Development of standard spectral generator for a spectrophotometer

H. Aoki[a,*] and S. Kawano[b]

[a]*The Graduate School for the Creation of New Photonics Industries, Hamamatsu 431-1201 Japan. E-mail: h_aoki@gpi.ac.jp*

[b]*National Food Research Institute, 2-1-12 Kannondai, Tsukuba 305-8642 Japan*

Introduction

In order to standardise near infrared (NIR) spectrophotometers, a standard sample, that has a similar spectrum to that of the products to be analysed, such as apples is needed. If an actual sample is used as a standard, it is very difficult to maintain the spectral properties for long periods, because changes in moisture (in particular), and other components occur, which affect the spectra. This is particularly true in the case of some kinds of samples, such as foods and biological cells, that contain a lot of water, which makes them subject to chemical change, and susceptible to temperature changes. In this laboratory we have attempted to develop a standard spectrum generator "SPO-G1", which could produce a spectrum identical to that of any sample (Figure 1).

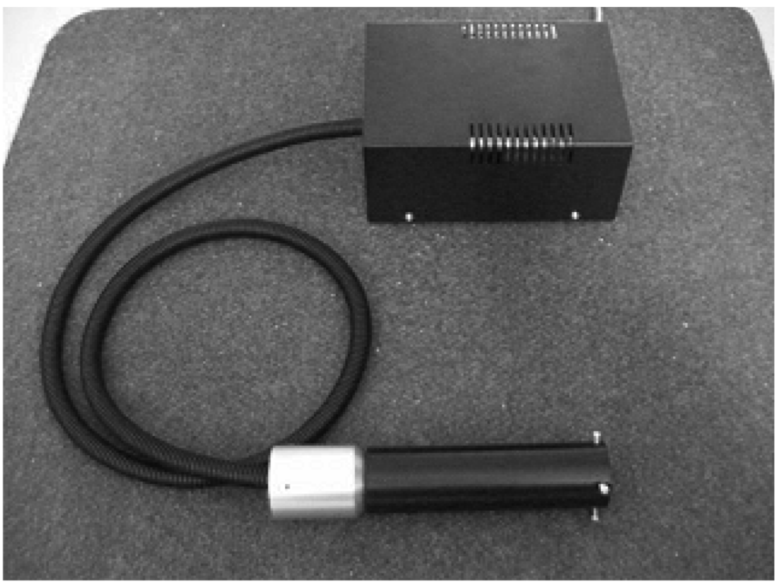

Figure 1. Spectrum Generator SPO-G1.

The spectrum generator could output spectra very similar to those of real samples in 2nd derivative mode. The spectrum produced by the generator does not depend solely on molecular vibrations. The generator consists of metal and silicon parts only, which are free from possible chemical changes of the components, and from mode changes of molecular vibrations. A standard spectrum generator producing a spectrum similar to that of a real product was developed, and in this study its performance was examined.

Materials and methods

A total of 100 apples (cv. Fuji) were used as samples in this experiment. Of these, 50 samples were selected as “Sample Set A” and the rest as “Sample Set B”. NIR spectra of the apple samples were measured with a miniature fibre-optic spectrometer (USB4000, Ocean Optics, Germany), using the interactance method. An average spectrum from “Sample Set A” was calculated, and the spectrum generator was adjusted to reproduce the average spectrum of set A. In this way the spectrum generator “SPO-G1” was able to generate a spectrum similar to the average spectrum of the “Sample Set A”.

The spectrum generated was also measured with the USB4000 spectrophotometer (Figure 2).

Comparison of the generated spectrum and the average spectrum of “Sample Set B” was performed. After NIR measurement, the Brix value of each sample was analysed by a digital refractometer (ATAGO, Model APAL-1, Tokyo, Japan). Multiple linear regression (MLR) was performed based on 2nd derivative spectra of “Sample Set A” and Brix values were used as reference data to establish a MLR calibration model for Brix value. The MLR calibration was applied to the 2nd derivative spectra of “Sample Set B”, and to the second derivative of the newly-generated spectra.

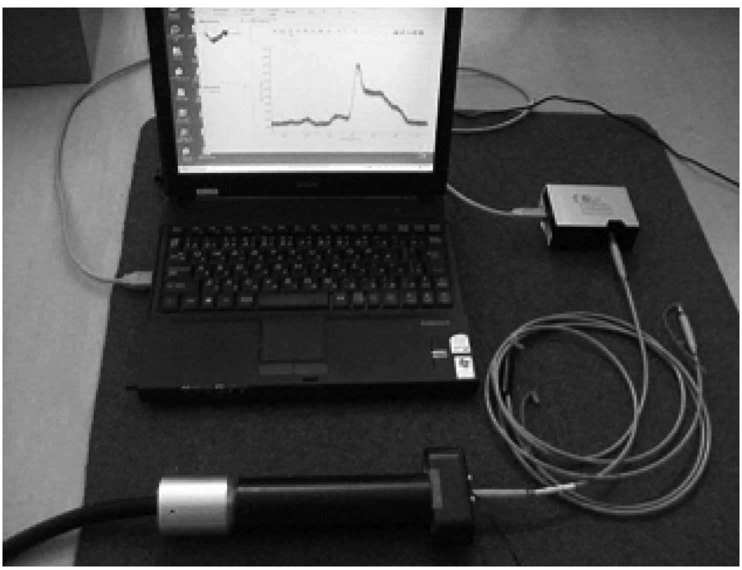

Figure 2. Spectrum collection for generator outputs.

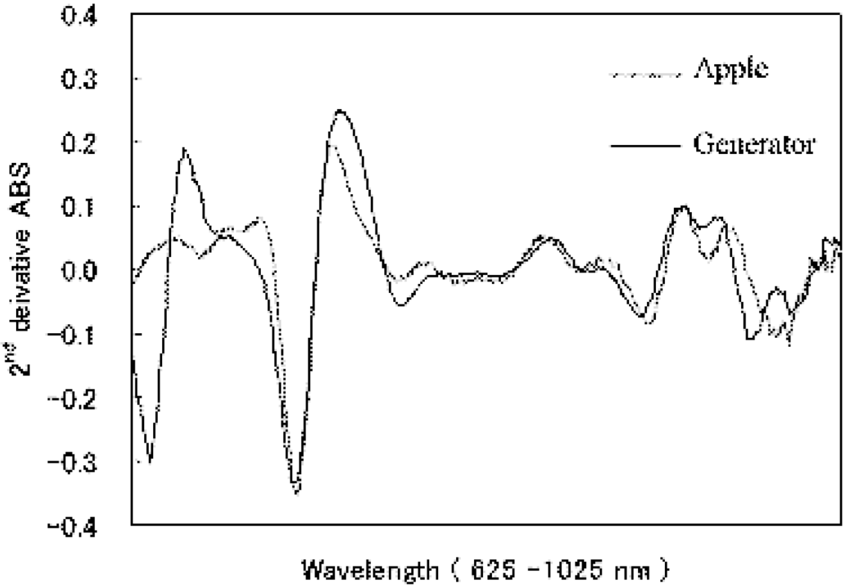

Figure 3. Second derivative spectra for Standard Spectrum Generator and real sample (apple).

Results and discussion

Results could be described as follows: (i) there were high similarities between the second derivative spectrum of the generated spectra and the average spectrum of "Sample Set B", both in absorption peak positions and intensity in the $d^2 \log 1/R$ spectra (Figure 3); (ii) when the calibration model developed using the "Sample Set A" was applied to the generated spectrum, the predicted Brix value with generator outputs gave values close to the range of the predicted Brix values of Sample Set A. The results were similar, with average of Brix for real samples of 15.21 (Figure 4). This supported the conclusion that the generated spectrum simulated a real apple spectrum, based on the output of the calibration; (iii) it was concluded that the spectrum generated by the spectrum

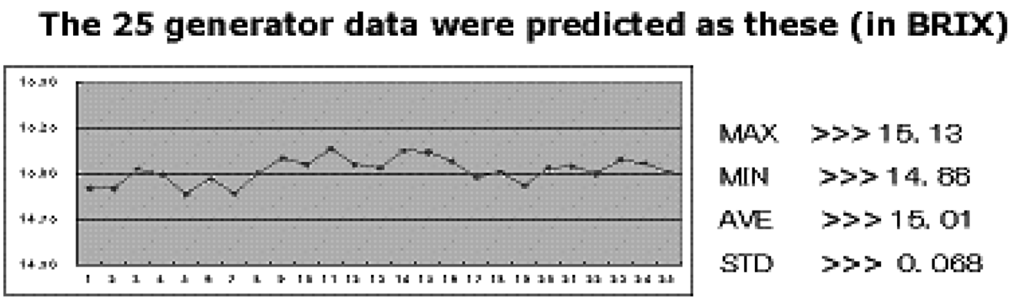

Figure 4. The 25 generator outputs were predicted closely similar to the real average of the apple Brix (15.21). Spectral data were collected at 5 minute intervals.

generator "SPO-G1" was sufficiently similar to the average apple spectrum that it could be used as a standard spectrum for apples; and (iv) in order to standardise NIR spectrophotometers using the spectrum generator "SPO-G1", the generated spectrum should be stable. Because the generator output is made by pure optical functions and does not depend on the absorbance of molecular vibrations the output should be free from vibration mode change, and also free the influence of temperature. Further study is needed for establishing the application of the spectrophotometer standardisation system using the spectrum generator "SPO-G1".