290 spectral profiles were obtained. Figure 14 shows the mean deviation of the absorber for three consecutive spectral lines as a function of time. The average deviation of three consecutive spectral lines of the absorber was used to describe the absorber’s mixing uniformity with good reproducibility, and the absorber’s overall mixing uniformity improved over time, as indicated by the decreasing trend of the average deviation of three consecutive spectral lines. After 160 min, the average deviation of the absorber’s three consecutive spectral lines was practically less than 0.03, indicating that the absorption had reached its terminal point.

### Table 2. Relevant Parameters and Cross-Validation Results from the RDX Content Modeling Process

| number of samples | \(R^2_c\) | RMSEC | spectral pretreatment methods | modeling interval/cm\(^{-1}\) | number of main factors |
|-------------------|-----------|-------|-------------------------------|-----------------------------|-----------------------|
| 23                | 0.9929    | 0.36  | first order derivative        | 4244.2–4557.4 cm\(^{-1}\), 6024.33–6106.74 cm\(^{-1}\) | 9                     |
In addition, microscopic pictures (Figure 15) of the mixed MDB propellant components at 20 and 160 min were taken, respectively, to verify their homogeneity. As shown in Figure 15, the MDB propellant components are composed of RDX with diameters ranging from tens of micrometers to 200 μm and NC with lengths ranging from tens of micrometers to 1 mm with a diameter of about 20 μm. Obviously, the difference in morphology and particle size of these two substances makes it
difficult for them to mix. At a mixing time of 20 min (Figure 15a), the two species, RDX and NC, were almost separated without much intersection, which corresponds to a large volatility of mean deviation of three consecutive spectral lines of the absorber shown in Figures 12 and 14. On the contrary, after mixing with 160 min, RDX and NC are more evenly mixed and have some intersection between them, which corresponds to a small volatility of mean deviation of three consecutive spectral lines of the absorber shown in Figures 12 and 14. These microscopic characterizations confirmed that MBSD could well represent the blending uniformity of MDB propellant components.

4. CONCLUSIONS

The components of the MDB absorber system were modeled using NIR spectroscopy combined with chemometrics. The model correlation coefficient was greater than 0.99. The results of the internal prediction validation demonstrated that the model prediction error was relatively small and stable. The MBSD method was demonstrated to analyze the sample components’ blend uniformity, and the MBSD value of RDX can be used to immediately reflect the sample’s total blend uniformity. The microscopic characterizations confirmed that MBSD could well represent the blending uniformity of MDB propellant components. The results demonstrated that using NIR spectroscopy, the mixing homogeneity of the MDB propellant components may be rapidly assessed. It can be expected that NIR spectroscopy and NIR technology have a great application in the characterization of the uniformity of various propellants.
Gazi Hao — National Special Superfine Powder Engineering Research Center of China, School of Chemistry and Chemical Engineering, Nanjing University of Science and Technology, Nanjing 210094, China; orcid.org/0000-0002-6508-5274; Email: hgznjust1989@163.com

Authors
Ben Liu — National Special Superfine Powder Engineering Research Center of China, School of Chemistry and Chemical Engineering, Nanjing University of Science and Technology, Nanjing 210094, China
Lei Xiao — National Special Superfine Powder Engineering Research Center of China, School of Chemistry and Chemical Engineering, Nanjing University of Science and Technology, Nanjing 210094, China
Zongkai Wu — Xi’an Modern Chemistry Research Institute, Xi’an 710065, China
Duo Li — Shanxi North Xing’an Chemical Industry Co. Ltd, Taiyuan 030008, China
Yubing Hu — National Special Superfine Powder Engineering Research Center of China, School of Chemistry and Chemical Engineering, Nanjing University of Science and Technology, Nanjing 210094, China
Guangpu Zhang — National Special Superfine Powder Engineering Research Center of China, School of Chemistry and Chemical Engineering, Nanjing University of Science and Technology, Nanjing 210094, China
Fengqi Zhao — Xi’an Modern Chemistry Research Institute, Xi’an 710065, China
Wei Jiang — National Special Superfine Powder Engineering Research Center of China, School of Chemistry and Chemical Engineering, Nanjing University of Science and Technology, Nanjing 210094, China; orcid.org/0000-0001-5663-9119

Complete contact information is available at: https://pubs.acs.org/10.1021/acsomega.2c00532

Notes
The authors declare no competing financial interest.

ACKNOWLEDGMENTS

This work was financially supported by the National Natural Science Foundation of China (grant nos. 21805139 and 12102194) and the Basic Product Innovation Technology Research Project of Explosives.

REFERENCES

(1) Wang, Z. S. Propellant and Explosive Science and Technology; Beijing Institute of Technology Press: Beijing, 2002.
(2) Wang, Z. S. Introduction to Energetic Materials; Harbin Institute of Technology Press: Harbin, 2006.
(3) Davanas, A. Development of modern solid propellants. J. Propul. Power 2003, 19, 1108–1128.
(4) Liu, S. E.; Chen, J. F.; Pan, B.; Zhao, M. L.; Gong, H. X.; Zhang, G. H.; Ren, X. B. Application of PNMA in HMX/Al-CMDB propellant. Chin. J. Explos. Propell. 2014, 37, 62–64+69.
(5) Li, L.; Wang, J. N.; Liu, Z. R. Effects of DNTF con-tents on dynamic mechanical properties of modified double-base propellant. Chin. J. Energ. Mater. 2010, 18, 174–179.
(6) Qi, X.-F.; Li, J. Q.; Zhang, X. H.; Xiao, X. J.; Zheng, W.; Liu, P. Influence of energetic potassium salt as eliminated-flame additive on performance of nitramine modified double-base propellant. Chin. J. Energ. Mater. 2013, 21, 334–338.
(7) Yin, Z. Z. Study on In-process Determination of Contents and Blend Uniformity of Primary Components in Modified Double Base Propellant Intermediate; Nanjing University of Science and Technology: Nanjing, China, 2016. https://kns.cnki.net/kcms/detail/detail.aspx?dbcode=CMFD&dbname=CMFD2017&filename=101622289. n h & un i p l a t f o r m = N Z K P T & v = w mktlff50GGL9UpRJwznDpAhV7WaioaX4lo003ZmHDN9V- u9QET Rn moiyT9S.
(8) Mattos, E. C.; Moreira, E. D.; Dutra, R. C. L.; Diniz, M. F.; Ribeiro, A. P.; Iba, K. Determination of the HMX and RDX content in synthesized energetic material by HPLC, FT-MIR, and FT-NIR spectroscopies. Quim. Nova 2004, 27, 540–544.
(9) Li, C. X.; Liu, B. A.; Cui, G. P. The research development of component analysis technology of modified double-base propellant in domestic. Shanxi Chem. Ind. 2012, 32, 49–52.
(10) US Department of Health and Human Services, Food and Drug Administration. Guidance for Industry-Powder Blends and Finished Dosage Units-Stratified In-process Dosage Unit Sampling and Assessment, 2003, [EB/OL]. [2010-6-15]. http://www.fda.gov/OHRMS/DOCKETS/98fr/98fr0493-d00001.
(11) Yan, Y. L. Foundation and Application of Near-Infrared Spectroscopy Analysis; China Light Industry Press: Beijing, 2005.
(12) Mauer, L. J.; Chernyshova, A. A.; Hiatt, A.; Deering, A.; Davis, R. Melamine detection in infant formula powder using near- and mid-infrared spectroscopy. J. Agric. Food Chem. 2009, 57, 3974–3980.
(13) Märc, J.; Karner, M.; Andre, M.; Rueland, J.; Huck, C. W. Online process control of a pharmaceutical intermediate in a fluidized-bed drier environment using near-infrared spectroscopy. Anal. Chem. 2010, 82, 4209–4215.
(14) Zhu, D. Z.; Huang, W. J.; Ma, Z. H.; Zhao, L.; Yang, X. D.; Wang, J. H. Wheat quality monitoring by NIR network. Sci. Agric. sin. 2010, 82, 4209–4215.
(15) Ji, P.; Feng, J.; Li, Z. W. Development of near infrared spectroscopic in tobacco industry. J. Anhui Agric. Sci. 2011, 39, 9848–9850.
(16) Lee, Y.; Chung, H.; Kim, N. Spectral range optimization for the near-infrared quantitative analysis of petrochemical and petroleum products: naphtha and gasoline. Appl. Spectrosc. 2006, 60, 892–897.
(17) Liu, Y. J.; Wang, J. X.; Xing, Z. N. Study on near infrared analysis model of initial distillation point of jet fuel based on iPLS and BP-ANN. J. Ord. Equip. Eng. 2020, 41, 212–215.
(18) Zhou, S.; Wang, Z.; Lu, L.; Yin, Q.; Yu, L.; Deng, G. Rapid quantification of stabilizing agents in single-base propellants using near infrared spectroscopy. Infrared Phys. Technol. 2016, 77, 1–7.
(19) Zhou, S.; Yin, Q.; Lu, L.; Wang, Z.; Deng, G. Application of near infrared spectroscopy in fast assay of liquid components in single-base propellant intermediates. Infrared Phys. Technol. 2017, 80, 11–20.
(20) Ma, L.; Zhou, L.; Xu, M.; Huang, X.; Zhang, Q.; Dai, S.; Qiao, Y.; Wu, Z. Investigation of the distributional homogeneity on chlorpheniramine maleate tablets using NIR-Cl. Spectrochem. Acta - A: Mol. Biomol. Spectrosc. 2018, 204, 783–790.
(21) Wahl, P. R.; Pucher, I.; Scheibelhofer, O.; Kerschhaggl, M.; Sacher, S.; khinast, J. G. Continuous monitoring of API content, API distribution and crushing strength after tableting via near-infrared chemical imaging. Int. J. Pharm. 2017, 518, 130–137.
(22) Zou, Q.; Deng, G. D.; Guo, X. D.; Jiang, W.; Li, F. S. Research on near-infrared online monitoring for blend uniformity of modified double-base absorbent powders. Acta Armamentarii 2014, 35, 977–981.
(23) Momose, W.; Imai, K.; Yokota, S.; Yonemochi, E.; Terada, K. Process analytical technology applied for end-point detection of pharmaceutical blending by combining two calibration-free methods: Simultaneously monitoring specific near-infrared peak intensity and moving block standard deviation. Powder Technol. 2011, 210, 122–131.
(24) Zou, Q.; Deng, G.; Guo, X.; Jiang, W.; Li, F. A green analytical tool for in-process determination of RDX content of propellant using the NIR system. ACS Sustain. Chem. Eng. 2013, 1, 1506–1510.
(25) Dong, M.; Wang, N. Adaptive network-based fuzzy inference system with leave-one-out cross-validation approach for prediction of surface roughness. *Appl. Math. Model.* 2011, 35, 1024–1035.

(26) Wold, S.; Sjostrom, M.; Eriksson, L. PLS-regression: a basic tool of chemometrics. *Chemom. Intell. Lab. Syst.* 2001, 58, 109–130.

(27) Wei, Y.; Fan, W.; Zhao, X.; Wu, W.; Lu, H. Rapid authentication of dendrobium officinale by near-infrared reflectance spectroscopy and chemometrics. *Anal. Lett.* 2015, 48, 817–829.

(28) Cheng, S.-C.; Lin, X. Y.; Li, Y.; Jian, G. X. Rapid test of modified double-base propellant component uniformity by NIR spectroscopy. *Chin. J. Energ. Mater.* 2016, 24, 343–347.

(29) Blanco, M.; Bano, G.; Bertran, E. Monitoring powder blending in pharmaceutical processes by use of near infrared spectroscopy. *Talanta* 2002, 56, 203–212.