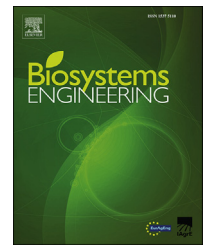


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Research Paper

Prediction of mineral contents in sugarcane cultivated under saline conditions based on stalk scanning by Vis/NIR spectral reflectance

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Mineral contents in the sugarcane juice are important qualitative variables to be used in the development of new products and to establish physicochemical criteria for food processing. The objective of this study was to estimate the mineral contents (K^+ , Na^+ , and Mg^{2+}) in sugarcane stalk samples by visible/near infrared (Vis/NIR) spectral reflectance measurements and multivariate data analysis. Four sugarcane varieties were cultivated under different saline conditions in a greenhouse. The spectral reflectance of stalk surface was measured with a portable spectrometer. The juice mineral compositions were determined by a reference laboratory method. Partial least squares regression (PLSR) was used for calibrating the estimation models. The most abundant mineral in the sugarcane juice was K^+ (310.01–561.48 mg 100 ml⁻¹) as compared to Na^+ (4.63–122.96 mg 100 ml⁻¹) and Mg^{2+} (6.93–18.78 mg 100 ml⁻¹). During the calibration process, the proposed models presented low root mean square errors (RMSE) for calibration (62.46, 25.70, 2.36, and 0.05 mg 100 ml⁻¹), and for cross-validation (90.08, 30.86, 3.79, and 0.06 mg 100 ml⁻¹) for K^+ , Na^+ , Mg^{2+} , and Na^+/K^+ ratio, respectively. Results were also satisfactory for the external validation with low root mean square error (27.30, 10.69, 0.57, and 0.03 mg 100 ml⁻¹), and mean bias error (−4.45, 6.57, 0.07, 0.01 mg 100 ml⁻¹), as well as high coefficients of determination (0.78, 0.89, 0.93, and 0.74), for K^+ , Na^+ , Mg^{2+} , and Na^+/K^+ ratio, respectively. Spectrometry combined to the PLSR technique resulted in an efficient, quick, and non-destructive method for evaluating sugarcane mineral contents.

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Nomenclature

B	matrix of regression coefficients or loadings (dimensionless)
$BIAS$	mean bias error (mg 100 ml ⁻¹)
F	matrix of Y-residuals (mg 100 ml ⁻¹)
h	number of latent variables (dimensionless)
j	denotes a specific wavelength (nm)
n	number of samples (dimensionless)
p	number of wavelengths (dimensionless)
R_{λ}^{cal}	calibrated spectral reflectance from the stalks (%)
R_{λ}^{dark}	spectral reflectance considering light absence (dimensionless)
R_{λ}^{stalk}	spectral reflectance from the stalks (dimensionless)
R_{λ}^{ref}	spectral reflectance from the specular reflectance standard (dimensionless)
R^2	coefficient of determination (dimensionless)
$RMSE$	root mean square error (mg 100 ml ⁻¹)
VIP	variable importance for the projection (dimensionless)
w	loading weight (dimensionless)
X	matrix of predictor variables or scores (mg 100 ml ⁻¹)
Y	matrix of response variables (mg 100 ml ⁻¹)
Y_o	values measured by the spectrophotometer (mg 100 ml ⁻¹)
Y_p	values predicted by the model (mg 100 ml ⁻¹)
Z	fraction of variance in the prediction explained by the latent variable (dimensionless)

1. Introduction

The sugarcane (*Saccharum officinarum*) constitutes one of the most promising cultures in Brazil (Leal et al., 2009), regarding its value for sugar production by food industry and as renewable energy source for ethanol (biofuel) production. For this reason, sugarcane productive chain had a great socioeconomic importance in Brazil (Pinto, Bernardes, Stape, & Pereira, 2005), which is one of the major producing countries in the world (Silva et al., 2013).

The increasing demand for sugarcane derived products has encouraged scientific researchers to improve the knowledge about plant–environment interactions (Batista et al., 2013; Silva et al., 2012; Teodoro et al., 2015), and to develop technologies that allow evaluation of sugarcane quality directly in a field (Nawi, Jensen, & Chen, 2012; Taira, Ueno, & Kawamitsu, 2010; Valderrama, Braga, & Poppi, 2007). Among several qualitative variables evaluated in the sugarcane industry, the sugar, fibre, and mineral contents are the most important.

Studies for evaluation of the sugarcane nutritional requirements during the growth period in field, in addition to information about nutritional balances on sugarcane crops are limited (Oliveira, Freire, Oliveira, Oliveira, & Freire, 2011). The sugarcane cultivation under saline conditions affects the mineral contents of plant aerial parts, since this crop is moderately sensitive to salinity (Shanoon, 1997). This is

demonstrated by toxicity symptoms, low sprout emergence, and overall growth reduction, leading to low biomass (Akhtar, Wahid, & Rasul, 2003; Cha-um & Kirdmanee, 2009; Plaut, Meinzer, & Federman, 2000; Wahid, Rao, & Rasul, 1997).

Considering that nutrients are essential for the proper metabolic functioning of plants and to ensure desirable commercial production, studies that aim to mineral quantification in aerial parts of sugarcane crops are very relevant. The results of these researches will assist in decision making about new fertilizing methods, besides improving the existent ones. Thus, it will be possible to maximise the yield quality, minimise the amounts of chemical fertilisers applied, and reduce the risks of environmental impact (Cuzzolino, Cynkar, Shah, & Smith, 2011a; Menesatti et al., 2010).

According to Nawi, Kamal, Chen, and Jensen (2014), the in-field determination of sugarcane qualitative variables is very important for assessing the crop growth and development, harvesting management, adoption of precision agriculture techniques, and payment purposes to growers. However, current methods for measuring qualitative variables are based on manual harvesting of samples in the field, extraction of juice, and laboratory analysis. This practice is destructive, time consuming, and labour demanding, which is also subject to measurement and sampling errors. Therefore, an efficient and accurate method of predicting in-field sugarcane mineral contents by directly scanning the stalk skin using spectroscopy would be beneficial to the industry and growers, since they are important for the development of new products and the establishment of physicochemical criteria for food processing (Kocher et al., 2014; Nogueira, Ferreira, Carneiro Júnior, & Passoni, 2009; Okuno & Tamaki, 2002).

Past studies have demonstrated that spectroscopic methods can be applied to predict internal quality of crops based on non-destructive measurements (Bureau et al., 2009; ElMasry, Wang, ElSayed, & Ngadi, 2007; Nawi, Chen, Jensen, & Mehdizadeh, 2013; Sánchez, De La Haba, Guerrero, Garrido-Varo, & Pérez-Marín, 2011; Zhang, Zheng, Li, Deng, & Ji, 2015). The analysis of sugarcane using the visible/near infrared (Vis/NIR) spectroscopy coupled with the multivariate statistical techniques offers the possibility of replacing standard laboratory analyses.

Although scientific researches already have been carried out for determination of ash content, fibre content, moisture content, soluble solids, polarisable sugars, reducing sugars, and commercial cane sugar in sugarcane juice (Madsen, White, & Rein, 2003; Nawi et al., 2012, 2013, 2014; Taira et al., 2010; Valderrama et al., 2007), as well as the estimation of nitrogen concentration in sugarcane leaf (Abdel-Rahman, Ahmed, & Van Den Berg, 2010), there are no applications for the sugarcane crop combining reflectance measurements together with multivariate data analysis for estimating the mineral contents in sugarcane juice.

The objective of this study was to estimate the mineral contents (K^+ , Na^+ , and Mg^{2+}) in sugarcane cultivated under saline conditions based on stalk scanning by Vis/NIR spectral reflectance measurements and multivariate data analysis.

This work is part of a project whose main objective will be to evaluate the salt stress effects on the physiology of the sugarcane varieties. The present paper focused on predicting the mineral contents of sugarcane juice from spectral

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