POSTER SUMMARY

EXPLORATION OF A SPECTROSCOPIC/CHEMOMETRIC APPROACH FOR THE IDENTIFICATION OF COLOURANT TYPES IN SUGARCANE PROCESSING STREAMS

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Abstract

The Sugar Milling Research Institute NPC (SMRI) is investigating rapid and cost-effective analytical methods for identifying the colourant types present in sugarcane processing streams. A possible approach that has been identified is the use of multivariate classification, a sub-group of chemometrics, which is a mathematically-based method that is used to extract information from data-rich sources, such as the spectra obtained through spectroscopy. Spectroscopy is a technique that enables the qualitative and quantitative analysis of compounds by measuring the amount of radiation produced, or absorbed, by molecular or atomic species. Fourier Transform Infrared (FTIR) spectroscopy measures the absorption of a sample by using mid-infrared radiation.

Thirty-five raw sugar samples were prepared for analysis by grinding the crystals to form a fine powder, using a mortar and pestle. The FTIR spectra of the 35 samples were collected using an Agilent Carey 630 FTIR spectrometer. The infrared spectral profiles of the raw sugar samples were studied to determine whether it is possible to detect the presence of colourant contaminants. As expected, it was found that the peaks in the spectra of the raw sugar samples were mainly due to the sucrose molecule and since these peaks are intense, they may obscure the peaks of any colourant component that is present in the samples. The spectra did not have obvious characteristic peaks associated with non-sugar components, such as colourants. However, similar studies have shown that the minor spectral differences could possibly assist with the identification of colourant types, by using a combined spectroscopic/chemometric approach.

A Principal Component Analysis (PCA), a multivariate classification technique, was used to explore the potential of using infrared spectral data to predict the types of colourants present in raw sugar. Raw sugar samples were used in this laboratory study to assess the feasibility of a spectroscopic/chemometric approach. Once the feasibility of the approach is confirmed, the project team will evaluate which factory stream would be most appropriate for the practical application of this approach in a processing environment. A possible benefit of this combined spectroscopic/chemometric approach, over the traditional analytical chemistry methods, is the rapid prediction of the presence or absence of colourants. Synthetic colourant samples (caramel, melanoidin and hexose alkaline degradation products) synthesised in the SMRI laboratory were added to a raw sugar solution and lyophilised to ensure that the sample matrix of the synthetic colourant samples was comparable to those of the raw sugar samples. The infrared spectra of these solid synthetic colourant samples were obtained, in addition to the infrared spectra of the 35 raw sugar samples.

A PCA was performed by using the collected infrared spectral data. Various pre-processing options and different wavelength regions were explored and the principal component score diagrams were generated. The preliminary results suggest that there may be potential in using a spectroscopic/chemometric approach for determining the relative contribution of particular colourant types to the colour of a raw sugar sample. This approach will enable an understanding of the colourant profiles of sugarcane processing streams and could possibly be used to gain an insight into the occurrence of colourant types that make the greatest contribution to the colour of raw sugar.

Keywords: Colour, colourants, chemometrics, spectroscopy, PCA, raw sugar