# Reduction of spectral data for rapid quality evaluation

# Károly J. Kaffka and László S. Gyarmati

University of Horticulture and Food Industry, Ménesi ut 45, Budapest, H-1118 Hungary.

# Introduction

A new method was introduced at the 3rd International Conference on Near Infrared Spectroscopy<sup>1</sup> for rapid qualification of different flavour and aroma samples using their near infrared spectra. A " quality point" was defined on a two-dimensional " quality plane" given by the centre of gravity of the spectral points of the spectrum represented in a polar coordinate system.

This "polar qualification system" (PQS) was successfully applied for qualifying different food products. Some examples are introduced in order to demonstrate the versatility and usefulness of this PQS.

### Materials and methods

In the first example, minced lean pork and minced fat bacon were mixed in different rates. In the second example, ground roasted coffee and ground coffee substitute were mixed in different rates. In the third example, skimmed and fat milk powders were mixed giving different fat contents. In the fourth example, original goose liver samples with different fat content were used. In the fifth example, healthy and mouldy red peppers were investigated and in the sixth example allspice samples irradiated with different doses were used.

In the polar coordinate system, the radius is the function of the spectral value while the angle is a function of the wavelength. The spectral value at a given wavelength can be taken from the log(1/R) spectrum, or from any of its transformed spectra; furthermore the spectra to be used in PQS can be taken in reflectance or in transmittance mode. Scanning type spectrophotometers are preferred. In the experiments described in this paper a Spectralyzer 1025 type research composition analyzer was used.

#### Results

The results of the aforementioned examples are demonstrated in Figures 1–6. It can clearly be seen that changing the composition of a sample the "quality point" shifts parallel with the direction of the absorption peak of the changing component and *vice versa*. From the direction of the quality shift conclusion, can be drawn with regards to which component has changed.

## Discussion

It was established that PQS could be used for determining the quality of different food products and given the distance between the quality points of the investigated sample and the standard sample, it can be used to determine acceptability.

It was demonstrated that from the position of the quality point and its shift in the quality plane further conclusions can be drawn concerning composition and changes in composition.







Figure 2. Quality points of coffee and coffee substitute mixtures. 1640–2000 nm, second derivative.



Figure 3. Quality points of milk powder with different fat content. 1500–1860 nm, log (1/R).



Figure 4. Quality points of goose-liver samples with different fat content. 1660–2020 nm, log (1/*R*).



Figure 5. Quality points of paprika powder samples containing different amounts of mould and some dried mould samples. 1110–1380 nm, first derivative.



Figure 6. Quality points of allspice samples irradiated with different doses. 1185-1245 nm, log (1/*R*).

From Near Infrared Spectroscopy: The Future Waves © IM Publications Open LLP 1996 As major advantages it was experienced that the place of the quality point is practically independent from the noise of the spectrum; so no smoothing is needed in preparing spectra. It was also experienced that PQS has some multiplicative scatter correction (MSC) effect.

The PQS is a drastic but meaningful data-reduction method based on geometrical view, therefore it is easy to imagine and at the same time it gives a good pictorial representation of the quality.

The results show a very promising future for near infrared spectroscopy in the field of qualitative analysis.

#### Reference

 K.J. Kaffka and L.S. Gyarmat, "Qualitative (Comparative) Analysis by Near Infrared Spectroscopy" in *Proceedings of 3rd International Conference on Near Infrared Spectroscopy*, Brussels, Belgium, Vol. 1, pp. 135-144 (1991).