



Rapid estimation of compost enzymatic activity by spectral analysis method combined with machine learning



Somsubhra Chakraborty^{a,*}, Bhabani S. Das^b, Md. Nasim Ali^a, Bin Li^c, M.C. Sarathjith^b, K. Majumdar^d, D.P. Ray^e

^a IRDM Faculty Centre, Ramakrishna Mission Vivekananda University, Kolkata 700103, India

^b Department of Agricultural and Food Engineering, IIT, Kharagpur 721302, India

^c Department of Experimental Statistics, Louisiana State University, 61 Agriculture Administration Building, Baton Rouge, LA 70803, USA

^d Soil Testing Laboratory, Kalimpong 734301, India

^e National Institute of Research on Jute and Allied Fibre Technology, Kolkata 700040, India

ARTICLE INFO

Article history:

Received 20 August 2013

Accepted 11 December 2013

Available online 4 January 2014

Keywords:

Compost

Fluorescein diacetate hydrolysis

Artificial neural network

Savitzky–Golay

Visible near infrared diffuse reflectance spectroscopy

ABSTRACT

The aim of this study was to investigate the feasibility of using visible near-infrared (VisNIR) diffuse reflectance spectroscopy (DRS) as an easy, inexpensive, and rapid method to predict compost enzymatic activity, which traditionally measured by fluorescein diacetate hydrolysis (FDA-HR) assay. Compost samples representative of five different compost facilities were scanned by DRS, and the raw reflectance spectra were preprocessed using seven spectral transformations for predicting compost FDA-HR with six multivariate algorithms. Although principal component analysis for all spectral pretreatments satisfactorily identified the clusters by compost types, it could not separate different FDA contents. Furthermore, the artificial neural network multilayer perceptron (residual prediction deviation = 3.2, validation $r^2 = 0.91$ and RMSE = $13.38 \mu\text{g g}^{-1} \text{h}^{-1}$) outperformed other multivariate models to capture the highly non-linear relationships between compost enzymatic activity and VisNIR reflectance spectra after Savitzky–Golay first derivative pretreatment. This work demonstrates the efficiency of VisNIR DRS for predicting compost enzymatic as well as microbial activity.

© 2013 Elsevier Ltd. All rights reserved.

1. Introduction

While resource recovery and subsequent composting play a key role in agriculture, horticulture, soil science, and waste management; constant monitoring of compost quality is time consuming and laborious. Microbial enzymatic activity which is an indicator of overall microbial activity of compost, is currently estimated by the non-specific fluorescein diacetate hydrolysis (FDA-HR) assay (Ntougias et al., 2006). Furthermore, FDA-HR assay is also used to predict the suppressive capacity of compost on plant pathogens (Inbar et al., 1991). Nonetheless, the estimation procedure is expensive, time-consuming, and strictly lab based. The visible, near-infrared (VisNIR) diffuse reflectance spectroscopy (DRS), an emerging tool in precision agriculture, may be a promising alternative to estimate compost microbial activity in a rapid and cost-effective manner.

The DRS approach consists of measuring reflectance values for a given sample as a function of wavelength (λ) over 350–2500 nm

Abbreviations: VisNIR, visible near-infrared; DRS, diffuse reflectance spectroscopy; FDA-HR, fluorescein diacetate hydrolysis.

* Corresponding author. Tel.: +91 8670125707; fax: +91 33 2477 2020.

E-mail address: som_pau@yahoo.com (S. Chakraborty).

region of the electromagnetic spectra. These reflectance values (also, known as spectral signatures) mainly arise from atomic electronic transitions and vibrational stretching and bending of structural groups of molecular atoms. While the fundamental vibrations of most organic molecules occur in mid-infrared (MIR) region, NIR spectra are dominated by weak overtones and combinations of fundamental vibrational bands. The active bonds in organic matter in the VisNIR region (350–2500 nm) are the O–H, C–N, N–H, and C=O groups (Malley et al., 2002). There is a growing body of literature on the use of near infrared spectroscopy (NIRS) for empirical calibrations, to simultaneously predict compost physical, chemical, and biological properties (Michel et al., 2006; Chakraborty et al., 2013).

Machine learning is a data based procedure allowing computers to 'learn' and 'recognize' the patterns of the empirical data (Mitchell, 1997). Several prediction methods have been developed in statistics and machine learning. Specifically, artificial neural network (ANN) based models, tree-learning techniques, rule-learning algorithms, and the traditional modeling approach such as linear regression, are the most widely used (Wu et al., 2013). Chemometric data reduction methods such as partial least squares regression (PLS), principal component regression (PCR), stepwise

multiple linear regression etc. have been used to calibrate VisNIR spectra with several compost properties. The reported predictive accuracy of DRS-compost studies suggested that this hyperspectral technique by means of its rapidity, non-destructive analysis with minimal sample pretreatment might replace standard laboratory methods for some compost applications (McWhirt et al., 2012; Chakraborty et al., 2013). Additionally, VisNIR DRS is field portable and might remove the constraints of quantifying compost FDA-HR in the lab.

Since there is a limited number of studies on the use of NIRS for compost FDA-HR assay, more investigations on the applicability of VisNIR DRS for compost FDA-HR assay involving a sample set having diversified compost samples are warranted. The objectives of this study are (i) to compare 35 different combinations of seven spectral pretreatments and five state-of-the-art machine learning algorithms to unravel the relationship between FDA-HR assay and compost VisNIR spectra, and (ii) to determine whether ANN model could assist in improving the DRS prediction accuracy. Since conventional PLS-based sensors are complicated for field use, the overarching goal of this study was to identify some other options to conventional VisNIR-PLS models, which would aid in designing a practical sensor configuration for a field person.

2. Materials and methods

2.1. Sample collection

This study included one hundred compost samples from five full scale composting facilities (referred to as Dairy, Vermi, PDOM, Dairybio, and Hostel) of Ramakrishna Mission Ashrama, Narendrapur, India (22°26'21"N, 88°23'45"E). To offset some spatial heterogeneity that may occur within a single pile, each sample represented a mixture of three subsamples collected across the same pile. For each subsample, a hole was made with a hand shovel and samples near the top, middle, and bottom were collected and mixed in a polyethylene bucket. Subsequently, samples were placed in low-density polyethylene zip-lock bags and transported to the laboratory inside a cooler box (−4 °C). Upon arrival at the lab, the samples were sieved (10 mm), homogenized, air-dried at 45 °C, ball milled, and stored in plastic bags at room temperature for VisNIR scanning and FDA-HR assay. A “fresh” aliquot of each sample was kept in 4 °C and subsequently used for compost physicochemical analyses (EC, water holding capacity, pH, moisture content, organic carbon, and volatile solids) within one week of sample collection. Note that, air-dried samples were preferred for FDA-HR assay over “fresh” aliquot since Mondini et al. (2004) demonstrated that the use of air-dried samples improves the consistency and the applicability of the enzymatic methods for the characterization of the composting process.

2.2. Compost physicochemical characterization

In this study, AR grade (Sigma) chemicals were used without further purification. All solutions were prepared with MilliQ™ (18.2 M Ω) water and sterilized by filtration (0.44 μ m pore) or by autoclave at 120 °C. Compost water holding capacity (WHC) was estimated following modified ASTM method D 2980-71 (American Society of Testing Materials, 1971). Electrical conductivity and pH were determined following method 04.11-A 1:5 Slurry (USDA-USCC, 2002) using a Mettler-Toledo pH meter (Mettler-Toledo Inc., Columbus, OH, USA) and Systronics 306 EC meter (Systronics India Ltd., Ahmedabad, India), respectively. Moisture content was estimated via method 03.09-A (USDA-USCC, 2002) while total volatile solid was estimated following Wu and Ma (2001). The organic matter (%) of compost samples was analyzed following TMECC

method 0.50.7-A loss on ignition (LOI) (USDA-USCC, 2002). All characterizations were done in four replicates. Details of WHC and volatile solid estimation are elaborated in Supplementary Material (SM).

2.3. Compost fluorescein diacetate hydrolysis assay

The FDA-HR assay is considered non-specific since it is sensitive to the activity of several enzyme classes including lipases, esterases, and proteases. Activity of these enzymes causes the hydrolytic cleavage of FDA (colorless) into fluorescein (fluorescent yellow-green). In present study, the FDA-HR assay was carried out following the method given by Schnurer and Rosswall (1982). Briefly, 5 g of well-mixed, air-dried compost was mixed with 50 mL potassium phosphate buffer (pH 6.7; 8.1 g KH_2PO_4 , and 1.3 g $\text{K}_2\text{HPO}_4\text{L}^{-1}$) and 0.5 mL FDA (2 mg FDA mL^{-1} acetone $^{-1}$). The mixture was incubated at 25 °C under continuous horizontal shaking at 120 rpm. The reaction was stopped after 30 min by adding 50 mL acetone and the extracts were filtered through Whatman-42 cellulose filter (GE healthcare, Little Chalfont, UK). The extinction of the extracts was determined against a blank at 492 nm using a Fisher Scientific Evolution 60S UV-Visible Spectrophotometer (Thermo Scientific Barnstead, Dubuque, IA). Moreover, seven standards in the range of 1–6 μ g fluorescein mL^{-1} were prepared. Four analytical replicates and triplicate controls were used. These FDA-HR ($\mu\text{g g}^{-1} \text{h}^{-1}$) values were used as dependent variables in the subsequent modeling studies.

2.4. Spectral scanning and pretreatments

In the laboratory, the 100 compost samples were scanned using a field portable ASD FieldSpec® VisNIR spectroradiometer (Analytical Spectral Devices, CO, USA) with a spectral range of 350–2500 nm. The spectroradiometer had a 2-nm sampling interval and a spectral resolution of 3- and 10-nm wavelengths from 350 to 1000 nm and 1000 to 2500 nm, respectively. Samples were allowed to assume room temperature, evenly distributed in a opaque polypropylene sample holder and scanned from top with an ASD contact probe connected to the FieldSpec® with a fiber optic cable, having a 2-cm-diameter circular viewing area and built-in halogen light source (Analytical Spectral Devices, CO, USA). Full contact with the sample was ensured to avoid outside interference. Each sample was scanned four times with a 90° rotation between scans to obtain an average spectral curve. Each individual scan was an average of 10 internal scans over a time of 1.5 s. The detector was white referenced (after each sample) using a white spectral panel with 99% reflectance, ensuring that fluctuating downwelling irradiance could not saturate the detector. Raw reflectance spectra were processed via a statistical analysis software package, R version 2.11.0 (R Development Core Team, 2008) using custom “R” routines (Chakraborty et al., 2013) for direct extraction of smoothed reflectance at 10 nm intervals.

This study used seven spectral pretreatment methods to prepare the compost smoothed spectra for analysis, and six multivariate algorithms to develop the predictive models. Spectral pretreatments helped in reducing the influence of the side information contained in the spectra. The pretreatment transformations applied were- gap segment derivative (segment size = 7 and gap size = 7) (GSD), Norris gap derivative across a seven-band window (NGD), Savitzky–Golay first derivative using a first-order polynomial across a ten band window (SG), standard normal variate transformation (SNV), normalization by range (NRA), log (1/reflectance) (ABS), and multiplicative scatter correction (MSC). All pretreatment transformations were implemented in the Unscrambler X 10.3 software (CAMO Software Inc., Woodbridge, NJ). All

Download English Version:

<https://daneshyari.com/en/article/6355383>

Download Persian Version:

<https://daneshyari.com/article/6355383>

[Daneshyari.com](https://daneshyari.com)