CALIBRATION TRANSFER FROM REFLECTANCE TO INTERACTANCE-REFLECTANCE WITHOUT STANDARDS: USE OF MATHEMATICAL PRETREATMENTS

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The use of fibre optic probes for NIR quality control in the industry is becoming very important, as it provides a powerful tool to reduce sample analysis time and it facilitates the implementation of on-line analyses. However, most of the applications of fibre optics and probes have been done on suspensions, clear liquids and films, chemical and pharmaceutical products and also on fruits and animal products. Traditional applications of near infrared spectroscopy in agriculture have been developed in reflectance mode and calibration transfer could be an interesting way to reduce efforts. Classical methods for calibration transfer between different instruments involve the use of sealed reference cups, but, as fibre optic analysis does not use cups, it is necessary to develop new methods for calibration transfer without standards (Blank et al., 1996).

In this paper, we have studied how the most used mathematical pretreatments (three methods of Multiplicative Scatter Correction, Standard Normal Variate, Detrending and derivatives) and their combinations applied to calibration development can contribute to reduce spectral differences between instruments. Calibration equations were obtained for three sets of cereals (barley, wheat and maize) scanned in reflectance mode and then they were validated with samples analysed in reflectance and interactance-reflectance mode (fibre optic). Preliminary results show how some combination of pretreatments reduce the differences in the predicted values, measured as standard error of differences, facilitating the use of calibrations obtained in reflectance for samples analysed by interactance-reflectance. However, the application of pretreatments is not enough to satisfy the control limits for calibration transfer suggested by Shenk et al. (1992), and it should be necessary to combine them with a specific algorithm for instruments standardisation.

Literature References

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