Rapid detection and visualization of organic spelt (*Triticum spelta L.*) flour adulteration using hyperspectral imaging and multivariate analysis

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I. INTRODUCTION

The hexaploid spelt (*Triticum spelta* L.) was the predominant cereal food cultivated in Europe from the 5th century and has been substituted by wheat (*Triticum aestivum* L.) since the 20th century [1]. Food adulteration is the presence of an extraneous and cheaper constituent. Driven by high profit, food adulteration has become a global challenge during the past years [2]. As organic spelt flour (OSF) is a species of wheat, the discrimination between OSF and organic wheat flour (OWF) should also be effectively evaluated. In addition, OSF is nearly same in color to SF and similar to rye flour (RF) as well, which makes them more difficult to be identified after adulteration. With the increasing requirement on the subtle adulterations in food, it is of critical importance to develop a more sensitive, accurate, and rapid approach for non-destructive identification and visualization of OSF. Hyperspectral imaging has been applied not only to the determination of their locations based spatial distribution but also the authentication and quantification of spectral properties based chemical component [3, 4]. In this study, we present an approach termed first-derivative and mean centering iteration algorithm (FMCIA), which has the latent capacity to select an optimum wavelength combination in full spectral range. In order to demonstrate the effectiveness of the proposed algorithm, partial least squares discriminant analysis (PLSDA), partial least squares regression (PLSR) and multiple linear regression (MLR) models are constructed to evaluate the inveracity of RF, OWF and SF in OSF, respectively.

II. MATERIALS

The organic spelt and organic common wheat were produced from organic system where the organic food standards such as non-using synthetic fertiliser and pesticide were strictly implemented. OSF samples were adulterated by respectively mixing with RF, OWF and SF in the range of 3-75% (w/w), at approximately 3% increments. All these acquired samples were respectively placed in circular transparent plastic jars one by one and imaged using the laboratory-based pushbroom hyperspectral imaging system mentioned by Kamruzzaman, ElMasry [5]. The fundamental purpose of extraction of spectral data from the test samples is to identify the region of interest (ROI) and obtain the average spectrum representing the ROI.

III. METHODS

Calibration models were established using a classification method, PLSDA, and another two typical linear methods, namely PLSR and MLR. PLSDA was employed for qualitative assessment of RF, OWF, SF and OSF while the quantitative analysis of OSF adulteration was explored by PLSR and MLR. A calibration phase and a validation phase calculating for the determination coefficients and the root mean square error in calibration (R^2_C, RMSEC), in cross validation (R^2_{CV}, RMSECV) and in prediction (R^2_P, RMSEP) are employed in the models for presenting model performance. The parameters of specificity, sensitivity and classification error are also included to evaluate PLSDA model. In this study, the characteristic wavelengths were qualified using the FMCIA for identification and quantification of adulterants in OSF. The superiority of hyperspectral imaging is to visualize the distribution of the substance in samples. The mass concentration of adulteration can be computed in each pixel of ROI based on simplified models using characteristic wavelengths.

IV. RESULTS

To improve the processing speed and realize on-line monitoring, it is of vital importance to qualify several optimal wavelengths instead of hundreds of variables. Wavelength selection can also improve the model prediction ability and furnish more robust models as well as models that can be transfered more readily. In this study, FMCIA was put forward for selection of characteristic variable in the spectral range of

957 to 1625 nm. The variables corresponding to the peak and trough of coefficient presented higher differences and would play an important role in established models. By means of this approach, eight sensitive wavelengths (1145, 1192, 1222, 1349, 1359, 1396, 1541, and 1567 nm) were finally survived.

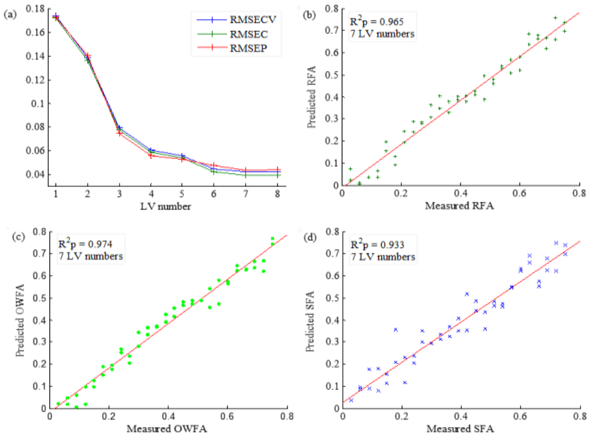

Fig. 1. (a) Selection of the latent variable (LV) numbers in PLSR model; measured and predicted values of (b) RFA, (c) OWFA, and (d) SFA in OSF estimated by PLSR model for the validation set using the selected characteristic wavelengths.

The overall performance of FMCIA-MC-PLSDA model was very high (mean R^2_{CV} = 0.958). Furthermore, the discrimination accuracy of different flour samples was 100% in FMCIA-MC-PLSDA model. Both MLR and PLSR models using only feature wavelengths showed very good performance, and the property of models pretreated by MC was much better than models without pre-processing. The FMCIA-MC-PLSR model was considered the best model for measuring OSF adulterants. As shown in Fig. 1, with the qualification of seven LVs, the OWFA in OSF was detected to obtain highest accuracy (R^2_P = 0.974) followed by RFA (R^2_P = 0.965) and SFA (R^2_P = 0.933). The FMCIA-MC-PLSR model were transferred in each pixel of an image to count the dot product of the spectral values of all pixels. Fig. 2 showed five typical distribution maps of adulteration percentages of SF in OSF by predicting variations in adulteration proportion based on FMCIA-MC-PLSR model. With the increase of adulteration level from 3% to 75%, the overall image colors changed from blue (low level) to red (high level), which indicated the corresponding adulteration in proportion to spectral differences of pixels

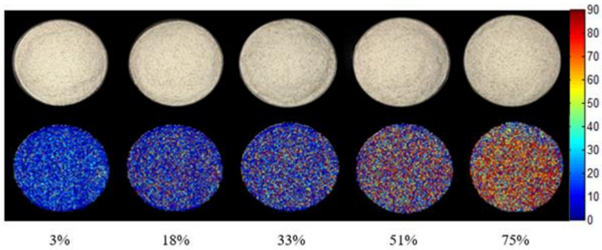

Fig. 2. Prediction maps of adulteration percentages of SF in OSF based on FMCIA-MC-PLSR model.

V. CONCLUSIONS

The results demonstrate that the FMCIA is an effective method of selecting characteristic wavelengths. The efficient multispectral imaging system can be established to detect OSF adulteration for a real-time practical application based on hyperspectral imaging in tandem with multivariate analyses. Based on the feature wavelengths, the optimum model performances with the visualization of adulteration were found in the FMCIA-MC-PLSDA model for qualitatively discriminating OSF (mean R^2_{CV} = 0.958), and the FMCIA-MC-PLSR model for quantitatively measuring adulterants (mean R^2_P = 0.957), respectively.

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