External detection of liquid explosives in bottles using NIR

Hideo Itozaki and Yuji Yamauchi
Graduate School of Engineering Science, Osaka University,
1-3 Machikaneyama Toyonaka, Osaka 630-8531 Japan.
E-mail: Itozaki@ee.es.osaka-u.ac.jp

Introduction

Liquid explosives have been used in terrorism recently.[1] Inspection of bottles has become very important, because these liquid explosives and/or their raw materials can be carried in bottles easily. Hydrogen peroxide is a typical raw material of liquid explosives. It was difficult to evaluate the concentration of hydrogen peroxide in the liquid in the bottle, because of the similarity of its optical properties to those of water.[2] However, using near-infrared spectra and multivariate statistical analysis, concentrations of a small order of hydrogen peroxide in the bottle can be evaluated from outside of the bottle instantly. Hydrogen peroxide has been detected in not only a clear PET or glass bottle, but also a colored glass bottle. Hydrogen peroxide mixed with soft drink such as coffee or orange juice with pulp was also easily detected by this method. This technique can be applied to inspection of bottles at airport security and elsewhere, where such security is needed.

Materials and methods

Drinks in PET bottles were inspected. Hydrogen peroxide was mixed with these drinks and the concentration was estimated by NIR. NIR light was irradiated into the bottle via optical fiber, where it was absorbed by the liquid, and then detected by another optical fiber. The reflected light was then sensed by the spectroscope. The spectroscope consists of an optical grating and a linear array sensor. It detects 256 wavelengths from 600 nm to 1000 nm simultaneously. The equipment is illustrated in Figure 1.

The intensity of the spectrum is weak and there are many harmonic overtones and overlapping spectra. The absorbance spectra were pretreated by developing the second differential, in order to separate background and other noise. Multivariate statistical analysis, such as multilinear regression, and partial least square regression has been used to analyze these complicated spectra to obtain information from them.[3] The quality of the calibration models was checked by the standard error of calibration (*SEC*) and the standard error of prediction (*SEP*).[4]

Figure 1. Bottle inspection device.

Results and discussion

The concentration of hydrogen peroxide diluted in water can be estimated accurately. Spectra were modified, not only by the concentration of hydrogen peroxide, but also by bottle shape, volume of liquid, bottle material such as PET or colored glass, types of beverage, and other factors. Figures 2

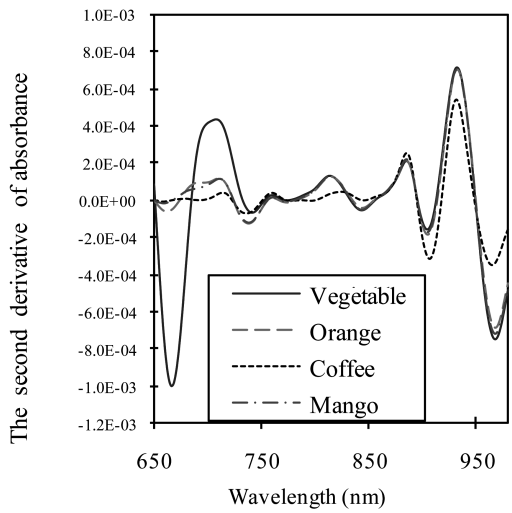

Figure 2. Schematic diagram of bottle inspection.

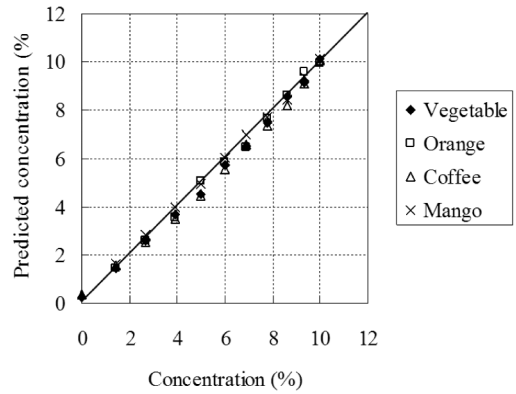

Figure 3. Concentration of hydrogen peroxide in vegetable juice, Orange juice, coffee and mango juice 100 mL.

and 3 show that concentration of hydrogen peroxide in vegetable juice, orange juice, coffee and mango juice (with pulp) can be measured using NIR spectroscopy.

PLSR is much better than MLR to get calibration equations, because it uses more data from the measured spectra. The system developed can detect explosives, such as hydrogen peroxide in bottles. Future threats arising from other types of liquid explosives can be met by obtaining calibration equations for them, and installing them in this NIR device. We hope that NIR bottle checkers like this will soon be installed in airports, and the restrictions on carrying bottles will be removed for the convenience of passengers.

Acknowledgment

This research is partially supported by the ministry of education, culture, sport, science and technology of Japan.

References

1. H. Schubert and A. Kuznetsov (Eds), in *Detection of Liquid Explosives and Flammable Agents in Connection with Terrorism*. Springer, Dordrecht, Germany, pp. 1–233 (2008).
2. W.F. McClure, "Near-infrared spectroscopy", *Anal. Chem.* **66**, 43A (1994).
3. H. Martens and T. Naes, *Multivariate Calibration*. John Wiley & Sons, Chichester, UK, p. 438 (1989).
4. P. Merckle and K.A. Kovar, *J. Pharm. Biomed. Anal.* **17**, 365 (1998).