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Short Communication

Classification of washing powder brands using near-infrared spectroscopy combined with chemometric calibrations

Hongguang Zhang, Qinmin Yang, Jiangang Lu *

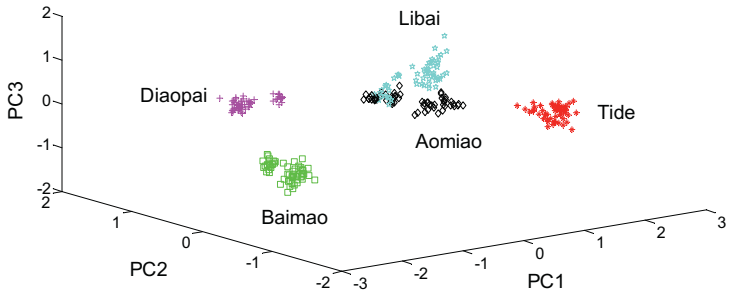
State Key Laboratory of Industrial Control Technology, Department of Control Science and Engineering, Zhejiang University, Hangzhou 310027, China

HIGHLIGHTS

- NIR spectroscopy used for classification of brands of washing powder.
- Washing powder brands classified using chemometric calibrations.
- Models of PLS-DA, BP-NN and LS-SVM were tested in classification.
- Results showed successful washing powder brands classification.

GRAPHICAL ABSTRACT

NIR spectroscopy and chemometric calibrations including PLS-DA, BP-NN and LS-SVM models were used to classify brands of washing powder. From the scatter plot of PC1 × PC2 × PC3, it can be found that washing powder samples of different brands distributed separately in the three-dimension space. Combined with BP-NN model and LS-SVM model, NIR spectroscopy successfully classified all the washing powder samples according to their brands.



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ABSTRACT

In this study, near-infrared (NIR) spectroscopy is applied for rapid and objective classification of 5 different brands of washing powder. Chemometric calibrations including partial least square discriminant analysis (PLS-DA), back propagation neural network (BP-NN) and least square support vector machine (LS-SVM) are investigated and compared to achieve an optimal result. Firstly, principal component analysis (PCA) is conducted to visualize the difference among washing powder samples of different brands and principal components (PCs) are extracted as inputs of BP-NN and LS-SVM models. The number of PCs and parameters of such models are optimized via cross validation. In experimental studies, a total of 225 spectra of washing powder samples (45 samples for each brand) were used to build models and 75 spectra of washing powder samples (15 samples for each brand) were used as the validation set to evaluate the performance of developed models. As for the comparison of the three investigated models, both BP-NN model and LS-SVM model successfully classified all samples in validation set according to their brands. However, the PLS-DA model failed to achieve 100% of classification accuracy. The results obtained in this investigation demonstrate that NIR spectroscopy combined with chemometric calibrations including BP-NN and LS-SVM can be successfully utilized to classify the brands of washing powder.

* Corresponding author. Tel./fax: +86 571 8795 2829.
E-mail address: jglu@iipc.zju.edu.cn (J. Lu).

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Introduction

Since washing powder was invented in 1907 by Henkel (German), it has been widely used in various fields throughout the world for decades, particularly in people's daily life. As a kind of synthetic detergent, washing powder is a complex formulation containing more than 25 different ingredients [1]. Generally, the main compositions of washing powder can be categorized into four major groups: surfactants, builders, bleaching agents and auxiliary agents. Though washing powder is indispensable in people's daily life, it has certain toxicity and may bring risk to human health. Therefore, its quality is crucial to human health, and safety and authenticity of washing powder have attracted considerable attention throughout the world, especially in China. Some literatures have reported that several famous brands of washing powder have been faked [2,3]. Currently, in Chinese market, there are many brands of washing powder available including both Chinese brands (Diaopai, Baimao, Libai, etc.) and foreign brands (Aomiao, Tide and so on). The quality and price of them are reasonably different. Famous brands of washing powder have high quality and are accepted widely in China. However, nowadays immoral merchants are selling unqualified washing powder which is labeled as famous brands for illegal commercial benefits. These phenomena are especially common in small towns and countryside of China and those unqualified products not only constitute a fraud for consumers, but also represent significant safety risk for human health.

However, the discrimination of washing powder brands is conventionally carried out on the basis of visual and olfactory difference. It is subjective and may lead to unreliable results. An objective and accurate assessment of washing powder samples can be obtained based on the determination of the content of different constituents within them by using gas chromatography (GC), high performance liquid chromatography (HPLC) and mass spectroscopy (MS). However, these philosophies are time-consuming, laborious, expensive, and require reagents. Hence, it is almost impossible for them to be enforced conveniently.

In the meantime, as a fast, low-cost and reliable technique, near-infrared (NIR) spectroscopy [4,5] has been widely utilized for the discrimination and/or classification of various materials, including cigarettes [6,7], alcoholic beverages [8,9], fuel samples [10,11], polymers [12], and food products [13–16]. As for analysis of washing power, only few researchers have quantified some main constituents in washing powder samples by using Fourier transform infrared spectroscopy (FT-IR) [1,17–19]. Moreover, to our best knowledge, there have not been any reports on the classification of washing powder samples of different brands using NIR spectroscopy.

Therefore, in this study, the feasibility of the classification of washing powder samples with respect to their brands is investigated via NIR spectroscopy along with chemometric calibrations. Firstly, principle component analysis (PCA) is conducted to visualize the difference between washing powder samples prepared from different brands and extract their principal components (PCs) used as the inputs of BP-NN model and LS-SVM model. Then a comparison is implemented among one linear model-PLS-DA model and two nonlinear models-BP-NN model and LS-SVM model. In addition, cross validation is utilized to optimize the parameters of each model and the performance of each model is evaluated based on the classification accuracy of the washing powder samples in the validation set.

Experimental studies

Samples preparation

In this work, all samples of washing powder were obtained from local supermarkets. Five most available brands of washing powder were considered including Tide, Aomiao, Diaopai, Baimao, and Libai. For each brand, 60 samples have been collected and we reached a total of 300 washing powder samples. In order to get an equalization room temperature, all washing powder samples were stored in the laboratory kept at 21 °C for more than 24 h before the experiment. All samples were sieved to guarantee all particles' size to be smaller than 0.45 mm and no additional pretreatments were conducted before NIR spectra recording. To develop calibration models, 225 samples (45 for each brand) were randomly selected as calibration set and the remaining 75 samples (15 for each brand) were used as validation set.

Near infrared instrument and measurement

The NIR spectra were collected by using a NIRQuest 512 near infrared spectrometer (OceanOptics, USA) in reflectance mode with a fiber optical, which is controlled by SpectraSuit software. Each spectrum was the average of 32 scanning spectra and obtained at 2.3 nm intervals from 900 to 2100 nm, resulting in 512 variables for each spectrum.

In order to reduce the variation introduced by instrumental factors, uniform plastic petri dishes (diameter, d = 35 mm; height, h = 10 mm) were employed to load the washing powder samples. A 'Y' style of fiber optical designed specifically by OceanOptics Co. was used to collect the spectra of samples and a probe was fixed 10 mm above the surface of the washing powder vertically. The spectrum of a Spectralon (OceanOptics, USA) was used as reference and the dark spectrum was collected when the light source was shielded. Both reference and dark spectra were gathered to transform the reflectance spectra of samples into absorbance mode and they were collected after every 5 samples measurements. All spectra data were stored as ASCII format files for further analysis.

Data pretreatment

To reduce the noise and correct baseline drift, different spectral pretreatment methods were employed. The standard normal variate (SNV) was utilized to remove the multiplicative interferences of scatter, particle size, and the change of light distance [20]. Savitzky–Golay smoothing and derivative were used to decrease the noise of spectra data and baseline drift [21]. To determine the optimal preprocessing method for this application, different preprocessing methods mentioned above were compared.

Based on comparison among these pretreatment methods, SNV is superior to other methods for this application. Therefore, the NIR spectra were preprocessed by SNV before the calibration stage in this study.

Principal component analysis (PCA)

As a commonly used chemomtric calibration in the present NIR spectroscopy analysis, PCA can record as much as possible the variance of the original variables while significantly reducing the dimensionality of the data. Specifically, it can extract information from the original data sets by constructing new uncorrelated variables known as principal components (PCs) [22]. The number of PCs needed to represent the most information contained in original data is always far less than the number of original variables. Thereafter, these PCs can be used to investigate the grouping phenomenon among samples, particularly in classification problems. Besides, these PCs can also be used as input of BP-NN and LS-SVM models to reduce the modeling time.