Bioresource Technology 133 (2013) 398–404

Contents lists available at SciVerse ScienceDirect

Bioresource Technology

journal homepage: www.elsevier.com/locate/biortech

Integration of NIRS and PCA techniques for the process monitoring of a sewage sludge anaerobic digester

James P. Reed *, Desmond Devlin, Sandra R.R. Esteves, Richard Dinsdale, Alan J. Guwy

Sustainable Environment Research Centre, Faculty of Health, Sport and Science, University of Glamorgan, Pontypridd, Wales CF37 1DL, UK

HIGHLIGHTS

- ▶ FT-NIRS with PCA and PLS-R to monitor stability of sewage sludge anaerobic digestion.
- ▶ Control charts were successfully produced for the sewage sludge digester.
- ▶ Use of FT-NIRS derived data allows realtime monitoring of key parameters.
- ▶ Advanced warning of digester instability is possible with use of feed characteristics.

ARTICLE INFO

Article history:
Received 16 November 2012
Received in revised form 10 January 2013
Accepted 16 January 2013
Available online 6 February 2013

Keywords:
Anaerobic digestion
FT-NIRS
PLS-R
PCA
Process monitoring

ABSTRACT

This study investigates the use of Hotelling's T^2 control charts as the basis of a process monitor for sewage sludge anaerobic digestion. Fourier transform near infrared spectroscopy was used to produce partial least squares regression models of volatile fatty acids, bicarbonate alkalinity and volatile solids. These were utilised in a series of principle component analysis models along with spectral data from digestate and feedstock samples to produce a pseudo steady state model, which was then used with an independent test set to evaluate the system. The system was able to identify disturbances to the digester due to a temporary alteration of the type of feedstock to the digester and separately, halving of the hydraulic retention time of the digester. It could also provide advance warning of disturbances to the digester. This technique could be used to improve the performance of sewage sludge anaerobic digesters by enabling optimisation of the process.

1. Introduction

The anaerobic digestion (AD) process is a complex multi-stage bioprocess utilising at least 4 trophic groups of bacteria. For stable operation, the intermediate byproducts such as volatile fatty acids (VFA) should not be allowed to accumulate as this will lead to a reduction in bicarbonate alkalinity (BA) and an eventual drop in pH inhibiting the methanogenic bacteria and potentially further acidogenesis and acetogenesis. The reliable monitoring of these key intermediates is thus essential for the optimisation of the AD process. However, monitoring these parameters in a timely manner is difficult due to the nature of the standard methods available. These methods require that a sample is taken and the analysis is then predominantly carried out off line or at only particular times during the day or week. Therefore a delay or temporal dislocation is introduced in the process monitoring scheme that does not allow rapid response to changes in the stability of the digester. Spanjers and van Lier (2006) surveyed approximately 400 full-scale AD plants and found that at 95% of the plants in-line instrumentation was limited to pH, temperature, water flow, biogas flow, level and pressure. They concluded that there is a clear need for further development of in-line measurement techniques for anaerobic process variables. It is not sufficient however, to only monitor the digestate itself. Variations in feedstocks can and will affect the digester stability. Nielsen and Angelidaki (2008) carried out a study on process imbalances in Danish centralised co-digestion plants. They found that imbalances occurred frequently and were likely to have occurred due to inadequate knowledge of the substrate composition, degradation characteristics of the waste, inadequate process surveillance (particularly of VFA) and inexpedient mixing of the different waste products in pre-storage tanks. As an example of the economic consequences of these imbalances, Steyer et al. (2006) described that in 2004 a Danish co-digestion plant using pig manure and industrial wastewater unintentionally overdosed on industrial waste. This led to reduced gas production and a decrease in gas quality that prohibited its use in the plants

* Corresponding author. Tel.: +44 1443 654389.
E-mail address: jpreed@glam.ac.uk (J.P. Reed).

0960-8524/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.biortech.2013.01.083

Table 1
Selected results for FT-NIRS derived PLS-R calibrations for anaerobic digestion.

Authors	Substrate	Parameter	RMSEP[a]	R^2
Hansson et al. (2002)	MSW	Propionic acid	0.21 g l^{-1}	0.88
Holm-Nielsen and Esbensen (2011)	Pig manure	VFA	857.5 mg l^{-1}	0.92
		Propionic acid	224.47 mg l^{-1}	0.95
		Acetic acid	577.58 mg l^{-1}	0.89
Jacobi et al. (2009)	Maize silage	VFA	0.82 g kg^{-1} FM	0.94
		Propionic acid	0.87 g kg^{-1} FM	0.89
		Acetic acid	0.27 g kg^{-1} FM	0.69
Lesteur et al. (2011)	MSW	BMP	28 ml CH4 g^{-1} VS	0.76
Reed et al. (2011)	Sewage sludge	VFA	184.9 mg l^{-1}	0.69
		BA	257.7 mg $CaCO_3$ l^{-1}	0.71
		VS	0.087 g l^{-1}	0.60
		Proportion of WAS	7.09%	0.97
Ward et al. (2011)	Cattle manure + food waste	BA	1230 mg l^{-1} HCO_3^-	0.87

[a] Root mean squared error of prediction.

Table 2
Operating conditions for the three reactors (Reed et al., 2011).

No.	Feedstock	OLR[a] (g VS l^{-1} d^{-1})	Temperature (°C)	HRT (days)	Day
1	Mixed sewage sludges	2.6	35	15	1–11
2	WAS only	2.8	35	15	12–13
3	Mixed sewage sludges	2.8	35	15	14–25
4	Mixed sewage sludges	2.6	30	15	26–33
5	Mixed sewage sludges	2.6	35	15	34–39
6	Mixed sewage sludges	2.5	25	15	40–49
7	Mixed sewage sludges	5.7	25	7.5	50–54
8	Mixed sewage sludges	5.8	20	7.5	55–57

[a] OLR = Organic Loading Rate.

CHP engines. It took 3 months for the plant to recover, incurring an operational loss of $150,000 US.

1.1. Fourier transform near infrared spectroscopy

Fourier transform near infrared spectroscopy (FT-NIRS) is increasingly being utilised to investigate the performance of anaerobic digesters. There have been two main approaches to achieve this. The first is the use of partial least squares regression (PLS-R) with some success to produce calibrations for performance parameters (Table 1) with the second being the use of principle component analysis (PCA). PCA has been used with FT-NIRS to distinguish between different periods of instability (Dias et al., 2008; Hansson et al., 2003; Reed et al., 2011) and to distinguish between waste activated sludge, primary sludge and treated and untreated sewage biosolids (Reed et al., 2011). This is possible because PCA can be used as a tool to understand the variability of the spectra over time and hence the variability of the substrate that the spectra represents. A weakness of the PLS-R approach is that it only provides information that has been asked for. Instability of the process could arise that is not immediately apparent from the monitored parameters. Conversely, the PCA approach may be able to follow disturbances, but on its own would not provide an explanation for the disturbance. However, a combination of approaches could be used to provide the plant operator with a wide view of the process, whilst maintaining a good diagnostic ability.

PCA can be used to produce control charts that are able to represent the stability of a process by the use of a single parameter Hotelling's T^2. A PCA model based on historical data representing steady-state or base-line operation of the digester can be produced. New spectra can then be applied to the baseline model and their scores on each principle component (PC) obtained. These scores can be converted into the Hotelling's T^2 statistic for the measured sample and plotted on a control chart to build a timeseries that represents the stability of the digester over time. This is possible because the Hotelling's T^2 statistic is a measure of the deviation of the sample properties away from the baseline operation of the digester. The greater the value of T^2 the further the sample properties are from the baseline operation of the system. However, it is not sufficient to rely on T^2 as it is only a measure of the in-model variation of the sample. To monitor deviations that are not accounted for by the model it is necessary to use the Q residuals of the sample. The Q residuals represent variance unaccounted for by the model (MacGregor and Kourti, 1995).

Garcia-Alvarez (2009) investigated the use of PCA as a method of fault detection in a simulated WWTP using Hotelling's T^2 control charts. Ruiz et al. (2011), used multiway PCA with case-based reasoning to develop a method of assessing the state of a sequencing batch reactor using online data for pH, oxidation reduction potential, dissolved oxygen and temperature. Rosen and Lennox (2001) also used PCA as the basis of a monitor for wastewater treatment. However, an important limitation of these approaches has been the lack of availability of key performance data such as VFA, BA, or VS as previously this has been unavailable in a timely manner. As

Table 3
Parameters used to construct PCA models shown in Table 4.

No.	Parameter
1	Hotelling's T^2 (feed)
2	Organic Loading Rate
3	Temperature
4	pH
5	VFA
6	BA
7	VS
8	Hotelling's T^2 (digestate)