Application of near infrared spectroscopy as a process analytical technology

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Food and pharmaceutical industries have a significant role related to global economy and hence such industries need to meet health and safety requirements, increasingly demanding environmental legislation, security, and sustainable production requirements. The determination of the chemical and physical properties and the detection and quantification of microbiological contaminations in these industries is a crucial step. The traditional methods used are laborious, time-consuming and/or requires expensive equipment and/or reagents. Near-infrared (NIR) spectroscopy has recently become increasingly important as a process analytical technique (PAT) due to its speed, low cost, and non-destructive characteristics. This spectroscopic technique is widely used for the analysis of different materials and its modes are transmittance, interactance, transflectance, diffuse transmittance and diffuse reflectance [1]. Many studies have been conducted to apply NIR to quality and safety measurements for food and agricultural materials, including fruits, vegetables, food and beverages as well as for pharmaceutical materials, namely for the detection, identification and quantification of bacteria in liquid suspensions and tablets.

It is difficult to analyze spectral data from complex functional groups of the materials directly because they contain many superposed overtones and combination bands. However, through the extraction of appropriate information from data sets using chemometric analysis - a multivariate statistical technique - it is possible to interpret spectroscopic data. This enables researchers to identify chemical and biological structures and determine the chemical/biological compound concentrations in the different materials. External environmental factors such as illumination and temperature play an important role when samples are measured. To eliminate undesirable effects from the external environment, pre-processing methods, such as averaging, centring, smoothing, standardization, normalization, transformation, multiplicative scatter correction (MSC), and standard vector normalization (SNV), must be conducted prior to chemometric analysis. The most frequently used multivariate statistical techniques are principal component analysis (PCA) and partial least-squares (PLS) [1].

At our lab several works are being carried out using NIR spectroscopy. The ability of this technique to detect and quantify bacterial contaminations in saline solutions (NaCl 0.9%) and pharmaceutical preparations was tested. Five different bacterial species usually responsible for microbial contamination of pharmaceutical products were used. The methodology was successfully tested in saline solutions (NaCl 0.9%) and validated in three different pharmaceutical preparations (contact lens solution, cough syrup and topic anti-inflammatory solution) [2]. The potential of NIR spectroscopy to determine the concentration of different compounds in white wines and cookies is also examined.

References

[1] Min, H, Cho, B-K, Spectroscopic techniques for nondestructive detection of fungi and mycotoxins in agricultural materials: A Review, *J. Biosystems Eng*. 40(1), 67-77, 2015.

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