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Near-infrared spectral measurements and multivariate analysis for predicting glass contamination of refuse-derived fuel

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Abstract

This paper investigates how glass contamination in refuse-derived fuel can be quantitatively detected using near-infrared spectroscopy. Near-infrared spectral data of glass in four different background materials were collected, each material chosen to represent a main component in municipal solid waste; actual refuse-derived fuel was not tested. The resulting spectra were pre-processed and used to develop multi-variate predictive models using partial least squares regression. It was shown that predictive models for coloured glass content are reasonably accurate, while models for mixed glass or clear glass content are not; the validated model for coloured glass content had a coefficient of determination of 0.83 between the predicted and reference data, and a root-mean-square error of validation of 0.64. The methods investigated in this paper show potential in predicting coloured glass content in different types of background material, but a different approach would be needed for predicting mixed type glass contamination in refuse-derived fuel.

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Keywords: NIR spectroscopy, RDF, glass detection, food waste, biomass

Nomenclature

NIR	Near-InfraRed
PLSR	Partial Least Squares Regression
RDF	Refuse-Derived Fuel

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1. Introduction

In the hierarchy of waste management, energy recovery from waste is preferred over disposing of waste to landfills [1]. Additionally, refuse-derived fuel (RDF) for combined heat and power plants is a partial replacement for fossil fuels as the carbon dioxide emissions per unit energy are lower for RDF than for fossil fuel, despite containing components of fossil origin [2]. RDF can contain incombustible substances such as glass, and the processes which sort incombustible substances from municipal solid waste have inefficiencies. At the combustion temperatures typically encountered in a fluidized bed boiler of a combined heat and power plant, glass can melt and form agglomerations with the boiler sands, which leads to defluidization of the boiler bed. Glass detection methods would be beneficial for improving boiler operating conditions, such as optimising the maintenance schedule for the bed sands and the use of additives for reducing agglomeration rates [3].

Near-infrared (NIR) spectroscopy is a sensing technology that is fast, non-destructive and can be applied to moving samples. The fundamental principle behind the use of infrared spectroscopy is that covalent chemical bond vibrations in a sample absorb certain wavelengths in the infrared spectrum; overtones and combinations of these vibrations absorb wavelengths in the NIR region of the spectrum. In NIR reflectance spectroscopy, a sensor captures wavelengths in the NIR region that are reflected from the sample; the sensor is connected to a spectrometer which can calculate the absorbance spectrum, this indicates the chemical composition of the sample. A review of existing literature found that NIR spectroscopy has a large variety of applications. In applications relevant to the research presented in this paper, NIRS has been investigated for use in waste management [4] and solid waste sorting [5] and can also be used to detect ceramic glass contaminants in glass recycling processes [6]. One difficulty identified in using NIR spectroscopy to detect glass in RDF is that waste is heterogeneous in composition, and it is difficult to detect changes in NIR spectral absorbance when the background material varies. Four homogeneous background materials were selected to represent RDF for glass detection test samples in the experimental part of this research. Paper and food waste have been identified as majority components in municipal solid waste [7]. Food consists of four key molecules: water, lipids, carbohydrates and proteins. Three types of food were chosen as background materials to represent each of the non-water molecular types: shredded coconut, dry rice and whey powder. It has previously been shown that food composition can be predicted using NIR spectroscopy [8,9]. NIR hyperspectral imaging has been used to find plastic, glass and rubber foreign bodies among grain samples [10]. NIR spectroscopy has been used extensively in the pulp and paper industry for a variety of purposes including detection of cellulose, lignin and fibre content as well as kappa number distributions [11,12,13] and has also shown potential in the analysis of various fuels [14,15]. Wood shavings were used in this work to represent paper in the test samples as the shavings were already available in the lab, saving time in the experimental phase of this research. Previous work has shown that glass content can be detected in woody biomass using NIR spectroscopy [16].

This research has identified a gap in existing literature, namely the lack of research in the public domain relating to the use of NIR spectroscopy to detect glass contamination in RDF. Thus this paper presents the findings of research into using NIR spectroscopy to detect glass in background materials which each represent a component of RDF. The research focused on developing multivariate predictive models of glass content using NIR absorbance spectra collected experimentally; this approach can then be applied for on-line detection of glass contamination.

2. Methodology

The testing and modelling process involved preparing multiple samples of soda-lime glass in each of the representative background materials and capturing NIR absorbance spectra for each sample. The spectral data were pre-processed and multivariate predictive models were developed using partial least squares regression.

2.1. Sample preparation

Each sample contained 1500 cc of one of the four types of background material and one type of silica based soda-lime glass, i.e. clear or coloured. The glass pieces used were selected by size using two sieves, one with 16 mm mesh and one with 4 mm mesh; particles which passed through the first sieve and captured by the second were used in testing. As per the Beer-Lambert Law, the spectral absorbance of a sample is proportional to the volumetric

concentration of individual components within the penetration depth [17]. The volume fraction of glass content in each sample of background material was increased incrementally from 0% up to a maximum of 5%; nominal values included 0%, 0.05%, 0.1%, 0.2%, 0.5%, 1%, 2%, 3%, 4% and 5% by volume. With each increase in glass fraction, the sample was shaken to replicate random distribution of glass particles in RDF.

2.2. NIR spectra acquisition

The samples were placed in a circular tray, as shown in Figure 1 (a), which was spun to replicate the movement of a conveyor belt; the linear velocity at the point below the sensor was measured as 0.9 ms^{-1} with a standard deviation of 0.1 ms^{-1}. NIR relative absorbance spectra were recorded using a Fourier-Transform NIR spectrometer positioned above the samples, as shown in Figure 1 (b). The wavenumber range recorded was 12000 cm^{-1} to 4000 cm^{-1} and the resolution was 8 cm^{-1}, with the average of 32 scans taken for each absorbance spectrum.

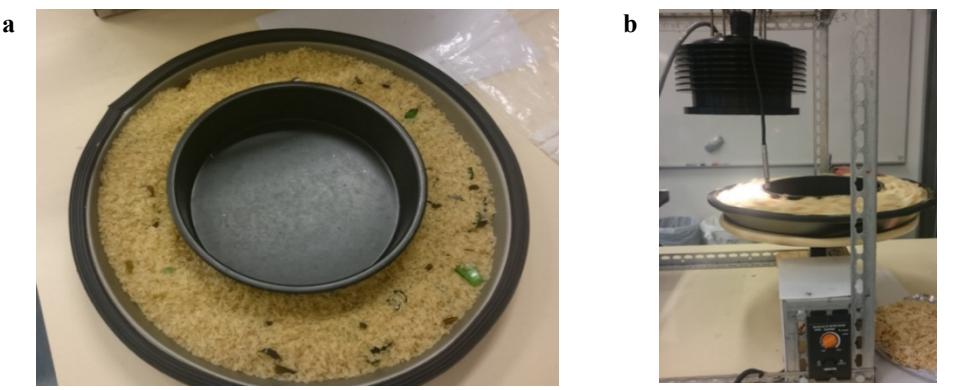

Fig. 1. (a) 1500 cc dry rice with 3.95% coloured glass in test tray; (b) Equipment set-up with NIR sensor above rotating tray

2.3. NIR spectra pre-processing

Standard normal variate transforms and Savitzky-Golay smoothing are two pre-processing techniques commonly used to remove additive and multiplicative effects in spectral data [18]. In this research, a standard normal variate transform was applied to each spectrum to normalize the data around the mean with respect to the standard deviation. Savitzky-Golay smoothing was used to remove noise in the data; 11 points was found to be the ideal number of smoothing points for this data. The raw spectral data for all samples is shown in Figure 2 (a), while the pre-processed spectra are shown in Figure 2 (b).

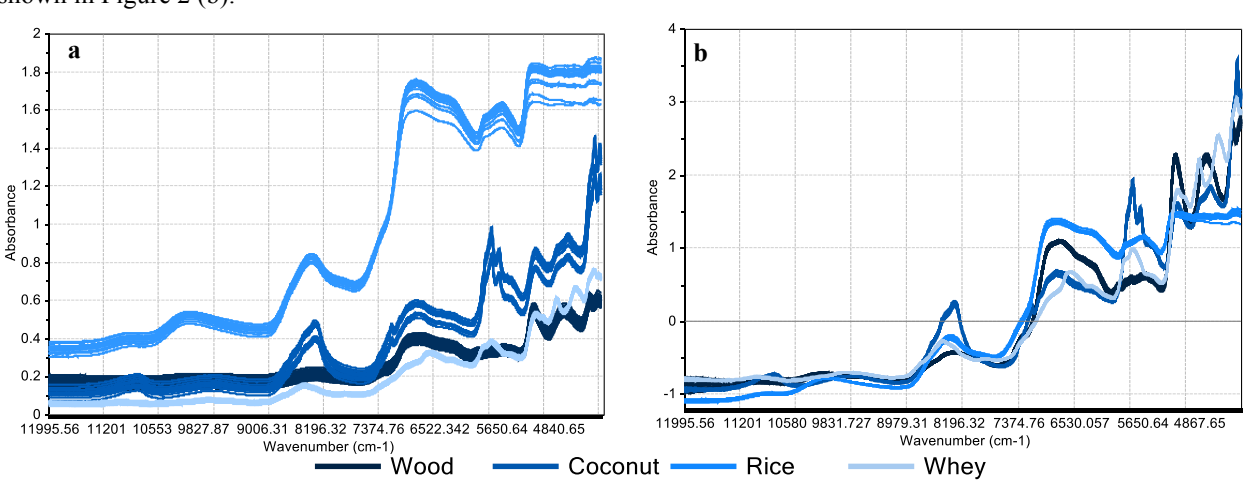

Fig. 2. (a) Raw spectra; (b) Pre-processed spectra.

2.4. Multivariate Analysis

Three regression models were developed using a partial least squares regression (PLSR) algorithm, which is commonly used in spectral data analysis [19]: one for all 131 samples, including 17 with 0% glass; one for the 45 samples with clear glass; one for the 66 samples with coloured glass. The number of samples warranted the use of a full cross-validation. Three of the 131 samples were identified as outliers using the influence plot of samples in Figure 3, and confirmed by inspecting the raw spectra. It was noted that there was higher influence from all of the food-type background material samples than the wood samples. This was expected given the larger number of the wood-based samples. Martens' Uncertainty Test [20,21] was used to identify significant wavenumbers for the development of the model. The effects of O-H bonds are not significant in this region [22], so the moisture content of the samples was not investigated.

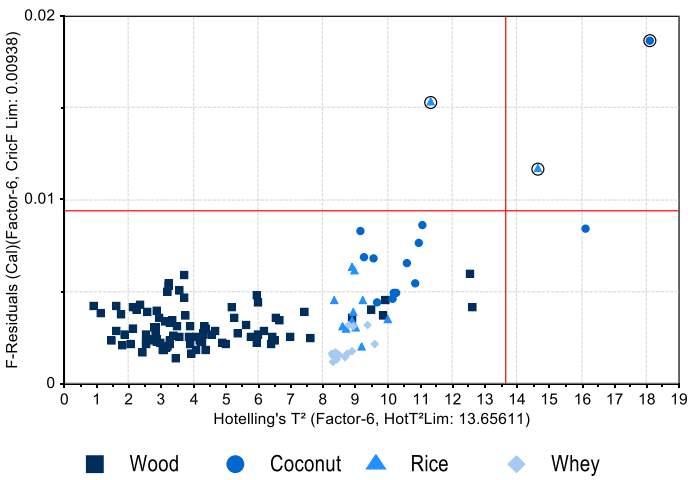

Fig. 3. Influence plot.

3. Results and Discussion

The parity plot of the PLSR model developed from using coloured glass in all four types of background material is illustrated in Figure 4. The parity plot for the calibration model is shown in blue, while the validation model is

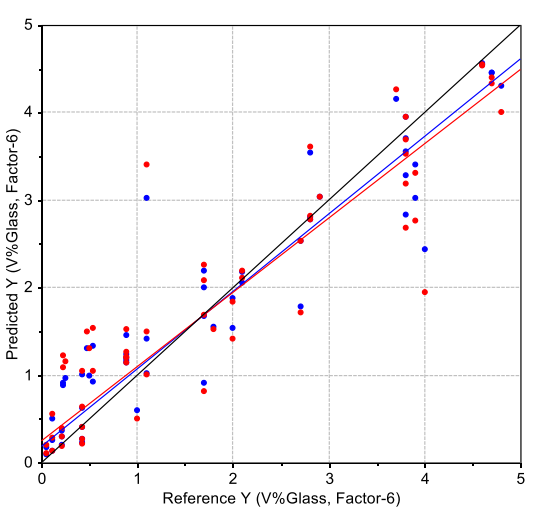

Fig. 4. Parity plot of prediction model including both clear and coloured glass content.

shown in red; the black line shows the target for parity between the predicted values and reference value for glass content. Six factors were required to explain 83% of the data variance in the validation model, as determined by inspection of the corresponding explained variance plot. Inaccuracies in prediction are due to a variety of sources. The randomized distribution of the glass particles results in an unknown amount of glass being within the penetration depth of the NIR sensor. Uncertainties in the volume fraction measurements would also have introduced some error in the reference values. The regression coefficients used in the model of coloured glass content are shown in Figure 5.

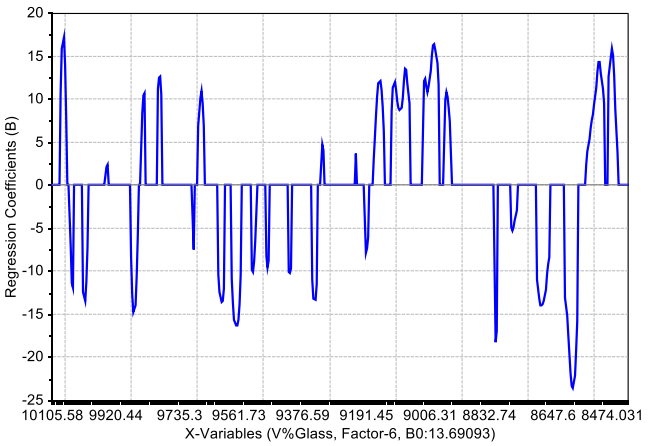

Fig. 5. Regression coefficients for model of coloured glass content.

To develop a better understanding of prediction capabilities, models for clear glass and mixed glass were also developed. Five factors were required to explain only 36% of the variance in the validation model for clear glass content. The validated prediction model for mixed glass content required seven factors to explain 63% of the variance. The number of factors required was determined by inspecting the respective explained variance plots. The accuracy of the three models is summarized in Table 1. The data is from the parity plots for each model; for a parity plot, the ideal coefficient of determination is 1, the target for root-mean-square error is 0, the ideal slope is 1, and the ideal offset is 0.

Table 1. Comparative summary of performance statistics for the validated models.

Type of glass in prediction model	Coefficient of Determination	Root-Mean-Square Error of Validation	Slope	Offset
Clear & coloured glass	0.63	0.95	0.67	0.49
Clear glass	0.36	1.26	0.42	1.04
Coloured glass	0.83	0.64	0.85	0.25

It is apparent that the predictive capability for coloured glass content is good in the presence of varying background material, while the predictive capability for mixed and clear glass content is not very good. This is believed to be due to the colourants used, some of which have been shown, in other applications, to affect the absorbance spectrum. Sulphur oxides are used for colouring glass brown and amber; sulphur dioxide residues are able to be detected in organic matter [23] in a wavenumber range which corresponds to that modelled in this research. The coloured glass sample spectra in the modelled range of wavenumbers is illustrated in Figure 6, where slight separation of the spectra by volumetric glass content is apparent. However, it is evident that the chemical differences between background materials dominate the absorbance effects of glass content. Further research is required into comparing the accuracy of the individual homogeneous background materials used in this study, and actual RDF which is heterogeneous.

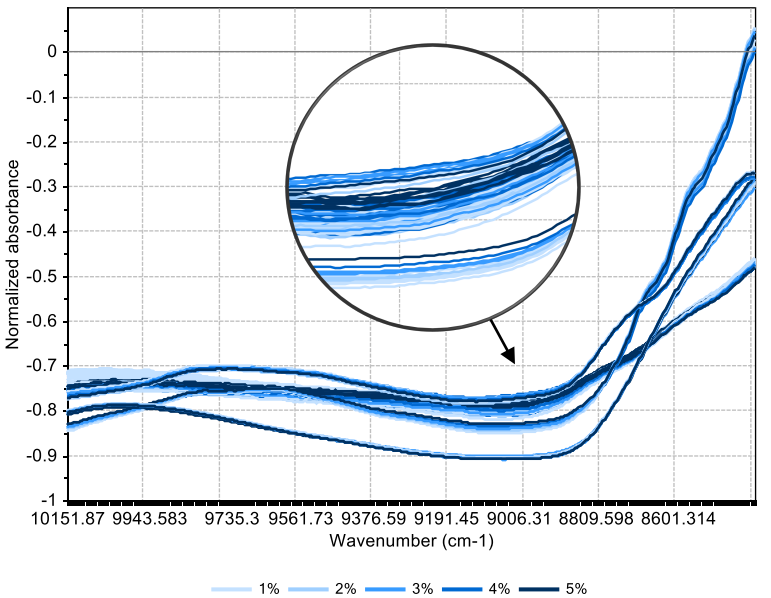

Fig. 6. Pre-processed NIR spectra showing variation by volumetric fraction of glass.

The wavenumber range on the left hand side of Figure 6 corresponds to the second overtone vibrations of N-H bonds, while the range on the right hand side corresponds to second overtone vibrations of C-H bonds [22]. It is possible that these chemical groups have formed inclusions during the glass manufacturing process and are detected by the NIR sensor. Further research is required to explain this and provide insight into how this might happen and whether these are the molecular groups detected.

A previous study has been performed on a single background material, wood shavings, with clear glass cullet [16]; the results obtained indicated a very high model accuracy. A key difference between that study and this work, other than the use of multiple background materials to build the models, is in the sample preparation. The preparation technique used in this work provides a more accurate representation of the presence of glass in RDF. In this study the glass cullet was randomly distributed throughout each background material whereas in the earlier work the pieces of clear glass were spread evenly on top of wood shavings. It is therefore unsurprising that the models presented here are less accurate, given the limited penetration depth of the NIR light into the background materials.

4. Conclusions

It was shown that predictive models of coloured glass content are reasonably accurate, while models of mixed glass or clear glass content are not. The most accurate validated model predicted coloured glass content with a coefficient of determination of 0.83, a parity plot root-mean-square error of 0.64, a slope of 0.85 and an offset of 0.25. This type of model has potential applications in predicting coloured glass content in different kinds of homogeneous background materials and possibly heterogeneous materials. These methods have limited applicability in the intended use of detecting mixed type glass in RDF, due to the presence of clear glass in municipal solid waste. However, different approaches might have more success, such as different pre-processing techniques to filter out the dominating chemical effects of the background material absorbance. Scanning each sample multiple times and re-randomising for each scan would give some measure of the variability present in the distribution of glass particles. More robust models would involve testing with a larger variety of unique background materials, heterogeneous samples and actual waste. Further research should also focus on understanding which chemical groups in the glass are detected by the NIR spectrometer.

References

[1] Hansen W, Christopher M, Verbuecheln M. EU waste policy and challenges for regional and local authorities. Ecological Institute for International and European Environmental Policy: Berlin, Germany. 2002.

[2] Obermoser M, Fellner J, Rechberger H. Determination of reliable CO2 emission factors for waste-to-energy plants. Waste Manag Res 2009;27:907–913.

[3] Khan AA, de Jong W, Jansens PJ, Spliethoff H. Biomass combustion in fluidized bed boilers: Potential problems and remedies. Fuel Process Technol 2009;90:21–50.

[4] Smidt E, Böhm K, Schwanninger M. The application of FT-IR spectroscopy in waste management. InFourier transforms - new analytical approaches and FTIR strategies. InTech 2011.

[5] Bonifazi G, Serranti S, Bonoli A, Dall'Ara A. Innovative recognition-sorting procedures applied to solid waste: the hyperspectral approach. WIT Transactions on Ecology and the Environment. 2009;120:885-94.

[6] Bonifazi G, Serranti S. Imaging spectroscopy based strategies for ceramic glass contaminants removal in glass recycling. Waste Manag 2006;26:627–639.

[7] Patumsawad S, Cliffe KR. Experimental study on fluidised bed combustion of high moisture municipal solid waste. Energy Convers Manag 2002;43:2329–2340.

[8] Hell J, Prückler M, Danner L, Henniges U, Apprich S, Rosenau T, Kneifel W, Böhmdorfer S. A comparison between near-infrared (NIR) and mid-infrared (ATR-FTIR) spectroscopy for the multivariate determination of compositional properties in wheat bran samples. Food Control 2016;60:365–369.

[9] Cen H, He Y. Theory and application of near infrared reflectance spectroscopy in determination of food quality. Trends Food Sci Technol 2007;18:72–83.

[10] Gowen AA, O'Donnell CP. Near infrared hyperspectral imaging for foreign body detection and identification in food processing. Spectrosc Eur 2013;25:6–11.

[11] Antti H, Alexandersson D, Sjöström M, Wallbäcks L. Detection of kappa number distributions in kraft pulps using NIR spectroscopy and multivariate calibration. Tappi journal. 2000;83:102-8.

[12] Brink M, Mandenius CF, Skoglund A. On-line predictions of the aspen fibre and birch bark content in unbleached hardwood pulp, using NIR spectroscopy and multivariate data analysis. Chemometrics and Intelligent Laboratory Systems. 2010;103:53-8.

[13] Poke FS, Raymond CA. Predicting extractives, lignin, and cellulose contents using near infrared spectroscopy on solid wood in Eucalyptus globulus. Journal of Wood Chemistry and Technology. 2006;26:187-99.

[14] Skvaril J, Kyprianidis KG, Dahlquist E. Applications of near-infrared spectroscopy (NIRS) in biomass energy conversion processes: A review. Applied Spectroscopy Reviews. 2017;1-54.

[15] Skvaril J, Kyprianidis K, Avelin A, Odlare M, Dahlquist E. Fast Determination of Fuel Properties in Solid Biofuel Mixtures by Near Infrared Spectroscopy. Energy Procedia. 2017;105:1309-17.

[16] Skvaril J, Kyprianidis K, Avelin A, Odlare M, Dahlquist E. Utilization of Near Infrared (NIR) Spectrometry for Detection of Glass in the Waste-based Fuel. Energy Procedia, Clean, Efficient and Affordable Energy for a Sustainable Future: The 7th International Conference on Applied Energy (ICAE2015) 2015;75:734–741.

[17] Svanberg S. Atomic and molecular spectroscopy: basic aspects and practical applications. 3rd ed. Springer Science & Business Media. 2001.

[18] Rinnan Å, van den Berg F, Engelsen SB. Review of the most common pre-processing techniques for near-infrared spectra. TrAC Trends in Analytical Chemistry. 2009;28:1201-22.

[19] Dumancas GG, Ramasahayam S, Bello G, Hughes J, Kramer R. Chemometric regression techniques as emerging, powerful tools in genetic association studies. TrAC Trends in Analytical Chemistry. 2015;74:79-88.

[20] Martens H, Martens M. Modified Jack-knife estimation of parameter uncertainty in bilinear modelling by partial least squares regression (PLSR). Food quality and preference. 2000;11:5-16.

[21] Martens H, Høy M, Westad F, Folkenberg D, Martens M. Analysis of designed experiments by stabilised PLS Regression and jack-knifing. Chemometrics and Intelligent Laboratory Systems. 2001 Oct 28;58(2):151-70.

[22] Eldin AB. Near Infra Red Spectroscopy. InWide Spectra of Quality Control. InTech 2011.

[23] He J, Zhang C, He Y. Application of Near-Infrared Hyperspectral Imaging to Detect Sulfur Dioxide Residual in the Fritillaria thunbergii Bulbus Treated by Sulfur Fumigation. Appl Sci 2017;7:77.