Measurement 89 (2016) 1–6

Contents lists available at ScienceDirect

Measurement

journal homepage: www.elsevier.com/locate/measurement

Developing a Vis/NIR spectroscopic system for fast and non-destructive pesticide residue monitoring in agricultural product

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ARTICLE INFO

Article history:
Received 19 October 2015
Received in revised form 11 February 2016
Accepted 29 March 2016
Available online 1 April 2016

Keywords:
Chemometrics
GUI
Non-destructive
Pesticide residues
Safety
Vis/NIR spectroscopy

ABSTRACT

In this research, an optical system based on fibre optic Vis/NIR spectroscopy combined with chemometrics methods and software as a graphical user interface (GUI) was developed and presented for fast and non-destructive detection and determination of pesticide residues in agricultural products (a case study on diazinon in intact cucumbers). Vis/NIR spectra of cucumber samples without and with different concentrations of diazinon residue were analyzed at the range of 450–1000 nm. Partial least squares (PLS) regression models were developed based on chemical reference measurements and the spectral information of the samples after performing different pre-processing methods. Moreover, partial least squares-discriminant analysis (PLS-DA) models were developed based on different spectral pre-processing techniques to classify cucumbers with contents of diazinon below and above the maximum residue limits (MRL) as safe and unsafe samples, respectively. Finally, user-friendly software as a GUI was created based on the best PLS and PLS-DA models developed for prediction of diazinon contents in the samples and for classification of intact cucumbers by the absence/presence of diazinon residues, respectively. Evaluation of the system and software designed based on the best developed PLS and PLS-DA models indicated good performance for measuring and detection of diazinon residue in cucumbers. It was concluded that the designed system and software based on Vis/NIR spectroscopy combined with chemometrics methods can be utilized for fast and non-destructive safety control of intact cucumbers by the absence/presence of diazinon residues. It can also be generalized for detection of other pesticide residues in agricultural products if developing their appropriate models is feasible.

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1. Introduction

Typically, the detection of pesticides in complex matrices, such as agricultural products, involves a sample treatment using different methods such as solid-phase extraction, supercritical fluid extraction, microwave-assisted extraction, and accelerated solvent extraction [1,2]. Conventional techniques such as gas chromatography [3], high-performance liquid chromatography [4], thin-layer chromatography [5], supercritical fluid chromatography [6], gas and liquid chromatography combined with mass spectrometry [5,7], capillary electrophoresis [8,9], enzyme inhibition method [5,10], immunoassay method [5,11], and bio-sensor method [5,12], are also used to measure the concentration of pesticide residue in agricultural products. However, these techniques are destructive, difficult, highly time consuming, very expensive, environmentally unfriendly, and enable safety control of a few samples per batch as well as require sample preparation, well-trained personnel and advance laboratory. Therefore, there is a need for development of a non-destructive, simple, fast, low-cost, environmentally friendly with little sample preparation, and reliable detection technique of pesticide residue in agricultural products for controlling each individual sample [2,13].

One of the most promising non-destructive techniques is Near-infrared (NIR) spectroscopy which has been successfully applied for qualitative and quantitative analyses especially to quality control of intact fruits and vegetables [14–22]. This technique has non-contaminant and lossless nature, the low operating cost compared with the conventional techniques, and the fast response times. It also requires little or no sample preparation and can be used in processing lines [23]. There are also some researches about detection or determination of pesticide residues in such products [1,2,24–27]. All of these researches show the feasibility of using NIR spectroscopy for detection of pesticide residues.

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http://dx.doi.org/10.1016/j.measurement.2016.03.069
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This research aims to develop a visible/near-infrared (Vis/NIR) Spectroscopic system for fast and non-destructive safety control of agricultural products based on absence/presence of pesticide residues with a case study on diazinon detection and determination in cucumber. To this end, the feasibility of utilizing Vis/NIR spectroscopy combined with partial least squares (PLS) regression and different spectral pre-processing methods were investigated for measuring the residue content in the samples non-destructively. Moreover, the results reported by Jamshidi et al. [2], who have assessed the feasibility of using this technique combined with partial least squares-discriminant analysis (PLS-DA) for non-destructive classification of intact cucumbers by the absence/presence of diazinon residues based on containing the levels below/above the maximum residue limits (MRL), 0.1 mg kg^{-1}, established by FAO/WHO Codex Alimentarius [28], were used. Then, user-friendly software as a graphical user interface (GUI) was designed based on the best PLS and PLS-DA models developed for prediction of diazinon contents in the samples and for classification of intact cucumbers by the absence/presence of diazinon residues, respectively.

2. Materials and methods

2.1. Cucumbers preparation

A total of 120 cucumbers were harvested from the greenhouses near Karaj city in Alborz province of Iran. The 60% diazinon pesticide ($C_{12}H_{21}N_2O_3PS$) was used to obtain different pesticide residue contents in some samples as a pesticide-contaminated set. It was diluted to 1/500 and sprayed on some of the cucumbers. Some other samples were placed in the prepared solution for 1 h. A pesticide-free set of cucumbers was also used. All samples were stored at 5 °C until Vis/NIR spectroscopy.

2.2. Experiments

Before each experiment, cucumbers were left until their temperature had risen to the laboratory temperature. Vis/NIR measurements of the samples at the range of 450–1000 nm were conducted with a USB2000 fibre optic spectrometer (Oceanoptics Inc., USA), in interactance mode. Before spectra acquisition of the samples, white reference and dark spectra were collected to obtain the relative interactance. For each cucumber, Vis/NIR spectra at thirty scans from different positions on the sample were acquired by OOIBase32 software (Oceanoptics). The mean spectrum was calculated for each sample and stored for later data analysis.

After each spectroscopy experiment, the cucumbers were sent to the Chemical Analysis Center at Iranian Institute of R&D in Chemical Industries for measurement of diazinon content in each sample with a reference method, GC analysis. To this end, sample preparation was done based on British Standard BS EN 15662:2008 [29]. Then, an Agilent 7890A gas chromatograph (Agilent Technologies Inc., Santa Clara, CA, USA) was used to measure the concentration of pesticide residue in each sample [2].

2.3. PLS analysis

The overall Vis/NIR spectra of the samples were converted to absorbance values ($\log(1/R)$). Principal component analysis (PCA) was used to determine the outlier samples. After removing the outliers (14 samples), all the 106 remained samples were utilized for quantitative analysis in order to measure the diazinon content.

PLS regression models were developed based on GC measurements and the spectral information of the cucumbers. Before modeling, multiplicative scatter correction (MSC) and standard normal variate (SNV) were used to correct both multiplicative and additive effects of the Vis/NIR spectra. First and second derivatives of the spectra (D_1, D_2) were also performed to increase the spectral resolution. The algorithm used most often for derivation is Savitzky–Golay. The data within a moving window are fitted by a polynomial of a given degree. Therefore, it is important to select the proper width of the moving window. In general, it should not exceed one point five times as the half width of the absorbance peak in the spectra [30]. To this end, Savitzky–Golay algorithm with five smoothing points and polynomial order of two was used for derivation.

Then, PLS models were developed with full cross-validation and investigating the maximum of 10 latent variables (LVs). Comparison of the calibration models was done based on having the lowest standard error of cross-validation (SECV) and the highest correlation coefficient of cross validation (r_{cv}). All analyses were conducted using the Unscrambler software X10.3 (CAMO Software AS, Norway).

2.4. Software design

To complete the spectroscopic system for safety assessment of the cucumbers, the best PLS model developed for prediction of diazinon contents in the samples was used. Moreover, the best PLS-DA model developed by Jamshidi et al. [2] was also used to discriminate the safe samples (all samples without or with diazinon concentrations $\leqslant$0.1 mg kg^{-1}) from the unsafe cucumbers (all samples with diazinon concentrations >0.1 mg kg^{-1}), respectively. Therefore, user-friendly software as a GUI was created based on the best PLS and PLS-DA models to predict diazinon contents in the samples and to classify the cucumbers by the absence/presence of diazinon residues, respectively.

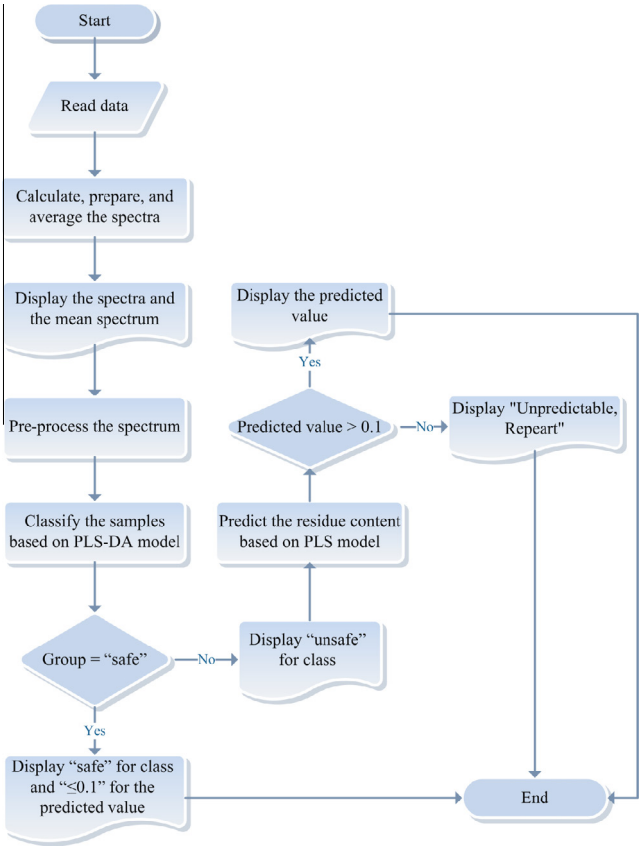

Fig. 1. Software flowchart.

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