



Transfer of a near infrared spectroscopy laboratory application to an online process analyser for in situ monitoring of anaerobic digestion

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HIGHLIGHTS

- We confirm the potential for robust in situ monitoring of anaerobic digestion.
- Total volatile fatty acid concentration can be visualised by near infrared spectroscopy.
- Validation of the models was performed on an independent spectra time series.
- Piecewise direct standardisation allows pooling of spectra from different instruments.

ARTICLE INFO

Article history:

Received 23 June 2012

Received in revised form 4 November 2012

Accepted 5 November 2012

Available online 15 November 2012

Keywords:

Anaerobic digestion

Near infrared spectroscopy

Piecewise direct standardisation

Process monitoring

ABSTRACT

A near infrared (NIR) spectroscopy online process analyser was used for in situ monitoring of anaerobic digestion of energy crops and livestock residues. Spectra were measured on a lab instrument and subjected to piecewise direct standardisation for a spectra transfer. The transfer was used in conjunction with samples for which data was recorded online for the partial least squares regression of volatile solids, ammonium, total inorganic carbon, and volatile fatty acids parameters in the fresh matter of a digester slurry. Validation was performed on independent time series spectra. The results confirmed that the procedure is robust in terms of NIR monitoring of these parameters in order to support the high potential for cross-linking different spectrometers, which may help in making this technology practical.

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1. Introduction

Organic matter selectively absorbs near infrared (NIR) radiation, and this can yield information about its molecular bonds, the foremost of which are the CH, OH, and NH bonds (Siesler, 2008). A common assumption regarding spectroscopic measurements in the NIR region is that the amount of light that is absorbed by the sample at different wavelengths is proportional to the concentration of its chemical functional groups (Griffiths and Dahm, 2008). The concentrations of the functional groups are in turn related to the concentrations of the different physicochemical parameters which allows for their quantitative determination. The use of NIR technology to quantitatively measure parameters that are usually

obtained from wet chemistry analyses requires a model for extracting this information from spectroscopic signals, such as multivariate calibration (Feudale et al., 2002). After the models have been independently (externally) validated, they can be used for analysing unknown samples (Bouveresse and Campbell, 2008). However, several situations can arise in which an NIR model can be invalid. One scenario involves the occurrence of changes in the physical or chemical constitution of the sample that has to be analysed. In the case of anaerobic digestion (AD) monitoring, variations in pH, temperature, and analyte concentration of a slurry can change the hydrogen bonding within the sample, which in turn complicates the interpretation of overlapping NIR spectral bands (Shenk et al., 2008; Workman and Burns, 2008). Furthermore, the main challenge of a feedstock-robust calibration is the complex nature of the NIR spectra, which are characterised by inter-constituent interactions and the strong influence of a sample's scattering properties on its spectral signature (Osborne and Fearn, 1986). One strategy that can be used to avoid erroneous estimations is

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